

Supporting Information

Basic Phosphonium Ionic Liquids as Wittig Reagents

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1 Atomic charges used in classical MD simulations

The RESP charges for the phenolate anion and cations were calculated at TPSS-D3/def2-TZVPP level of theory. These charges were averaged for the equivalent atoms and scaled to 0.8. The resulting charges (with XYZ geometries) used in classical molecular dynamics simulations are provided below.

[PhO]⁻

C 0.54400 -18.26215 5.24379 -8.74200
C -0.35200 -17.86795 5.58199 -7.44191
C -0.04000 -16.89029 6.56351 -7.23988
C -0.30400 -16.30684 7.20682 -8.33793
C -0.04000 -16.70104 6.86862 -9.63802
C -0.35200 -17.67870 5.88711 -9.84005
H 0.08800 -18.32180 5.08159 -6.58778
H 0.05600 -16.58366 6.82658 -6.22860
H 0.08000 -15.54636 7.97029 -8.18078
H 0.05600 -16.24719 7.36902 -10.49215
H 0.08800 -17.98533 5.62404 -10.85134
O -0.62400 -19.24332 4.24662 -8.68763

[Et₄P]⁺

P 0.54400 2.27171 -20.20324 23.96469
C -0.24800 3.74185 -19.10324 24.08428
H 0.10400 4.54167 -19.43153 23.41076
H 0.10400 3.48993 -18.07024 23.81869
C -0.24800 1.87632 -20.87145 25.63285
H 0.10400 2.78515 -21.16224 26.17191
H 0.10400 1.35206 -20.12954 26.24591
C -0.24800 0.83915 -19.24262 23.32394
H 0.10400 0.52035 -18.47633 24.03968
H 0.10400 -0.02216 -19.89202 23.13018
C -0.24800 2.62969 -21.59630 22.81716
H 0.10400 1.74947 -21.85610 22.21815
C -0.04000 1.18778 -18.52869 22.00471
H 0.04800 0.28523 -18.18724 21.48518
H 0.04800 1.81929 -17.65051 22.18105

H 0.04800 1.72983 -19.19339 21.32245
C -0.04000 0.97447 -22.11622 25.53893
H 0.04800 -0.00916 -21.93091 25.98529
H 0.04800 0.81312 -22.41434 24.49672
H 0.04800 1.41844 -22.97099 26.06177
C -0.04000 4.31591 -19.08792 25.51321
H 0.04800 5.32258 -19.52012 25.54345
H 0.04800 4.38323 -18.06671 25.90524
H 0.04800 3.68812 -19.66503 26.20164
C -0.04000 3.05704 -22.86038 23.58598
H 0.04800 3.13242 -23.72670 22.91896
H 0.04800 4.03416 -22.72562 24.06368
H 0.04800 2.33674 -23.11139 24.37291
H 0.10400 3.43140 -21.26149 22.17563

[Pr₄P]⁺

P 0.54400 -12.94938 10.21330 -24.23140
 C -0.24800 -11.71061 10.48742 -25.56403
 H 0.10400 -12.14570 11.03728 -26.40632
 H 0.10400 -10.85388 11.06565 -25.19963
 C -0.24800 -13.08442 8.41035 -23.88973
 H 0.10400 -13.08107 7.82705 -24.81756
 H 0.10400 -12.24888 8.05709 -23.27476
 C -0.24800 -12.41527 11.09665 -22.70824
 H 0.10400 -11.50046 10.65869 -22.29301
 H 0.10400 -13.18556 11.05154 -21.92995
 C -0.24800 -14.58800 10.85907 -24.76385
 H 0.10400 -15.12490 11.32253 -23.92835
 C 0.00800 -12.13009 12.58300 -22.99293
 H 0.04800 -11.17642 12.71306 -23.51704
 H 0.04800 -12.91335 13.02703 -23.61779
 C 0.00800 -14.38666 8.07817 -23.13778
 H 0.04800 -15.02105 8.96501 -23.02747
 H 0.04800 -14.97120 7.31816 -23.66863
 C 0.00800 -11.17062 9.15284 -26.11075
 H 0.04800 -11.45310 9.00781 -27.15969
 H 0.04800 -11.56215 8.30128 -25.54272

C 0.00800 -15.47981 9.73411 -25.32129
 H 0.04800 -15.08857 9.34742 -26.26919
 H 0.04800 -15.54360 8.89221 -24.62255
 H 0.10400 -14.38937 11.59217 -25.53165
 C -0.14400 -12.05806 13.39978 -21.68937
 H 0.04800 -11.25777 13.03656 -21.03460
 H 0.04800 -11.86319 14.45898 -21.89241
 H 0.04800 -12.99722 13.33871 -21.12781
 C -0.14400 -9.63369 9.09550 -26.03215
 H 0.04800 -9.19171 8.88225 -27.01209
 H 0.04800 -9.21633 10.04634 -25.68169
 H 0.04800 -9.29837 8.31335 -25.34156
 C -0.14400 -16.91404 10.23176 -25.58005
 H 0.04800 -17.37527 10.61438 -24.66246
 H 0.04800 -16.92836 11.04106 -26.31893
 H 0.04800 -17.55330 9.42668 -25.95990
 C -0.14400 -14.09622 7.53713 -21.72550
 H 0.04800 -13.31793 6.76578 -21.74596
 H 0.04800 -13.75364 8.33397 -21.05558
 H 0.04800 -14.99129 7.09107 -21.27720

[Bu₄P]⁺

P 0.54400 19.65600 22.31701 3.72503
 C -0.24800 21.11417 22.00212 4.80214
 H 0.10400 21.72029 22.90654 4.92764
 H 0.10400 20.80834 21.66862 5.80031
 C -0.24800 19.68471 21.14520 2.30671
 H 0.10400 20.69778 21.02987 1.90484
 H 0.10400 19.33217 20.15083 2.60346
 C -0.24800 18.11304 22.07757 4.69846
 H 0.10400 17.98513 21.02948 4.99213
 H 0.10400 17.22800 22.36907 4.12154
 C -0.24800 19.71209 24.04397 3.09251
 H 0.10400 18.70962 24.48432 3.04514
 C 0.00800 18.12590 22.92184 5.98634
 H 0.04800 18.78495 22.48339 6.74432
 H 0.04800 18.47880 23.94103 5.79183
 C 0.00800 18.78280 21.63326 1.15782
 H 0.04800 18.36640 22.62439 1.37089
 H 0.04800 19.33929 21.70448 0.21636
 C 0.00800 22.02525 20.91200 4.20785
 H 0.04800 23.00614 21.31719 3.93438
 H 0.04800 21.58584 20.47343 3.30470
 C 0.00800 20.31194 24.10283 1.67536
 H 0.04800 21.37763 23.84715 1.68221
 H 0.04800 19.80870 23.40195 0.99962
 H 0.10400 20.33064 24.59892 3.78231
 C -0.09600 16.71800 23.02797 6.60128
 H 0.04800 16.32263 22.04062 6.86576

H 0.04800 16.01128 23.49021 5.90273
 C -0.09600 22.25952 19.76823 5.21209
 H 0.04800 21.80303 19.99029 6.18339
 H 0.04800 21.82865 18.82691 4.85239
 C -0.09600 20.17681 25.51126 1.06737
 H 0.04800 20.71030 26.25758 1.66696
 H 0.04800 20.58761 25.54866 0.05201
 C -0.09600 17.60082 20.67358 0.92646
 H 0.04800 16.85647 20.75716 1.72650
 H 0.04800 17.09271 20.88744 -0.02075
 C -0.14400 18.70231 25.94838 0.98750
 H 0.04800 18.02612 25.09211 1.09084
 H 0.04800 18.45427 26.66246 1.78102
 H 0.04800 18.48038 26.43035 0.02856
 C -0.14400 23.76227 19.52960 5.44958
 H 0.04800 24.32620 20.46859 5.41214
 H 0.04800 23.94397 19.07432 6.42979
 H 0.04800 24.18473 18.86042 4.69141
 C -0.14400 18.06970 19.20742 0.88053
 H 0.04800 19.15750 19.13979 0.76558
 H 0.04800 17.80106 18.67361 1.79922
 H 0.04800 17.61500 18.66918 0.04109
 C -0.14400 16.72884 23.88174 7.88291
 H 0.04800 15.72640 23.95960 8.31898
 H 0.04800 17.38753 23.44948 8.64475
 H 0.04800 17.08103 24.89977 7.68121

[Hex₄P]⁺

P 0.54400 -21.74281 13.64169 -30.04368
C -0.24800 -22.90779 13.82049 -28.63073
H 0.10400 -23.89936 13.42492 -28.87859
H 0.10400 -22.54876 13.28111 -27.74683
C -0.24800 -21.06168 15.29393 -30.48159
H 0.10400 -21.83931 16.06577 -30.45556
H 0.10400 -20.27199 15.59740 -29.78489
C -0.24800 -20.37218 12.51029 -29.56734
H 0.10400 -19.74680 12.94967 -28.78188
H 0.10400 -19.72224 12.28908 -30.42160
C -0.24800 -22.63001 12.94172 -31.49576
H 0.10400 -21.99505 12.24329 -32.05265
C 0.00800 -20.91123 11.16944 -29.03523
H 0.04800 -21.30584 11.27345 -28.01809
H 0.04800 -21.72149 10.78655 -29.66607
C 0.00800 -20.45598 15.29338 -31.89747
H 0.04800 -20.62399 14.33560 -32.40297
H 0.04800 -20.89902 16.07802 -32.52130
C 0.00800 -23.08397 15.29771 -28.23276
H 0.04800 -24.11055 15.63869 -28.40881
H 0.04800 -22.41661 15.94854 -28.80909
C 0.00800 -23.06873 14.04903 -32.47197
H 0.04800 -23.84949 14.68103 -32.03368
H 0.04800 -22.22898 14.70015 -32.74026
H 0.10400 -23.49456 12.42726 -31.10295
C -0.09600 -19.80692 10.09676 -28.99683
H 0.04800 -18.98182 10.39682 -28.34087
H 0.04800 -19.38811 9.91937 -29.99394
C -0.09600 -22.77166 15.51757 -26.74087
H 0.04800 -22.56680 14.56876 -26.23205
H 0.04800 -21.89378 16.15993 -26.60743
C -0.09600 -23.63080 13.45551 -33.77711
H 0.04800 -24.51410 12.83565 -33.58565
H 0.04800 -23.92645 14.24358 -34.47900
C -0.09600 -18.93577 15.53609 -31.85707
H 0.04800 -18.40104 14.65614 -31.48175
H 0.04800 -18.54106 15.76168 -32.85428
C -0.09600 -22.58809 12.57084 -34.48544
H 0.04800 -21.57817 12.76212 -34.10520

H 0.04800 -22.80077 11.50613 -34.33627
C -0.09600 -23.95197 16.18832 -26.01386
H 0.04800 -24.91317 15.85298 -26.41976
H 0.04800 -23.91411 17.27908 -26.11350
C -0.09600 -18.58129 16.72068 -30.93908
H 0.04800 -19.46846 17.31641 -30.69586
H 0.04800 -18.14546 16.37674 -29.99416
C -0.09600 -20.34865 8.75276 -28.47550
H 0.04800 -20.74642 8.85020 -27.45894
H 0.04800 -21.15719 8.37476 -29.11148
C -0.09600 -17.55992 17.66073 -31.60593
H 0.04800 -16.53357 17.30868 -31.45171
H 0.04800 -17.72662 17.72866 -32.68699
C -0.14400 -17.65226 19.08677 -31.03191
H 0.04800 -18.67158 19.48218 -31.10770
H 0.04800 -17.36689 19.11033 -29.97403
H 0.04800 -16.99007 19.77628 -31.56783
C -0.09600 -22.56943 12.83189 -36.00304
C -0.09600 -19.24527 7.67901 -28.44084
H 0.04800 -18.41840 7.97753 -27.78641
H 0.04800 -18.82888 7.50238 -29.43911
C -0.14400 -19.78708 6.33491 -27.91985
H 0.04800 -19.00187 5.57074 -27.89527
H 0.04800 -20.18495 6.43214 -26.90331
H 0.04800 -20.59557 5.95706 -28.55600
C -0.09600 -23.94374 15.85947 -24.50940
H 0.04800 -23.80979 14.78558 -24.33643
H 0.04800 -23.13094 16.38113 -23.99138
C -0.14400 -25.26507 16.27627 -23.83712
H 0.04800 -26.12382 15.77979 -24.30313
H 0.04800 -25.27076 16.01557 -22.77265
H 0.04800 -25.42771 17.35742 -23.91303
H 0.04800 -21.59480 12.52323 -36.35121
H 0.04800 -22.75754 13.87471 -36.21173
C -0.14400 -23.66944 12.03025 -36.72343
H 0.04800 -23.24950 11.17703 -37.26820
H 0.04800 -24.40699 11.63819 -36.01392
H 0.04800 -24.20687 12.65242 -37.44813

[Oct₄P]⁺

P 0.54400 38.70542 37.61457 31.50833
C -0.24800 37.21567 36.55014 31.32612
H 0.10400 37.49095 35.49724 31.19673
H 0.10400 36.56794 36.61600 32.20772
C -0.24800 38.67682 38.92489 30.21689
H 0.10400 38.35636 38.52387 29.24859
H 0.10400 37.98682 39.73339 30.48398
C -0.24800 38.70502 38.38711 33.17830
H 0.10400 37.87642 39.09569 33.28994
H 0.10400 39.63551 38.93538 33.36454
C -0.24800 40.22491 36.59565 31.31194
H 0.10400 41.01596 36.92286 31.99625
C 0.00800 38.56145 37.32729 34.28634
H 0.04800 37.53217 36.95685 34.35323
H 0.04800 39.21125 36.46465 34.10000
C 0.00800 40.07054 39.55019 30.02161
H 0.04800 40.82663 39.03651 30.62624
H 0.04800 40.39039 39.49312 28.97492
C 0.00800 36.37710 36.96400 30.10255
H 0.04800 36.35879 36.17218 29.34506
H 0.04800 36.78149 37.86537 29.62808
C 0.00800 40.78230 36.69045 29.87948
H 0.04800 40.11226 36.20927 29.15794
H 0.04800 40.90786 37.73380 29.56842
H 0.10400 39.93779 35.57836 31.53350
C -0.09600 38.93787 37.90238 35.66444
H 0.04800 38.29044 38.74393 35.93600
H 0.04800 39.97225 38.26434 35.67675
C -0.09600 34.91869 37.26212 30.49720
H 0.04800 34.73856 37.04124 31.55544
H 0.04800 34.66837 38.31637 30.33282
C -0.09600 42.15618 36.00406 29.76587
H 0.04800 42.09064 34.93740 30.00889
H 0.04800 42.56096 36.08704 28.75080
C -0.09600 40.08100 41.03517 30.42946
H 0.04800 40.03338 41.15024 31.51831
H 0.04800 40.99176 41.53744 30.08399
C -0.09600 43.18012 36.63657 30.72664
H 0.04800 42.84229 37.61720 31.08067
H 0.04800 43.34308 36.00570 31.60787
C -0.09600 33.93058 36.41674 29.67224
H 0.04800 34.34022 35.42389 29.45415
H 0.04800 33.69866 36.89583 28.71422
C -0.09600 38.87956 41.78963 29.83036
H 0.04800 38.39722 41.20652 29.03762
H 0.04800 38.12099 42.00132 30.59250
C -0.09600 38.80529 36.83937 36.77081
H 0.04800 37.77830 36.46343 36.84195
H 0.04800 39.45863 35.98054 36.57935
C -0.09600 39.31098 43.13563 29.21899
H 0.04800 38.61101 43.46364 28.44210

H 0.04800 40.30391 43.06562 28.76042
C -0.09600 39.37054 44.24327 30.28725
H 0.04800 38.52302 44.93204 30.19556
H 0.04800 39.34655 43.82330 31.29926
C -0.09600 40.66020 45.07538 30.16086
H 0.04800 41.40443 44.77366 30.90664
H 0.04800 41.11685 44.95586 29.17177
C -0.14400 40.38138 46.57615 30.36470
H 0.04800 39.50990 46.90233 29.78571
H 0.04800 40.18272 46.80566 31.41777
H 0.04800 41.23480 47.18702 30.04906
C -0.09600 44.54423 36.83594 30.04031
H 0.04800 45.12834 37.62094 30.53396
H 0.04800 44.42402 37.12506 28.99004
C -0.09600 45.38234 35.54438 30.07280
H 0.04800 44.76761 34.67635 30.33687
H 0.04800 45.83950 35.34074 29.09779
C -0.09600 46.51917 35.63957 31.10728
H 0.04800 46.44038 36.55571 31.70358
H 0.04800 46.49936 34.79143 31.80110
C -0.14400 47.89944 35.64795 30.42436
H 0.04800 48.60174 36.30326 30.95205
H 0.04800 48.33889 34.64425 30.40043
H 0.04800 47.83059 36.00287 29.38976
C -0.09600 39.18552 37.41337 38.14833
H 0.04800 38.54015 38.25599 38.42144
H 0.04800 40.22057 37.77349 38.15866
C -0.09600 39.05328 36.35027 39.25464
H 0.04800 38.02635 35.97416 39.32591
H 0.04800 39.70673 35.49156 39.06302
C -0.09600 39.43363 36.92423 40.63214
H 0.04800 38.78832 37.76689 40.90530
H 0.04800 39.33952 36.16767 41.41945
C -0.14400 40.88807 37.43018 40.64656
H 0.04800 40.94936 38.45783 41.02247
H 0.04800 41.52132 36.80604 41.28731
H 0.04800 41.32410 37.41995 39.64114
C -0.09600 32.60160 36.21530 30.42379
H 0.04800 32.77258 35.89629 31.45825
H 0.04800 32.01724 37.14188 30.45644
C -0.09600 31.73090 35.14152 29.74521
H 0.04800 30.79812 34.97717 30.29659
H 0.04800 31.46322 35.43230 28.72300
C -0.09600 32.46672 33.79102 29.66561
H 0.04800 33.31249 33.75581 30.36169
H 0.04800 31.79959 32.95786 29.91438
C -0.14400 33.01939 33.53616 28.25097
H 0.04800 34.02148 33.09394 28.28776
H 0.04800 32.37607 32.84959 27.68895
H 0.04800 33.09021 34.46685 27.67658

[Ph₃EtP]⁺

C -0.24800 34.74001 35.49619 24.26694
H 0.10400 34.34203 36.34560 23.71222
H 0.10400 34.62991 35.68489 25.33459
C -0.24800 34.51657 32.60762 24.73497
H 0.10400 34.40738 32.78303 25.80497
H 0.10400 35.57339 32.48129 24.50094
C -0.24800 34.03656 33.70097 22.05417
H 0.10400 33.50005 32.79463 21.77438
H 0.10400 33.63340 34.54195 21.49044
C -0.24800 32.10775 34.20014 24.20934
H 0.10400 31.69769 35.04504 23.65654
H 0.10400 31.56109 33.29751 23.93731
P 0.54400 33.85014 34.00117 23.81630
C -0.04000 33.75981 31.32102 24.35607
H 0.04800 33.15242 30.95463 25.19150
H 0.04800 33.08687 31.48912 23.50755
H 0.04800 34.45192 30.51921 24.07463
C -0.04000 36.23536 35.33489 23.93597

H 0.04800 36.63409 34.39659 24.33810
H 0.04800 36.40605 35.32899 22.85341
H 0.04800 36.82827 36.15373 24.35914
C -0.04000 31.93779 34.45601 25.71840
H 0.04800 31.71030 35.50867 25.92149
H 0.04800 31.12139 33.85547 26.13547
H 0.04800 32.84958 34.20276 26.27123
C 0.00800 35.52728 33.53094 21.70713
H 0.04800 35.92481 32.59029 22.10495
H 0.04800 36.12951 34.34625 22.12389
C -0.09600 35.75070 33.52133 20.18345
H 0.04800 34.84150 33.81211 19.64501
H 0.04800 36.54418 34.21890 19.89211
C -0.14400 36.15732 32.12205 19.68520
H 0.04800 35.96449 31.35627 20.44514
H 0.04800 35.59921 31.84135 18.78474
H 0.04800 37.22433 32.08084 19.43842

[Ph₃PrP]⁺

C -0.00468 29.03621 -13.56209 -23.59999
H 0.07959 29.76332 -12.77722 -23.38829
P -0.15095 29.05808 -14.85513 -22.48699
C 0.25741 28.08595 -16.23705 -23.14802
C -0.21302 28.69828 -17.24282 -23.90460
C -0.21302 26.69061 -16.22689 -23.00849
C -0.04658 27.92369 -18.22337 -24.51963
C -0.04658 25.92056 -17.20833 -23.62775
C -0.08832 26.53634 -18.20487 -24.38579
H 0.13133 29.77590 -17.24635 -24.02875
H 0.13133 26.21000 -15.45167 -22.41886
H 0.11338 28.40327 -18.98690 -25.12274
H 0.11338 24.83975 -17.18973 -23.52582
H 0.11880 25.93436 -18.95962 -24.88166
C 0.25741 30.77369 -15.39598 -22.24176
C -0.21302 31.23456 -15.82205 -20.98827
C -0.21302 31.65248 -15.39283 -23.33715
C -0.04658 32.55456 -16.24018 -20.83120
C -0.04658 32.97115 -15.81319 -23.17140
C -0.08832 33.42450 -16.23715 -21.92188
H 0.13133 30.56706 -15.81527 -20.13354
H 0.13133 31.30075 -15.07420 -24.31228
H 0.11338 32.90365 -16.56273 -19.85502

H 0.11338 33.64376 -15.80831 -24.02363
H 0.11880 34.45325 -16.56179 -21.79722
C 0.25741 28.38707 -14.64290 -20.79214
C -0.21302 28.32177 -13.34654 -20.26987
C -0.21302 27.94489 -15.72272 -20.01358
C -0.04658 27.83311 -13.12945 -18.98195
C -0.04658 27.45217 -15.50433 -18.72834
C -0.08832 27.39805 -14.20815 -18.21106
H 0.13133 28.64591 -12.51260 -20.88739
H 0.13133 27.97931 -16.72983 -20.41847
H 0.11338 27.78470 -12.12058 -18.58338
H 0.11338 27.10684 -16.34337 -18.13165
H 0.11880 27.01017 -14.03958 -17.21095
H 0.07959 29.37527 -13.99898 -24.52765
C -0.07390 27.62222 -13.02960 -23.89776
H 0.04800 26.94782 -13.83750 -24.20370
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H 0.04800 28.00333 -12.42609 -25.96954
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H 0.04800 28.29884 -11.14491 -24.78762

[Ph₃BuP]⁺

C -0.00468 6.40284 22.07830 29.54685
H 0.07959 7.25779 22.57403 30.00820
P -0.15095 5.31962 23.13727 28.76173
C 0.25741 3.78588 22.25067 28.37020
C -0.21302 2.70923 22.25791 29.26445
C -0.21302 3.72850 21.44663 27.22268
C -0.04658 1.59088 21.46551 29.01718
C -0.04658 2.60886 20.65420 26.98156
C -0.08832 1.54126 20.66102 27.87994
H 0.13133 2.75504 22.86598 30.16157
H 0.13133 4.55889 21.44024 26.52266
H 0.11338 0.76966 21.45925 29.72590
H 0.11338 2.57392 20.02502 26.09736
H 0.11880 0.67629 20.03070 27.69984
C 0.25741 4.94059 24.52460 29.86972
C -0.21302 4.76234 25.82554 29.37885
C -0.21302 4.81667 24.28230 31.24744
C -0.04658 4.46343 26.86984 30.25176
C -0.04658 4.51694 25.33258 32.11356
C -0.08832 4.33961 26.62533 31.61970
H 0.13133 4.86930 26.02485 28.31818
H 0.13133 4.94317 23.27685 31.63367
H 0.11338 4.33308 27.87503 29.86260
H 0.11338 4.42221 25.13645 33.17719

H 0.11880 4.10824 27.44068 32.29862
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C -0.21302 7.12842 24.04716 26.85544
C -0.21302 4.80977 24.39592 26.25864
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H 0.13133 7.86593 23.65812 27.55300
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H 0.11338 8.58296 24.74091 25.42761
H 0.11338 4.46126 25.35268 24.36328
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H 0.04800 7.37681 21.13618 27.82480
C -0.09600 7.61952 19.84472 29.51668
H 0.04800 7.05443 19.45799 30.37239
H 0.04800 7.92062 18.98664 28.90500
C -0.14400 8.90259 20.49669 30.06465
H 0.04800 9.52338 19.76847 30.59890
H 0.04800 9.51114 20.92000 29.25745
H 0.04800 8.67059 21.30837 30.76354

[Ph₃HexP]⁺

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P -0.15095 31.79869 -31.49310 -16.96549
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H 0.13133 33.08147 -30.08353 -19.22497
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H 0.11338 35.34526 -30.23024 -20.19946
H 0.11338 36.38327 -33.26592 -17.33563
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C -0.21302 30.85269 -29.11993 -18.22360

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C -0.04658 30.07468 -28.43194 -19.15294
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H 0.13133 31.49892 -28.57209 -17.54416
H 0.11338 28.51442 -31.07509 -20.62285
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H 0.07959 32.01009 -33.33589 -15.71757
C -0.07390 31.50646 -34.13385 -17.58154
H 0.04800 30.81591 -33.98299 -18.41909
H 0.04800 32.52494 -34.11383 -17.98577
C -0.09600 31.25672 -35.54723 -17.02334
H 0.04800 31.90751 -35.75892 -16.16732
H 0.04800 30.22033 -35.66619 -16.68740
C -0.09600 31.52576 -36.62638 -18.08854
H 0.04800 30.86047 -36.50975 -18.95161
H 0.04800 32.55660 -36.57501 -18.45709
C -0.09600 31.30596 -38.04116 -17.52136
H 0.04800 31.97138 -38.23888 -16.67328
H 0.04800 30.27616 -38.17510 -17.17111
C -0.14400 31.57792 -39.12042 -18.58570
H 0.04800 31.42229 -40.12729 -18.18184
H 0.04800 30.91367 -39.00507 -19.44975
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H 0.07959 30.26543 -33.02485 -16.23559

[Ph₃OctP]⁺

C -0.00468 -23.68559 9.64981 -31.21736
H 0.07959 -24.00793 10.68906 -31.29208
P -0.15095 -24.79417 8.62896 -30.41727
C 0.25741 -23.99189 7.04665 -30.03734
C -0.21302 -23.34940 6.84890 -28.80973
C -0.21302 -23.90407 6.06220 -31.03219
C -0.04658 -22.62237 5.68301 -28.58199
C -0.04658 -23.17361 4.89934 -30.80016
C -0.08832 -22.53019 4.71068 -29.57652
H 0.13133 -23.40103 7.61404 -28.04254
H 0.13133 -24.40429 6.20786 -31.98518
H 0.11338 -22.10863 5.54639 -27.63641
H 0.11338 -23.09946 4.14506 -31.57763
H 0.11880 -21.94747 3.81173 -29.40259
C 0.25741 -25.31618 9.42019 -28.86890
C -0.21302 -26.62985 9.30289 -28.39385
C -0.21302 -24.37717 10.15861 -28.13056
C -0.04658 -27.00029 9.91376 -27.19740
C -0.04658 -24.75600 10.76601 -26.93446
C -0.08832 -26.06451 10.64538 -26.46566
H 0.13133 -27.36544 8.74596 -28.96385
H 0.13133 -23.35639 10.24556 -28.48630
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H 0.11880 -26.35544 11.12209 -25.53434
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C -0.21302 -27.05965 6.96359 -30.86867
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C -0.08832 -28.74228 7.45038 -32.53416
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H 0.13133 -26.67085 6.32162 -30.08375
H 0.11338 -28.42654 9.23577 -33.69981
H 0.11338 -28.78462 5.73057 -31.23386
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H 0.07959 -22.82717 9.68142 -30.56275
C -0.07390 -23.16050 9.06951 -32.54369
H 0.04800 -22.75380 8.06133 -32.40487
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C -0.09600 -22.03918 9.94477 -33.13373
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H 0.04800 -21.68954 9.55097 -34.09486
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H 0.04800 -23.39849 11.41291 -34.02734
H 0.04800 -22.79821 11.87628 -32.43027
C -0.09600 -21.42385 12.24360 -34.03199
H 0.04800 -20.51397 12.26656 -33.42149
H 0.04800 -21.15019 11.85005 -35.01755
C -0.09600 -21.88873 13.69883 -34.22643
H 0.04800 -22.75655 13.75474 -34.89342
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C -0.09600 -20.77450 14.56596 -34.84139
H 0.04800 -19.87070 14.55278 -34.22165
H 0.04800 -20.49570 14.20869 -35.83926
C -0.14400 -21.21923 16.03365 -34.98176
H 0.04800 -20.42058 16.65393 -35.40426
H 0.04800 -22.09117 16.12523 -35.63937
H 0.04800 -21.49166 16.46264 -34.01075

2 Liquid structure of the ILs at 420 K

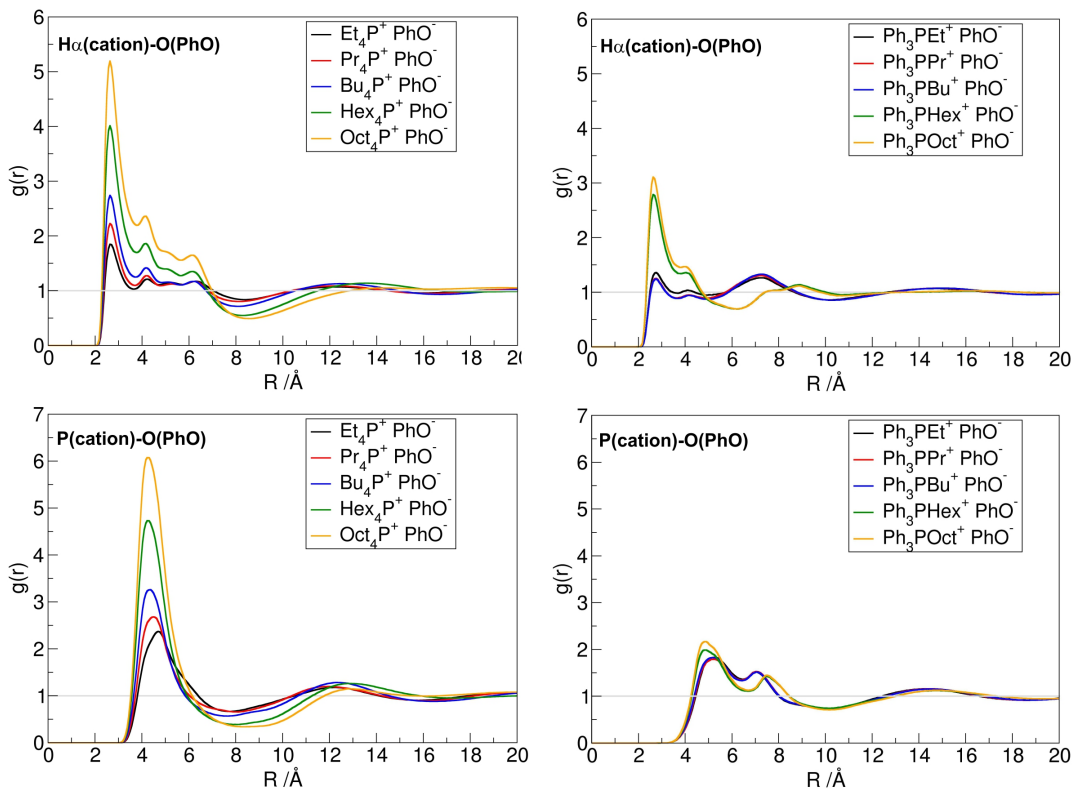


Figure S1: Relevant radial pair correlation functions for the liquid models investigated by classical molecular dynamics simulations, describing the anion-cation interactions.

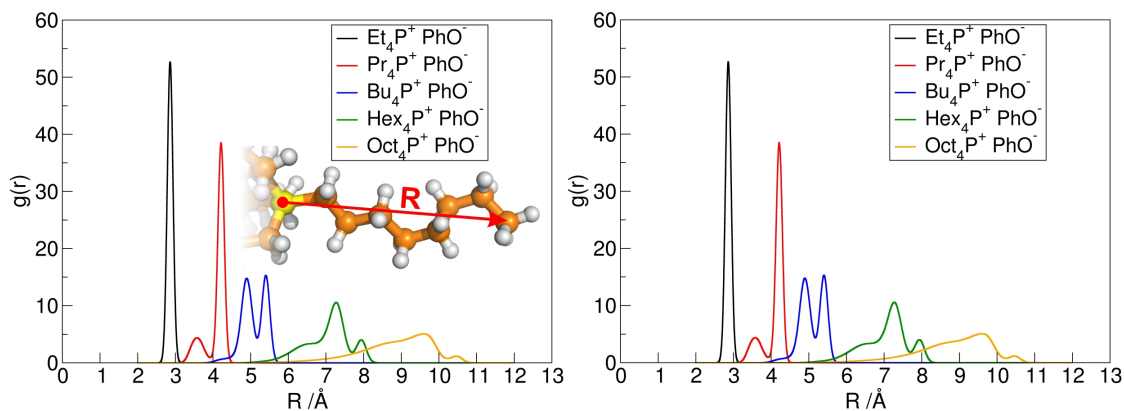


Figure S2: Distribution of the intramolecular distances between the phosphorous atom and the terminal carbon atom of the side chains in the investigated ionic liquids.

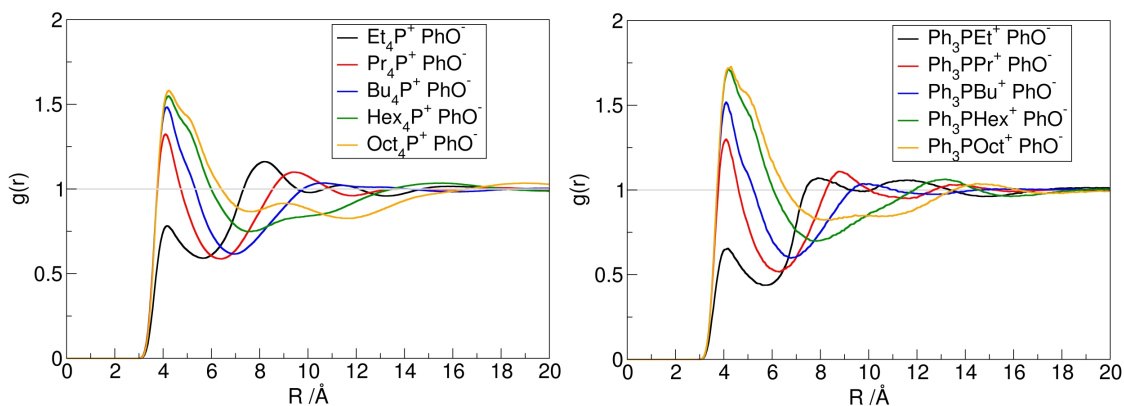


Figure S3: Radial pair correlation functions between the terminal carbon atoms of the side chains in the liquid models investigated by classical molecular dynamics simulations.

3 Complete tables with the Gibbs free energies at 298.15 and 420 K in THF and IL

Table S1: Gibbs free energy profiles at 298.15 K in THF for the Wittig reaction of $\text{Me}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_2O	12.3	10.9	-75.3	-58.3	10.1	-227.9
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_3CHO	19.8	28.8	-54.3	-35.2	40.3	-203.6
$\text{Me}_4\text{P}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	17.6	46.1	-38.8	-21.8	56.2	-185.8
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCHO	23.4	25.3	-48.4	-27.4	48.0	-207.3
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCMeO	20.5	41.9	-37.0	→	60.9	-189.7
$\text{Me}_4\text{P}^+\text{PhO}^-$	Ph_2CO	24.6	40.6	-40.9	→	61.8	-200.6
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_2O	16.9	8.8	-84.5	→	42.2	-253.4
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	31.8	27.8	-63.1	→	42.8	-221.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	30.7	36.5	-60.4	→	45.3	-217.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	28.9	52.4	-47.6	→	61.7	-200.2
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	32.2	22.9	-58.5	→	51.0	-228.5
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	33.7	22.1	-52.3	→	53.6	-218.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	34.6	71.8	-42.5	→	65.5	-203.7
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	33.3	46.6	-42.9	→	66.5	-202.9
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	30.4	44.5	-50.2	→	58.8	-217.9

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S2: Gibbs free energy profiles at 298.15 K in THF for the Wittig reaction of $\text{Ph}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_2O	-7.4	19.5	-93.2	→	-10.0	-261.4
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_3CHO	-0.7	27.9	-69.8	-51.9	13.9	-237.1
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	-1.0	48.6	-52.4	-38.2	28.8	-219.3
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCHO	5.1	25.5	-63.6	-39.9	26.6	-240.8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCMeO	-2.6	45.4	-52.3	-35.9	30.9	-223.2
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	Ph_2CO	5.5	36.4	-61.1	-34.7	32.7	-234.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_2O	-6.3	10.3	-107.6	-90.1	-15.4	-290.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	3.6	32.0	-82.3	-68.0	9.0	-258.5
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	1.7	29.3	-73.6	-63.7	13.3	-254.6
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	6.1	65.4	-54.2	-50.2	26.1	-237.4
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	8.9	21.0	-70.0	-61.8	14.7	-265.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	4.2	20.0	-69.6	-51.6	26.0	-255.5
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	3.5	46.3	-57.3	-44.0	26.8	-240.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	2.8	48.7	-55.2	-43.0	34.5	-240.2
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	0.4	41.6	-67.0	-44.7	25.7	-255.1

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S3: Gibbs free energy profiles at 420 K in THF for the Wittig reaction of $\text{Me}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_2O	18.9	21.0	-65.4	-48.0	20.1	-228.5
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_3CHO	27.6	42.3	-42.3	-22.5	53.5	-204.5
$\text{Me}_4\text{P}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	25.3	60.2	-25.9	-8.7	70.0	-186.3
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCHO	33.8	40.5	-35.3	-13.3	63.1	-208.0
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCMeO	29.9	57.3	-22.8	→	76.2	-190.3
$\text{Me}_4\text{P}^+\text{PhO}^-$	Ph_2CO	34.5	54.0	-27.8	→	76.5	-201.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_2O	23.7	18.2	-74.6	→	52.8	-256.5
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	39.6	39.5	-51.0	→	55.9	-222.5
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	38.0	49.7	-48.1	→	58.4	-218.7
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	35.6	59.0	-35.0	→	75.3	-202.6
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	42.4	37.8	-45.1	→	65.8	-230.0
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	44.0	37.3	-38.0	→	68.3	-219.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	44.4	87.2	-28.7	→	80.6	-205.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	42.7	62.0	-29.0	→	81.6	-204.4
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	39.6	58.2	-36.8	→	72.0	-219.9

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S4: Gibbs free energy profiles at 420 K in THF for the Wittig reaction of $\text{Ph}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS _{5→6}	6	7	TS _{7→8}	8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_2O	-0.7	29.8	-82.4	→	0.2	-263.4
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_3CHO	8.0	40.8	-56.4	-38.7	26.7	-239.4
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	7.8	62.3	-38.5	-24.5	42.1	-221.2
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCHO	16.1	40.9	-48.3	-24.9	43.4	-242.9
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCMeO	8.9	61.4	-36.4	-20.4	46.4	-225.2
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	Ph_2CO	16.9	51.8	-45.6	-19.1	48.2	-236.2
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_2O	0.7	21.3	-96.5	-79.1	-4.9	-294.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	12.8	45.1	-68.6	-54.6	22.0	-260.8
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	10.2	42.7	-59.4	-50.2	26.4	-257.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	15.0	79.3	-39.4	-36.0	39.7	-240.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	20.6	36.4	-54.4	-46.4	29.7	-268.3
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	15.5	35.3	-53.2	-35.7	41.3	-257.6
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	14.7	62.8	-41.1	-27.8	41.8	-243.6
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	14.3	64.5	-39.1	-26.8	50.0	-242.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	12.0	57.5	-50.9	-29.0	40.8	-258.2

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S5: Gibbs free energy profiles at 298.15 K in IL for the Wittig reaction of $\text{Me}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_2O	28.1	21.7	-59.3	-40.5	26.3	-215.0
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_3CHO	36.4	39.4	-37.9	-17.1	57.2	-190.3
$\text{Me}_4\text{P}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	34.4	56.7	-22.0	-3.6	73.3	-172.3
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCHO	39.0	35.5	-32.4	-10.1	63.6	-195.2
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCMeO	36.7	52.7	-20.4	→	78.1	-177.1
$\text{Me}_4\text{P}^+\text{PhO}^-$	Ph_2CO	39.9	51.9	-24.6	→	77.6	-188.4
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_2O	30.0	19.4	-69.7	→	57.8	-241.4
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	47.0	38.2	-47.8	→	59.0	-208.8
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	46.2	46.1	-45.3	→	61.2	-205.0
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	44.8	68.3	-32.2	→	77.8	-187.6
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	46.6	32.5	-43.8	→	66.6	-217.2
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	48.1	31.7	-37.8	→	68.2	-206.8
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	49.5	81.7	-27.2	→	81.6	-192.0
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	48.2	56.3	-28.0	→	82.2	-191.1
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	44.9	55.4	-35.0	→	74.1	-206.6

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S6: Gibbs free energy profiles at 298.15 K in IL for the Wittig reaction of $\text{Ph}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_2O	4.4	27.7	-82.0	→	2.3	-251.9
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_3CHO	11.3	38.8	-58.2	-39.1	29.1	-227.2
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	11.0	56.5	-40.7	-25.1	41.6	-209.0
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCHO	16.7	33.8	-51.9	-28.0	38.8	-231.5
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCMeO	9.0	53.9	-40.9	-23.1	43.2	-213.6
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	Ph_2CO	17.3	44.9	-49.5	-22.9	44.5	-224.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_2O	3.4	17.4	-97.8	-79.3	-4.7	-282.5
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	13.3	38.7	-72.2	-56.9	20.1	-249.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	12.1	36.2	-63.7	-52.6	24.3	-246.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	16.1	72.2	-44.0	-38.9	37.1	-228.8
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	18.7	28.0	-59.9	-51.4	25.0	-257.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	13.8	27.0	-60.0	-41.0	36.3	-247.5
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	13.0	53.2	-47.1	-33.5	37.5	-232.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	12.6	55.5	-44.9	-32.3	45.1	-231.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	10.3	49.5	-57.4	-34.8	36.0	-247.1

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S7: Gibbs free energy profiles at 420 K in IL for the Wittig reaction of $\text{Me}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_2O	34.6	31.8	-49.2	-30.1	36.2	-215.5
$\text{Me}_4\text{P}^+\text{PhO}^-$	CH_3CHO	44.0	52.9	-25.6	-4.4	70.4	-191.2
$\text{Me}_4\text{P}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	41.7	70.8	-9.2	9.5	86.9	-172.8
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCHO	48.9	50.2	-19.5	3.7	78.1	-196.2
$\text{Me}_4\text{P}^+\text{PhO}^-$	PhCMeO	45.6	67.6	-6.5	→	93.0	-178.0
$\text{Me}_4\text{P}^+\text{PhO}^-$	Ph_2CO	49.2	64.4	-12.1	→	91.7	-189.4
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_2O	36.6	28.6	-59.8	→	68.2	-244.7
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	54.5	49.7	-35.7	→	71.8	-210.1
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	53.2	59.3	-33.0	→	74.1	-206.6
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	51.0	74.5	-19.8	→	91.1	-190.2
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	56.1	46.9	-30.8	→	81.0	-219.2
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	57.7	46.3	-24.0	→	82.3	-208.3
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	58.7	96.6	-13.9	→	96.2	-194.1
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	56.9	71.1	-14.5	→	96.7	-192.9
$\text{Me}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	53.4	68.0	-22.3	→	86.6	-209.1

^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

Table S8: Gibbs free energy profiles at 420 K in IL for the Wittig reaction of $\text{Ph}_3\text{PR}^+\text{PhO}^-$ ($\text{R} = \text{Me}, \text{Et}$), taking **2** as reference, and considering the formation of $[(\text{PhO})_2\text{H}]^-$ from the phenol. The structures are shown in Figure 3. If *cis* and *trans* products are available, only those reactions are shown here, which involve the lower energy oxaphosphetane intermediate.

IL	substrate	5	TS_{5→6}	6	7	TS_{7→8}	8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_2O	9.5	37.0	-72.8	→	10.6	-255.7
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	CH_3CHO	18.2	52.3	-46.5	-27.8	42.0	-231.4
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	18.1	69.3	-28.7	-13.4	52.9	-213.0
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCHO	25.8	47.9	-38.5	-14.9	53.5	-235.8
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	PhCMeO	18.6	68.5	-26.9	-9.6	56.7	-217.7
$\text{Ph}_3\text{PMe}^+\text{PhO}^-$	Ph_2CO	26.6	58.9	-36.1	-9.3	57.9	-228.9
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_2O	9.3	27.7	-87.9	-69.6	-4.4	-288.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^a	21.3	51.2	-59.7	-44.9	31.6	-253.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	CH_3CHO^b	19.4	48.9	-50.8	-40.5	35.9	-250.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	$(\text{CH}_3)_2\text{CO}$	23.6	85.3	-30.6	-26.2	49.1	-233.7
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^a	29.0	42.5	-45.7	-37.4	38.4	-262.1
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCHO^b	23.7	41.3	-45.1	-26.7	50.1	-251.2
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^a	22.9	68.8	-32.3	-18.8	51.1	-237.2
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	PhCMeO^b	22.7	70.5	-30.2	-17.6	59.0	-236.0
$\text{Ph}_3\text{PEt}^+\text{PhO}^-$	Ph_2CO	20.5	64.1	-42.8	-20.8	49.5	-251.9

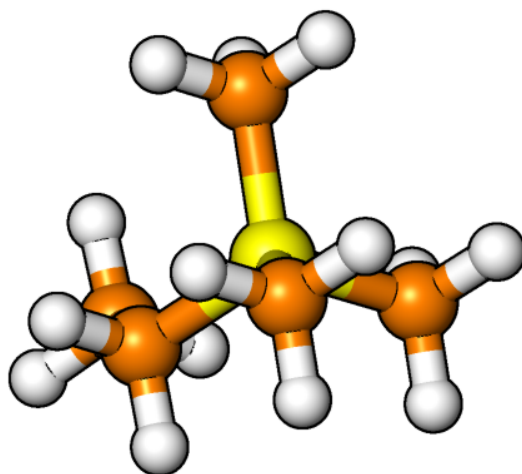
^a reaction Gibbs free energy profile for the formation of the *trans* structure

^b reaction Gibbs free energy profile for the formation of the *cis* structure

4 Geometries, names, and ball-and-stick representation of the calculated molecules and ions

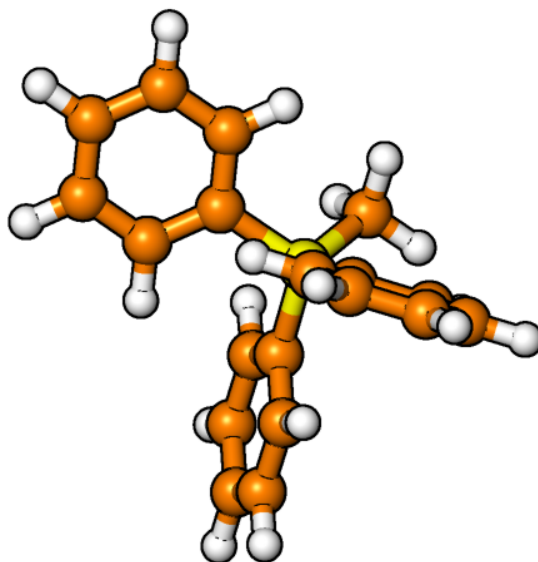
Names of the systems are given in symbols in the following order

- 1) The number of the geometry for the system is given in Figures 3 and 4 in the article
- 2) The notation for the phosphonium cations is given as follows:
Me₄P - A
Me₃PEt - B
PhP₃Me - C
PhP₃Et - D
- 3) The notation for the substituent on the carbonyl group is H, Me, or Ph.
- 4) If more than one geometric isomer exists, 'trans' corresponds to the *E*-product and "cis" to the *Z*-product



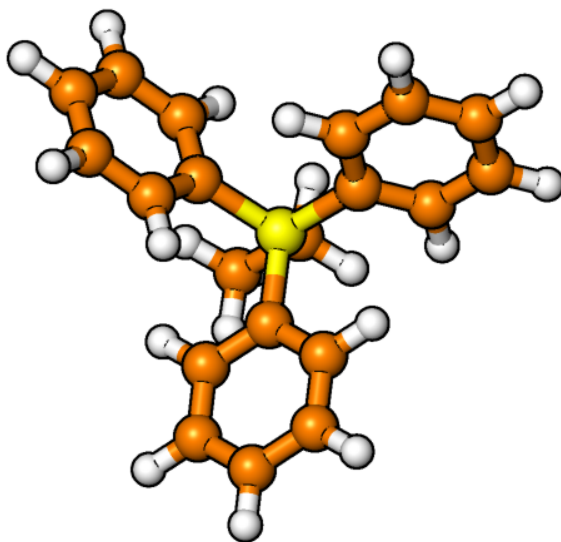
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H 4.589174 1.196567 -0.192359	H 5.417138 4.223390 -3.849558	C 2.051299 3.155989 -2.249353
H 3.303202 2.259269 0.396196	H 4.120201 5.282795 -3.261680	P 3.824283 3.021749 -2.518431
C 4.356360 2.213159 0.122027	H 3.818622 4.180610 -4.619728	H 5.775563 3.207246 -1.199169
H 5.266408 1.305431 -3.371849	C 4.344518 4.298808 -3.672696	H 4.496485 4.257137 -0.619325
H 3.684612 1.297996 -4.177196	H 1.527053 3.054627 -3.199293	C 4.710248 3.240362 -0.957886
H 3.851018 0.620539 -2.547504	H 1.814886 4.126713 -1.814200	



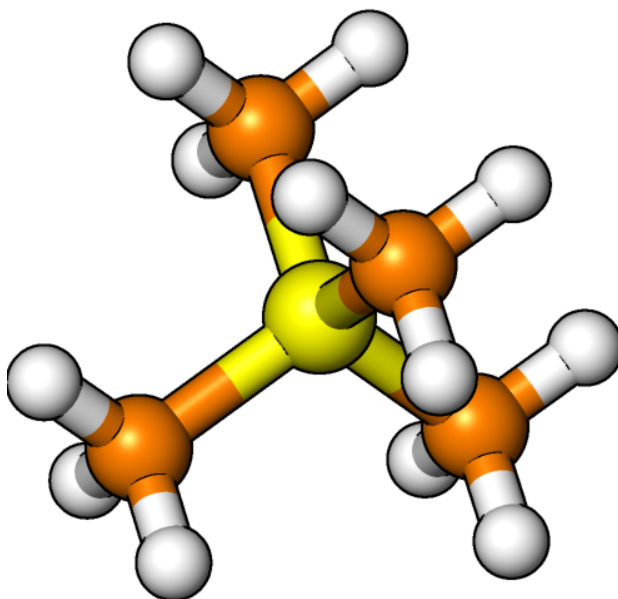
Methyltriphenylphosphonium

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C 3.640449 2.306413 4.489630	C 1.573430 -2.239798 3.601671	C -1.944162 -0.430737 3.610627
C 2.348336 2.232295 4.996661	C 0.706464 -1.831295 2.585928	C -3.195794 -0.012951 4.045118
C 1.371256 1.522644 4.311469	C 0.004374 -2.783137 1.836682	H -4.658464 1.554344 4.010625
C 1.693399 0.881739 3.112269	C 0.176789 -4.132431 2.103350	H -3.299181 3.044191 2.578773
C 2.996307 0.953001 2.606570	H 1.175820 -5.591191 3.319768	H -1.077776 2.332249 1.813131
C 3.963736 1.667894 3.295752	H 2.410318 -3.910723 4.647578	H -1.568717 -1.401174 3.900297
H 4.398046 2.863150 5.023669	H 2.117942 -1.508834 4.181684	H -3.789004 -0.663277 4.672851
H 2.098606 2.727988 5.924052	H -0.679606 -2.478302 1.055502	C 0.596625 0.195853 0.481432
H 0.365646 1.471732 4.704224	H -0.363304 -4.867441 1.523359	H 1.575670 -0.126465 0.133546
H 3.261951 0.452645 1.685535	C -3.682955 1.233926 3.672511	H -0.171221 -0.373290 -0.038536
H 4.968929 1.727525 2.902558	C -2.919801 2.073629 2.865427	H 0.467215 1.254362 0.265052
C 1.043123 -4.537573 3.115331	C -1.669124 1.666891 2.428207	



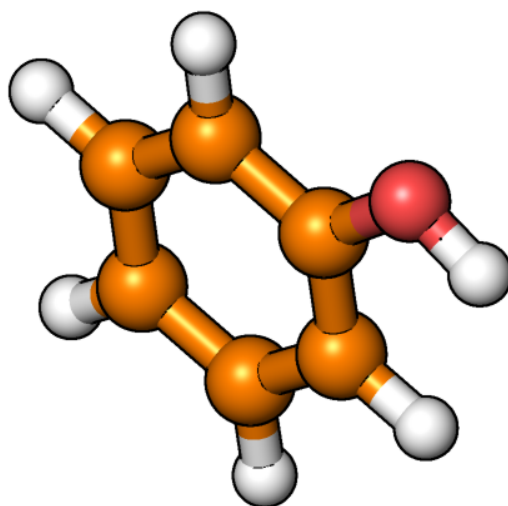
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C -0.479510 3.834947 4.364166	C 1.995687 -0.684429 2.758340	H -3.569192 -3.979141 3.515832
C -0.966414 2.647594 4.898675	C 2.677513 -1.652595 2.011299	H -4.240637 -1.729160 2.735506
C -0.735461 1.444279 4.246169	C 3.922066 -2.098137 2.431071	H -2.533297 -0.040197 2.221470
C -0.010701 1.430429 3.050723	H 5.461991 -1.934137 3.915686	H 0.548650 -2.855756 3.264441
C 0.484935 2.626208 2.519908	H 4.259768 -0.224056 5.237294	H -1.173776 -4.532950 3.784364
C 0.245776 3.824070 3.176642	H 2.054344 0.582134 4.501092	C 0.404837 0.115087 0.442924
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H -1.527738 2.657020 5.822364	H 4.447669 -2.843952 1.851141	H 1.244964 0.781146 0.239744
H -1.118956 0.523777 4.662354	C -2.813931 -3.241353 3.282485	C -0.893080 0.645433 -0.166925
H 1.055484 2.629686 1.601611	C -3.193421 -1.976266 2.842173	H -0.751618 0.799108 -1.235555
H 0.623952 4.748049 2.762608	C -2.229668 -1.025800 2.543913	H -1.711342 -0.060673 -0.038410
C 4.491010 -1.585477 3.592950	C -0.872065 -1.342692 2.682998	H -1.184315 1.598031 0.272774
C 3.816376 -0.624419 4.336602	C -0.495018 -2.609685 3.134735	



Methyltrimethylphosphonium

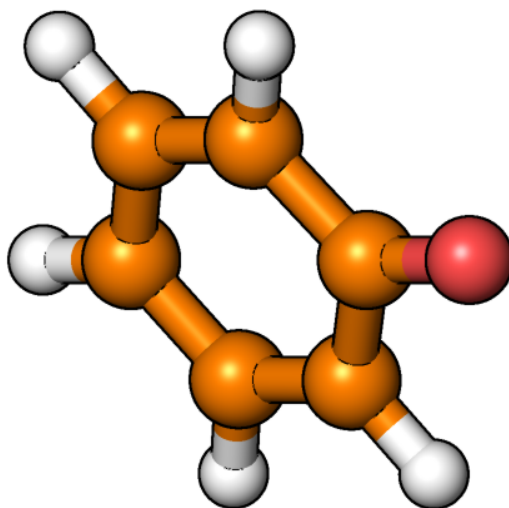
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H 1.737957 -2.716405 -3.111034	C -0.208113 -1.161887 -5.017142	H -0.902061 0.375666 -2.373120
H 0.311462 -2.300155 -2.139852	H 2.166596 0.885368 -5.092453	H -0.202533 1.573715 -3.480758
C 1.233482 -1.913737 -2.573634	H 2.897613 -0.726376 -4.952981	C 0.026047 0.751049 -2.803588
H -0.440049 -0.348038 -5.703765	H 3.038929 0.431307 -3.614610	



Phenol

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-307.07711856

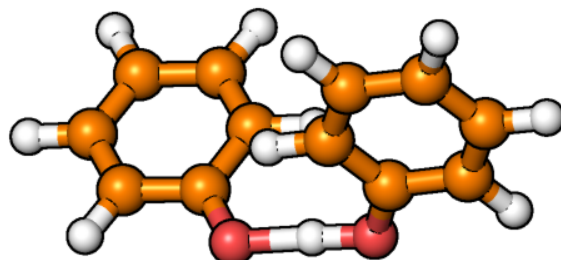
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O -4.760478 0.208110 -3.236777	C -4.760478 -1.129272 -5.251767	C -4.760478 1.224954 -6.722596
H -4.760478 -0.037345 -8.464694	C -4.760478 1.282551 -5.336302	C -4.760478 0.000222 -7.384239
C -4.760478 0.101017 -4.599264	H -4.760478 -2.133332 -7.141154	
H -4.760478 -2.047355 -4.675253	H -4.760478 2.146020 -7.290541	



Phenolate

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-306.50598851

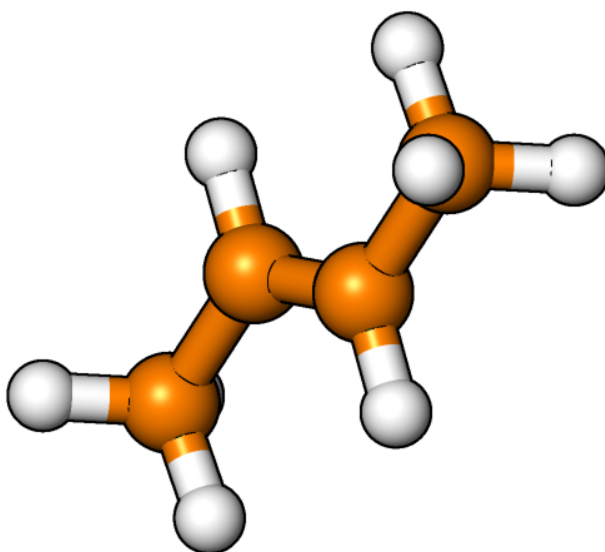
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H -4.760478 -2.132991 -7.136180	C -4.760478 -1.126909 -5.253024	
H -4.760478 2.149975 -7.298634	C -4.760478 1.289388 -5.344672	
H -4.760478 -2.045579 -4.674978	C -4.760478 -1.166944 -6.635938	



Phenol-phenolate complex

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-613.62900307

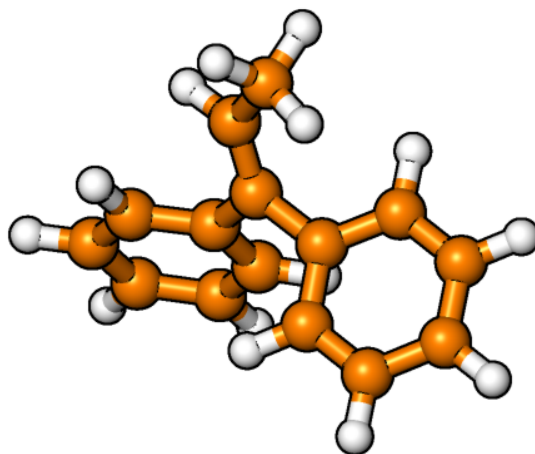
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H -0.070727 6.124843 -11.486514	C -0.326124 3.792935 -9.018112	C -4.541733 1.115323 -5.838752
H 0.709913 4.117147 -12.727782	C 0.113656 2.646147 -9.711125	C -4.120461 1.098246 -7.168631
H -0.732290 5.886308 -9.103340	H -0.141168 1.451721 -8.116453	C -3.571876 1.244777 -4.843819
H 0.820330 1.917539 -11.596638	O -0.510212 1.449363 -6.787882	C -2.780126 1.205180 -7.504618
H -0.610522 3.688431 -7.980231	H -5.591201 1.031298 -5.585953	C -2.227819 1.354482 -5.161249
C -0.018297 5.161338 -10.995703	H -4.855117 1.000106 -7.961687	C -1.772292 1.339422 -6.508474
C 0.417870 4.033024 -11.686625	H -3.872573 1.260975 -3.800645	
C -0.387469 5.021353 -9.658929	H -2.472879 1.187611 -8.542604	



(*E*)-but-2-ene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-156.99903797

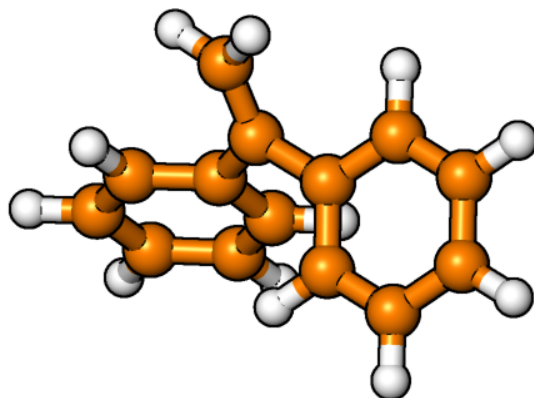
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H -1.244965 2.181616 -0.876845	H 0.955992 1.183653 0.000000	
H -1.244965 2.181616 0.876845	C 1.221591 -1.528164 -0.000000	
H 2.132995 -0.929347 -0.000000	C -1.221591 1.528164 -0.000000	



Prop-1-ene-1,1-diylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-579.17737105

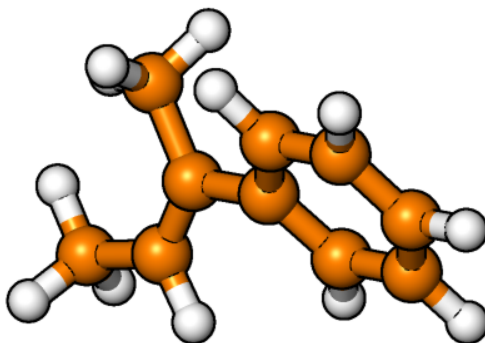
H -1.149426	4.364159	-1.607818	C 2.008472	4.646306	0.070197	H -3.030488	0.642000	0.484550
H -2.682623	3.753664	-2.245048	C 0.895346	4.602801	2.199740	C -1.549528	2.283239	-1.192077
H -1.180478	3.326777	-3.035444	C 1.135241	3.674114	-0.403705	C -0.814757	2.120147	-0.081728
C -1.636195	3.500906	-2.055904	C 0.031062	3.625446	1.727215	C 0.233832	0.320535	1.305942
H 2.564488	5.877539	1.740446	C 0.128433	3.157014	0.413504	C 0.165071	-0.865137	2.024359
H 2.785197	5.032491	-0.576954	H -2.169459	1.449179	-1.503324	C -1.051716	-1.519741	2.182475
H 0.796416	4.962530	3.215384	H 1.184188	0.823534	1.190365	C -2.199012	-0.973858	1.618103
H 1.239177	3.299974	-1.413056	H 1.064262	-1.279032	2.461404	C -2.128473	0.210128	0.896149
H -0.732937	3.218805	2.376748	H -1.106761	-2.440823	2.747033	C -0.909056	0.871554	0.715509
C 1.887596	5.118227	1.371524	H -3.154552	-1.464399	1.750503			



Ethene-1,1-diyl dibenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-539.91693530

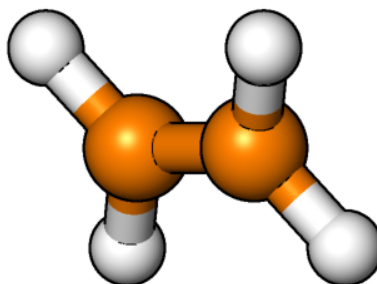
H 3.580835 5.512577 -0.233008	C 1.212390 3.395984 0.951518	C -1.652720 2.371521 -1.017130
H 2.497019 4.879165 -2.368705	C 0.579154 3.043858 -0.244879	C -0.589563 2.129449 -0.240912
H 2.748414 4.552418 1.893670	H -2.489718 1.688512 -1.057691	C 0.648134 0.221304 0.806339
H 0.604299 3.299932 -2.373522	H -1.710799 3.260485 -1.629152	C 0.688961 -0.918543 1.597109
H 0.857331 2.975775 1.882539	H 1.542187 0.555713 0.298858	C -0.455714 -1.356574 2.254314
C 2.743712 4.827078 -0.236327	H 1.616324 -1.466717 1.699625	C -1.640791 -0.642810 2.114919
C 2.132893 4.473965 -1.433905	H -0.422540 -2.242059 2.874975	C -1.681582 0.495170 1.320395
C 2.278523 4.284182 0.956718	H -2.533218 -0.966490 2.634206	C -0.541046 0.940263 0.645104
C 1.062040 3.589787 -1.437508	H -2.600262 1.059385 1.234361	



But-1-en-2-ylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-387.71714628

H -0.953181 4.715618 -0.087694	H -2.107009 1.895313 0.466514	C 1.338646 0.092896 0.389494
H -2.073795 4.328064 1.213733	H 2.138014 0.757910 0.684780	C 1.546122 -1.279193 0.450444
H -2.596697 4.187559 -0.452073	H 2.501305 -1.661106 0.786724	C 0.535422 -2.158608 0.082824
C -1.743208 4.031398 0.213983	H 0.698335 -3.227527 0.123979	C -0.683468 -1.649030 -0.352890
H 0.817135 3.960943 -0.637041	H -1.472695 -2.321816 -0.662506	C -0.889306 -0.278354 -0.410801
H 1.650463 2.520298 -1.221181	H -1.830083 0.102710 -0.782955	C 0.111262 0.623237 -0.025752
H 1.778854 2.990802 0.465914	C -1.322605 2.596415 0.202112	
C 1.091821 2.940878 -0.383187	C -0.111019 2.090609 -0.064419	

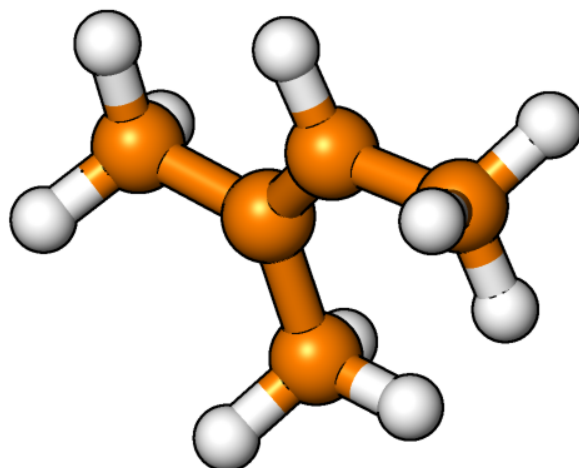


Ethylene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-78.47523886

H 7.572901 0.737496 -9.258346
H 7.572896 2.579897 -9.258595
C 7.570268 1.658777 -8.689227

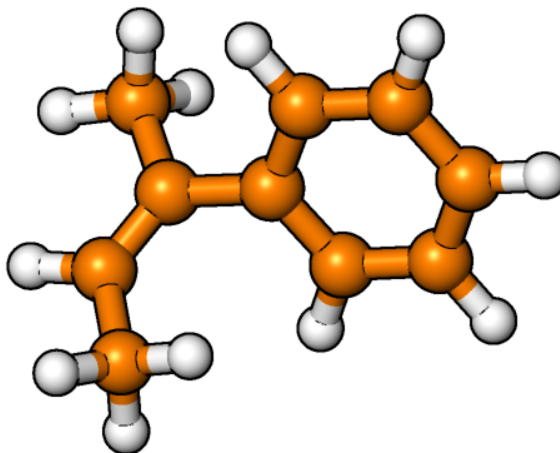
H 7.561503 0.737496 -6.795209
H 7.561508 2.579897 -6.794960
C 7.564135 1.658777 -7.364328



2-methylbut-2-ene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-196.25992740

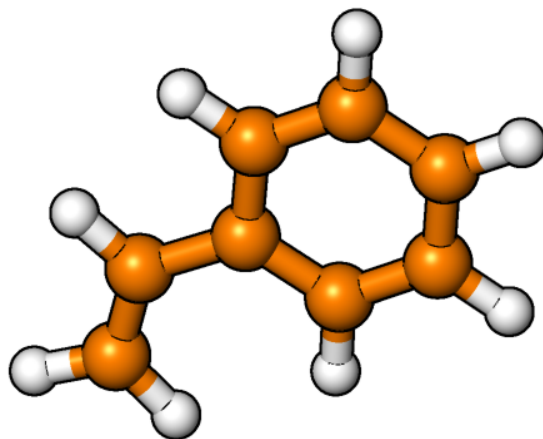
H 0.357561 2.384227 -0.876559	C 0.735510 -0.667560 -0.000000	H -1.865663 1.033069 0.875828
H 0.357561 2.384227 0.876559	H -0.822842 -2.177901 0.000000	H -1.957483 -0.495444 0.000000
H 1.746923 1.725024 0.000000	H 0.640231 -2.623494 0.875944	C -1.498147 0.489508 -0.000000
C 0.659925 1.802247 0.000000	H 0.640230 -2.623494 -0.875944	
C 0.003841 0.448609 -0.000000	C 0.262053 -2.088168 -0.000000	
H 1.816164 -0.549720 0.000000	H -1.865663 1.033069 -0.875828	



(Z)-but-2-en-2-ylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-387.71751732

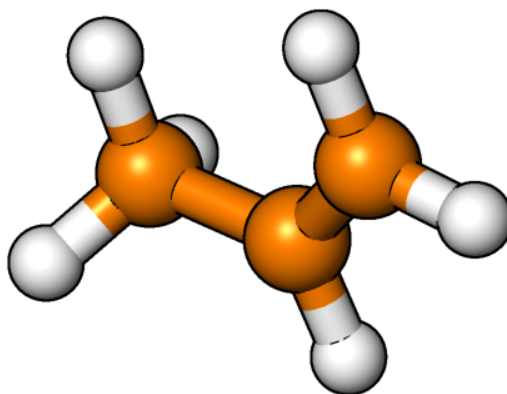
H -3.052007 2.350612 1.519672	H -1.587776 3.612082 -0.045305	C 1.090807 0.114274 0.698947
H -2.448860 0.802027 0.919153	H 1.689451 0.828932 1.247856	C 1.380335 -1.240292 0.797624
H -3.485131 1.812117 -0.091139	H 2.204525 -1.569609 1.417142	C 0.615996 -2.171950 0.103745
C -2.669396 1.829668 0.638414	H 0.844580 -3.227064 0.176586	C -0.440266 -1.736453 -0.687405
H 0.560680 3.929324 -0.742290	H -1.037115 -2.451978 -1.237775	C -0.731671 -0.380740 -0.779480
H 1.207387 2.558517 -1.661473	H -1.547462 -0.045323 -1.405864	C 0.023992 0.566389 -0.083417
H 1.721699 2.818408 -0.007535	C -1.468783 2.541431 0.096627	
C 0.860828 2.883893 -0.677501	C -0.274492 2.018082 -0.196579	



Styrene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-309.19628541

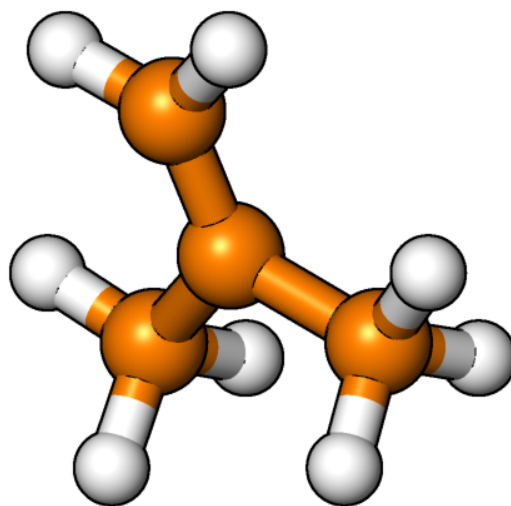
H -1.482363 3.701992 0.114748	H -1.454553 -2.441995 -0.456087	C 0.631492 -2.172978 -0.016792
H -2.324222 2.096910 -0.196597	H -1.988142 -0.053726 -0.343308	C -0.671147 -1.729110 -0.234424
H 0.631294 2.613556 0.421789	C -1.408412 2.626839 0.029028	C -0.971375 -0.378182 -0.169742
H 2.107869 0.819982 0.552602	C -0.240802 2.007112 0.196489	C 0.023513 0.566337 0.115084
H 2.644680 -1.582936 0.437672	C 1.326273 0.104087 0.330574	
H 0.862925 -3.228592 -0.068372	C 1.629611 -1.249846 0.266160	



Prop-1-ene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-117.73750661

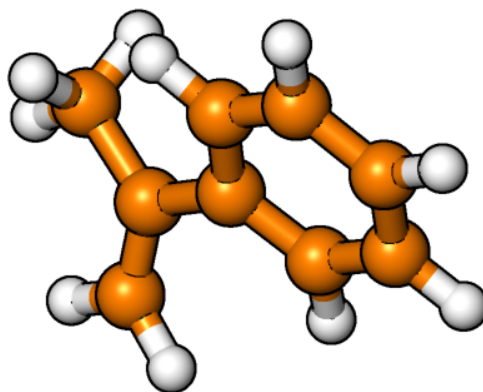
H 2.986872 3.416306 -4.191660	H 3.530959 0.387675 -4.540620	C 3.373877 1.272460 -2.663674
H 2.276505 2.419119 -5.469746	C 3.365951 1.309855 -3.990132	
H 4.001986 2.730358 -5.469010	H 3.539745 0.350027 -2.122944	
C 3.145646 2.537171 -4.816800	H 3.213937 2.166122 -2.071314	



2-methylprop-1-ene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-157.00088155

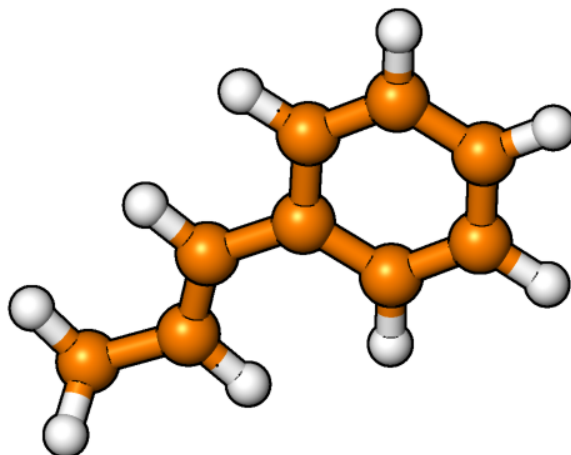
H 0.876761 -1.317645 -1.329168	H 0.000000 2.152845 -0.037567	C -0.000000 -0.000000 1.455361
H -0.876761 -1.317645 -1.329168	C 0.000000 -1.270614 -0.676212	C 0.000000 -0.000000 0.124962
H 0.000000 -2.152845 -0.037567	C 0.000000 1.270614 -0.676212	
H -0.876761 1.317645 -1.329168	H -0.000000 -0.923021 2.021004	
H 0.876761 1.317645 -1.329168	H -0.000000 0.923021 2.021004	



Prop-1-en-2-ylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-348.45784916

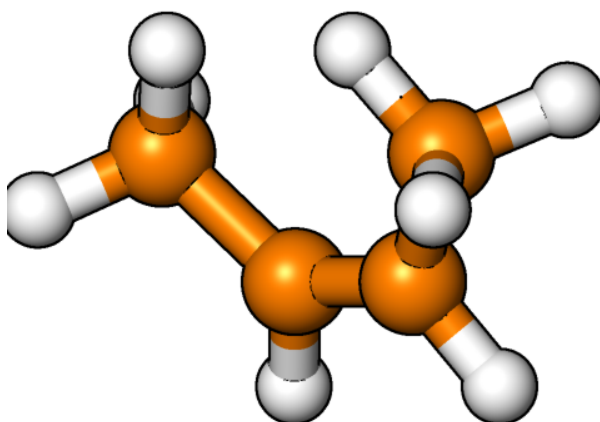
H 0.575961 3.989919 -0.379973	H 2.622520 -1.622222 0.492618	C 1.618891 -1.273832 0.286778
H 1.416807 2.685655 -1.234389	H 0.805886 -3.249501 0.057718	C 0.601084 -2.187112 0.046071
H 1.691533 2.934511 0.482113	H -1.480421 -2.421538 -0.432452	C -0.682198 -1.721130 -0.224047
C 0.927142 2.962973 -0.298413	H -1.937121 -0.012862 -0.485108	C -0.942428 -0.359653 -0.243279
H -2.250366 1.876803 0.583980	C -1.424609 2.516076 0.305963	C 0.067920 0.576100 0.014994
H -1.617840 3.580282 0.288453	C -0.213585 2.031757 0.017627	
H 2.164184 0.781942 0.457205	C 1.356655 0.090509 0.264141	



(*E*)-prop-1-en-1-ylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-348.45824444

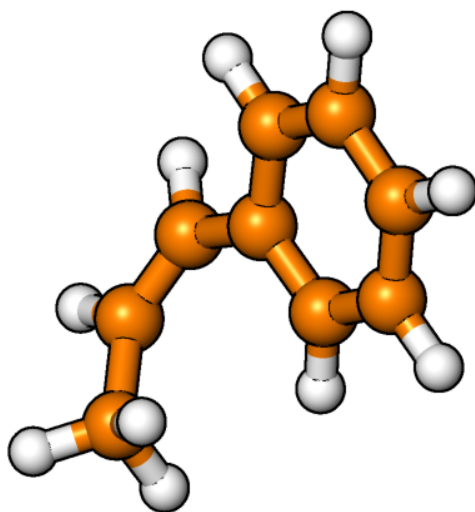
H -0.652816 4.624510 0.381868	H 2.659245 -1.574860 0.329758	C 1.636030 -1.245326 0.205198
H -2.305966 4.371165 0.959980	H 0.860352 -3.227680 -0.089079	C 0.629054 -2.172520 -0.028880
H -2.000187 4.524746 -0.759135	H -1.475081 -2.444991 -0.367484	C -0.682775 -1.730579 -0.185272
C -1.593362 4.115374 0.170348	H -2.008878 -0.061155 -0.234361	C -0.983050 -0.379966 -0.109652
H -2.302501 2.058753 -0.133075	C -1.406572 2.636379 0.071442	C 0.020808 0.569872 0.125006
H 0.641199 2.617727 0.415503	C -0.237212 2.010431 0.212740	
H 2.123147 0.825299 0.464676	C 1.332881 0.107969 0.281030	



(Z)-but-2-ene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-156.99738717

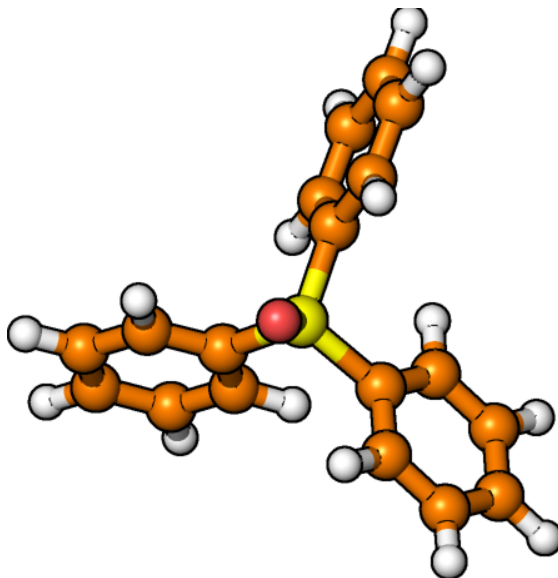
H -0.876346 -2.236251 -0.504925	H -0.000000 1.049721 -1.470516	C 0.000000 -0.665795 0.662626
H 0.876346 -2.236251 -0.504925	H -0.000000 -1.163372 1.627968	C 0.000000 0.665795 0.662626
H 0.876346 2.236251 -0.504925	H 0.000000 1.163372 1.627968	
H -0.876346 2.236251 -0.504925	C 0.000000 -1.582041 -0.521528	
H 0.000000 -1.049721 -1.470516	C -0.000000 1.582041 -0.521528	



(Z)-prop-1-en-1-ylbenzene

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-348.45573486

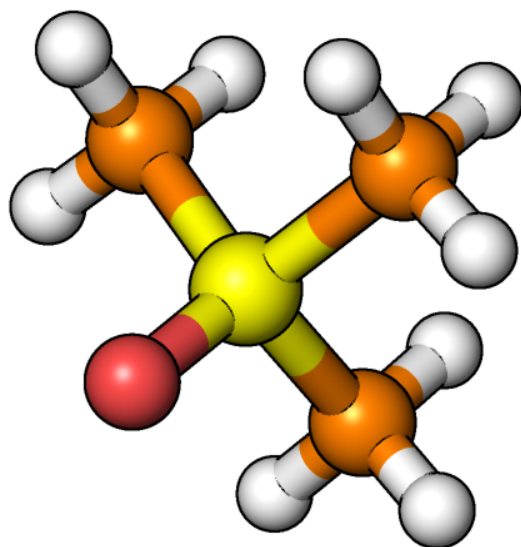
H -3.248095	2.662139	1.091699	H 2.623287	-1.439505	0.664636	C 1.618288	-1.189177	0.351212
H -2.618335	1.019998	0.909516	H 0.964006	-3.235077	0.261824	C 0.687608	-2.197971	0.125625
H -3.518567	1.782556	-0.401012	H -1.319577	-2.641883	-0.492736	C -0.595380	-1.863210	-0.291664
C -2.785570	1.963034	0.391719	H -1.941813	-0.291082	-0.824419	C -0.952378	-0.532552	-0.465692
H -1.543501	3.610396	-0.351168	C -1.517568	2.543490	-0.154354	C -0.034510	0.496480	-0.221398
H 0.472812	2.534650	-0.718888	C -0.359119	1.919434	-0.390473			
H 1.992680	0.919655	0.344687	C 1.262336	0.139096	0.170888			



Triphenylphosphine oxide

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1110.09569817

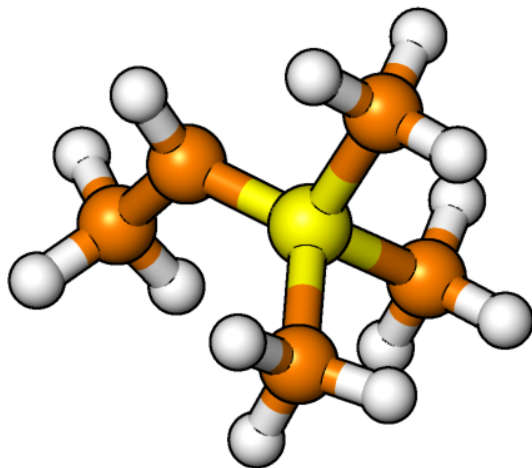
H -1.417429 -0.896107 4.666635	H 2.689362 -0.245240 -0.945345	H -0.465697 2.232128 -1.575884
H 0.000710 -1.299558 2.659010	H 0.173384 2.487426 1.213685	H -1.858027 2.639122 -3.585201
H -2.395742 1.470869 0.413806	H 1.996929 4.165518 1.226632	H -3.108250 0.766676 -4.630471
H -3.809011 1.874503 2.409050	H 4.172070 3.644847 0.149828	C -2.422137 -0.695160 -3.203163
H -3.319314 0.695066 4.537658	C 3.568727 1.672427 -0.474999	C -1.645858 -0.925715 -2.069524
C -1.624011 -0.369815 3.739567	C 2.543137 0.729660 -0.490074	C -0.948551 0.131547 -1.468333
C -0.823461 -0.593560 2.621572	C 1.308775 1.024454 0.105659	C -1.025461 1.415545 -2.022282
C -1.088614 0.080208 1.421057	C 1.118648 2.264856 0.727512	C -1.804671 1.642783 -3.156599
C -2.170254 0.966908 1.348999	C 2.147368 3.206701 0.739521	C -2.505192 0.589207 -3.744980
C -2.968817 1.189297 2.470771	C 3.370516 2.912321 0.136110	P 0.020400 -0.255036 0.020257
C -2.694341 0.524120 3.666188	H -2.958114 -1.517286 -3.667864	O 0.569142 -1.645635 0.022062
H 4.524514 1.439066 -0.934484	H -1.557419 -1.922566 -1.648150	



Trimethylphosphine oxide

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-535.73628249

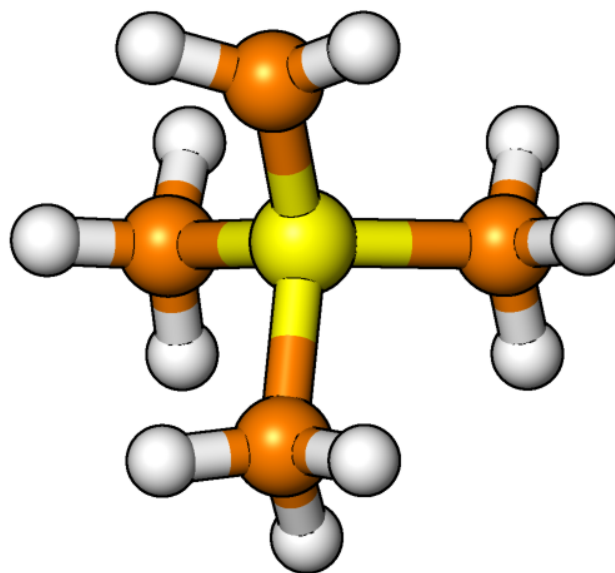
H -0.476034 -0.130727 2.310364	H -1.411082 1.035622 -1.447637	C -1.037798 0.011593 -1.477738
H -1.429638 1.034787 1.364450	H 1.909498 0.775560 -0.903979	C 1.279241 0.902666 -0.024051
H -1.899617 -0.679486 1.417349	H 0.854898 1.907065 -0.026520	P -0.008628 -0.378153 -0.032706
H -0.445508 -0.129712 -2.381538	H 1.898174 0.775112 0.863816	O 0.522113 -1.763125 -0.029607
H -1.880714 -0.678520 -1.507367	C -1.056547 0.010829 1.398993	



Ethylidenetriethylphosphorane

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-538.98159875

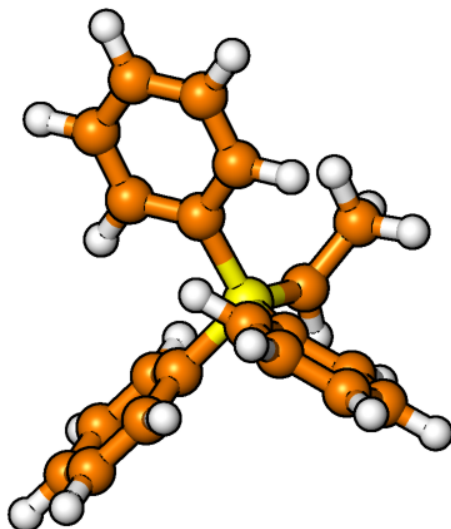
H -0.201181 -0.704519 1.390935	H 4.103938 1.330326 -2.042740	C 3.502291 1.329883 -1.134355
H 0.855286 -2.098158 1.209552	H 0.653681 -0.948829 -2.457214	C 1.297699 -0.069745 -2.470673
H -0.014152 -1.457327 -0.174146	H 0.674279 0.817494 -2.380613	C 3.591988 -1.487705 -1.621532
C 0.535266 -1.165528 0.725808	H 1.838531 -0.052921 -3.416781	P 2.445380 -0.143388 -1.055613
H 2.214272 0.216066 1.238808	H 4.001222 -1.311978 -2.618822	C 1.656833 -0.205370 0.410263
H 2.883603 2.223814 -1.100108	H 4.409371 -1.572984 -0.905188	
H 4.168191 1.331458 -0.271746	H 3.045703 -2.431789 -1.624422	



Trimethyl(methylene)phosphorane

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-499.73027647

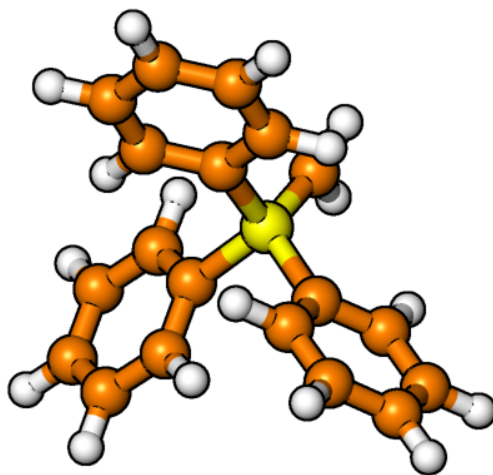
H 2.508391 -0.252715 1.066684	H 0.494931 1.368662 -2.889578	C 0.347184 1.027402 -1.865275
H 2.585375 2.694941 -0.478245	H 2.738941 0.013707 -3.418171	C 2.641214 -0.538373 -2.480883
H 3.966151 1.597180 -0.597179	H 3.624760 -0.887285 -2.165162	P 1.908858 0.475414 -1.117321
H 3.254757 2.266749 -2.075908	H 2.009395 -1.412117 -2.642522	C 1.655271 -0.132341 0.412956
H -0.352182 0.191092 -1.871381	H 0.819614 -0.800929 0.568835	
H -0.076423 1.828024 -1.262804	C 3.033871 1.902152 -1.073018	



Ethylenetriphenylphosphorane

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1113.34469607

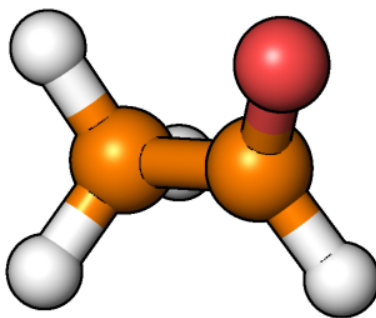
H -0.553083 1.991262 0.274978	C -1.744010 3.073745 3.601065	H 3.024575 0.136541 1.224466
H -0.450331 1.119506 -1.240480	C -2.952565 2.504188 3.984236	H 1.000115 0.818429 4.928099
H 1.000940 1.809021 -0.525658	H -1.543477 -4.629058 1.624058	H 3.126612 1.484422 5.979456
C 0.063369 1.287570 -0.290489	H -1.158410 -2.267766 0.970041	H 5.220732 1.472386 4.660345
H 0.624118 -0.868524 -0.085358	H 1.387667 -1.748474 4.367729	C 4.263332 0.793646 2.861967
H -4.086607 0.686261 4.140053	H 0.983112 -4.077733 5.039338	C 3.062253 0.420934 2.269270
H -2.306369 -0.723612 3.184661	H -0.480012 -5.531678 3.670882	C 1.879507 0.415619 3.005827
H 0.214059 2.721744 2.805828	C -0.906612 -3.997082 2.229175	C 1.912561 0.804870 4.347080
H -1.586382 4.138886 3.709013	C -0.692911 -2.676717 1.855638	C 3.110805 1.181884 4.940561
H -3.738582 3.124270 4.394600	C 0.133823 -1.850657 2.622562	C 4.288410 1.174755 4.198795
C -3.148867 1.134578 3.839442	C 0.735346 -2.368936 3.771136	P 0.346911 -0.118093 2.113463
C -2.143787 0.338685 3.305601	C 0.511516 -3.687587 4.147254	C 0.235835 -0.012851 0.452928
C -0.924554 0.901424 2.926354	C -0.308864 -4.504280 3.377824	
C -0.731084 2.275390 3.082714	H 5.176491 0.793672 2.281015	



Methylenetriphenylphosphorane

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1074.09159482

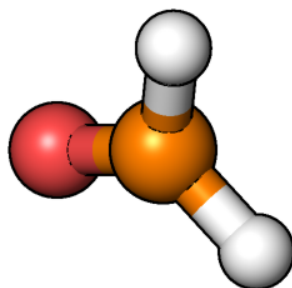
H 0.866833 -0.723435 -0.198008	H -1.046165 -2.275334 0.900590	H 3.038840 1.478617 6.022431
H -3.965844 0.681912 4.230909	H 1.367617 -1.756606 4.391711	H 5.190451 1.436367 4.799932
H -2.182795 -0.751899 3.313046	H 0.915832 -4.077957 5.063505	C 4.309153 0.749005 2.966097
H 0.186859 2.724525 2.494200	H -0.511507 -5.526182 3.652407	C 3.133461 0.382198 2.321887
H -1.613566 4.159378 3.374581	C -0.869335 -3.998774 2.185045	C 1.919809 0.388911 3.006056
H -3.691793 3.141810 4.256107	C -0.625685 -2.683924 1.809002	C 1.895165 0.788079 4.344498
C -3.060937 1.131172 3.843516	C 0.177024 -1.860499 2.602587	C 3.068186 1.164111 4.987494
C -2.055140 0.321854 3.328747	C 0.731491 -2.375340 3.776020	C 4.277471 1.141032 4.299953
C -0.881920 0.889105 2.833249	C 0.480617 -3.688812 4.152722	H 0.083464 0.945652 -0.014087
C -0.727118 2.276863 2.860933	C -0.320132 -4.502440 3.359030	P 0.412592 -0.132579 2.073459
C -1.739044 3.084497 3.363553	H 5.247205 0.738320 2.426348	C 0.327546 -0.014940 0.414644
C -2.906577 2.512648 3.858295	H 3.142213 0.102421 1.275527	
H -1.488411 -4.629746 1.560711	H 0.957541 0.813034 4.883709	



Acetaldehyde

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-153.65989776

H -2.333292 0.243833 -4.827668	H -1.337403 0.071776 -2.501848	C -1.995201 -0.722143 -2.865947
O -1.699770 -1.645970 -5.060940	H -1.664978 -1.686192 -2.485425	
C -2.008359 -0.712889 -4.366269	H -2.996907 -0.493610 -2.491588	

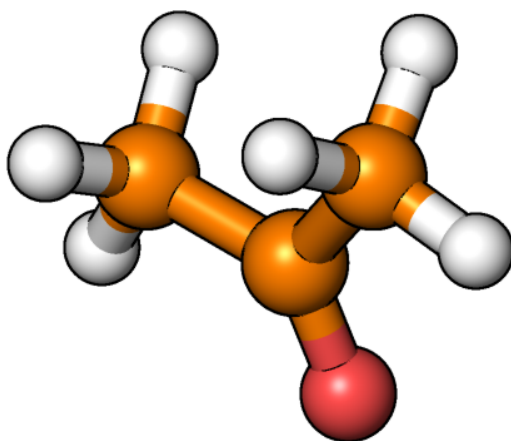


Formaldehyde

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-114.38863341

H 0.930538 1.207961 -1.249038
O 1.220841 3.005069 -0.379094

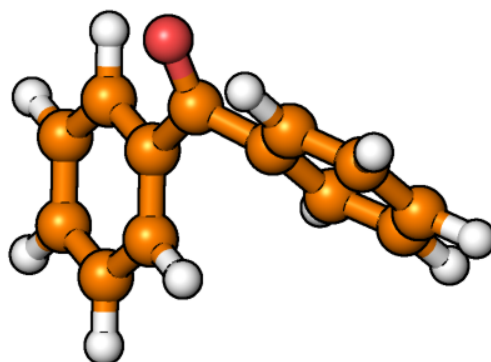
H 1.526404 1.230365 0.530705
C 1.226227 1.806045 -0.365803



Propan-2-one

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-192.92891550

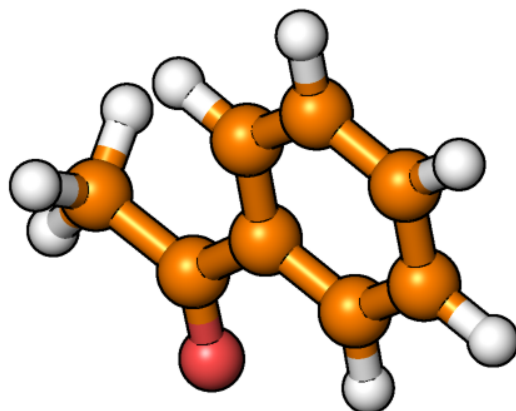
H -2.059682 0.466212 -3.969978	O -1.058068 -2.428896 -4.344947	H -1.813280 -0.924293 -1.731731
H -1.209187 -0.146787 -5.411951	C -1.060792 -1.414188 -3.687567	C -0.960533 -1.440959 -2.178244
H -0.310611 0.570940 -4.047804	H -0.064011 -0.907363 -1.853191	
C -1.165502 -0.048474 -4.330283	H -0.923832 -2.467419 -1.823680	



Benzophenone

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-575.84178224

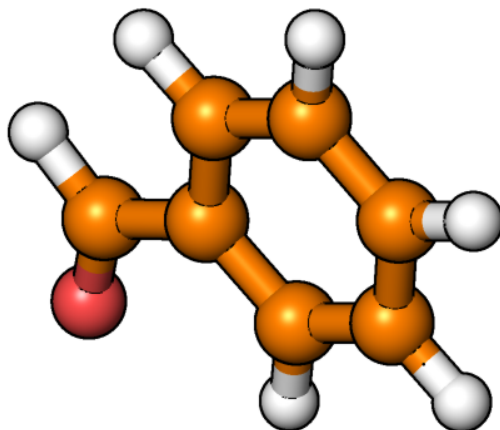
H -4.719616 0.337492 1.407322	C -1.393834 0.702135 0.874968	C 3.771650 -0.266704 0.888070
H -4.546999 -0.778212 -0.794622	C -1.289103 0.073287 -0.367687	C 2.641585 -0.807074 1.490092
H -2.701934 1.305587 2.462272	O -0.004330 -0.000244 -2.340457	C 3.667091 0.361920 -0.350066
H -2.348087 -0.910085 -1.941489	C -0.000700 -0.000407 -1.122426	C 1.404604 -0.704391 0.865935
H -0.516462 1.131320 1.336955	H 4.733261 -0.338448 1.379039	C 2.437193 0.446540 -0.983438
C -3.760949 0.265726 0.910637	H 2.722375 -1.308745 2.444857	C 1.292193 -0.074331 -0.375425
C -3.664049 -0.361691 -0.328737	H 4.547041 0.779398 -0.820741	
C -2.627050 0.804845 1.506539	H 0.530197 -1.134484 1.332679	
C -2.437963 -0.446353 -0.969453	H 2.341326 0.911208 -1.954455	



Acetophenone

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-384.38629604

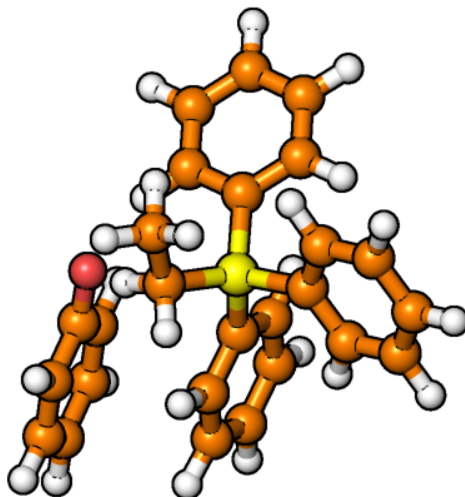
H -3.427340 0.535349 -6.470353	H -2.004851 -0.252114 -0.446590	C -0.743058 -0.563723 -2.158600
H -2.178256 1.132564 -7.587155	H 0.038448 -1.052925 -1.592392	C -2.895224 0.516385 -2.241717
H -2.676201 2.098445 -6.178628	H -3.788704 0.867894 -1.743341	C -0.599380 -0.385845 -3.524856
C -2.489052 1.088268 -6.547153	H 0.284286 -0.727944 -4.044614	C -2.751035 0.694508 -3.611840
O -0.389133 0.014476 -6.278841	H -3.538299 1.184522 -4.166760	C -1.602278 0.245026 -4.266769
C -1.401764 0.412665 -5.739977	C -1.892324 -0.112758 -1.513819	



Benzaldehyde

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-345.11891993

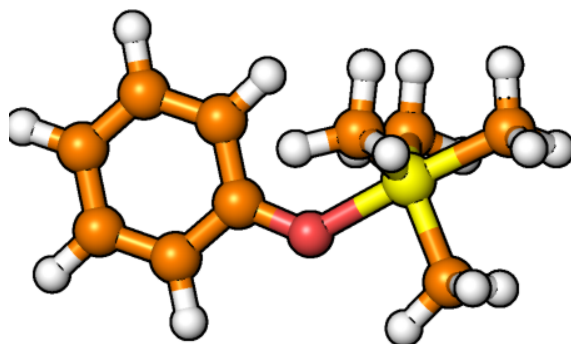
H 0.691152 -1.687771 -2.700952	H -1.534395 -3.934092 1.859683	C -0.877105 -3.271540 1.312446
O -0.716271 -3.105206 -2.954083	H 1.476490 -0.899211 -0.630441	C 0.819718 -1.561235 -0.078569
C -0.023214 -2.407871 -2.251628	H -1.535816 -3.932923 -0.631158	C -0.883181 -3.276199 -0.072222
H -0.021412 -2.411656 3.086613	C -0.023270 -2.412388 2.004121	C -0.032190 -2.418458 -0.774832
H 1.486190 -0.892050 1.849842	C 0.825373 -1.557003 1.310185	



2D

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1420.44786357

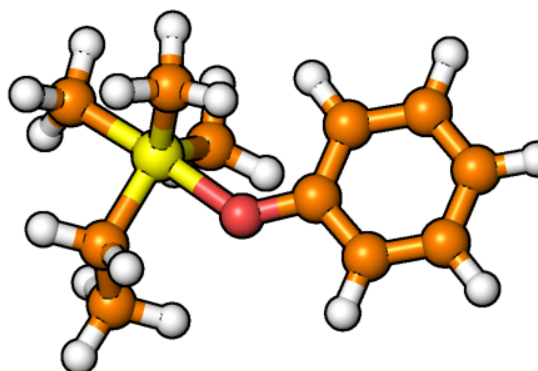
H 4.729751 6.138351 -0.838870	H 1.763173 6.127475 -1.922589	C 2.169742 2.953146 -2.948365
H 5.920587 4.835050 -0.700449	H 4.685868 5.361176 -4.992642	H 2.838175 4.443745 -0.463714
H 4.891009 5.247844 0.666243	C 2.742725 8.091909 -4.534270	P 3.567690 4.016621 -2.621533
C 4.916070 5.150205 -0.418676	C 2.065560 7.698418 -3.384785	H 4.071742 3.147377 -0.490751
H 8.183841 1.651300 -4.939464	C 3.684869 7.248173 -5.112257	C 3.840567 4.153799 -0.844536
H 6.018934 0.453078 -4.987002	C 2.323769 6.467169 -2.796170	O 1.102996 4.994939 -0.527204
H 8.326362 3.899964 -3.912767	C 3.958832 6.015437 -4.534805	H -2.501431 1.214659 -0.249861
H 4.009237 1.490950 -4.009020	C 3.285591 5.628467 -3.372872	C 0.199613 4.078158 -0.442499
H 6.325843 4.943899 -2.945638	H -0.777273 0.597347 -3.759868	H -0.996307 4.801414 -2.080298
C 7.302266 2.106477 -4.508490	H 0.520127 0.280748 -1.684243	H 1.080602 3.064688 1.242440
C 6.087730 1.433237 -4.535071	H -0.219955 2.456785 -5.297013	C -0.911730 4.022236 -1.332301
C 7.383762 3.369832 -3.930559	H 2.387635 1.770599 -1.153808	C 0.263547 3.037876 0.530246
C 4.952877 2.016436 -3.983631	H 1.648392 3.972881 -4.772121	H -2.678260 3.005336 -1.963295
C 6.255003 3.956322 -3.377777	C 0.058693 1.247488 -3.542111	H -0.605386 1.266971 1.355238
C 5.028649 3.281123 -3.398550	C 0.793640 1.058724 -2.380658	C -1.851820 3.011128 -1.260758
H 2.531878 9.052811 -4.985207	C 0.369059 2.294102 -4.404787	C -0.691127 2.033989 0.592875
H 1.322644 8.348316 -2.942122	C 1.845415 1.910164 -2.075861	C -1.755862 1.996613 -0.305034
H 4.204803 7.546075 -6.012764	C 1.420749 3.148080 -4.111365	



1B

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-806.845459567

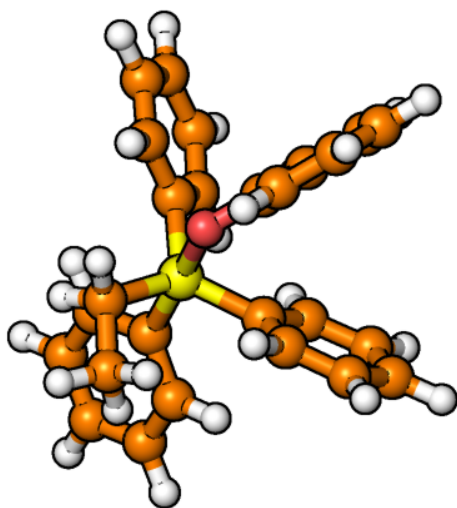
C -0.744949 0.576597 0.209379	H -1.690088 0.107727 0.446206	C 4.218548 4.427079 -3.538542
C 0.339133 0.469812 1.079559	O 2.921050 2.348641 -0.627123	H 3.460542 4.592384 -4.306291
C -0.587766 1.295973 -0.966265	C 5.105732 3.433361 -1.190324	H 4.555157 5.403817 -3.187372
H 0.237763 -0.087265 2.002658	H 5.361982 4.478136 -1.014434	H 5.068278 3.931635 -4.010979
H -1.417007 1.391382 -1.656270	H 5.879460 3.010163 -1.830989	C 3.207827 1.959874 -3.213283
C 1.549871 1.068831 0.778822	P 3.524976 3.384998 -2.105875	H 2.764112 1.112395 -2.705854
C 0.624751 1.903207 -1.280302	C 2.258588 4.650808 -1.716073	H 2.567328 2.278925 -4.034989
H 2.393689 0.988395 1.451095	H 1.621231 4.377806 -0.884308	H 4.168461 1.673459 -3.641958
H 0.707197 2.454476 -2.204994	H 2.792810 5.573067 -1.486747	H 5.055753 2.894763 -0.253708
C 1.724188 1.801698 -0.409869	H 1.653528 4.837607 -2.602813	



1C

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-846.102010908

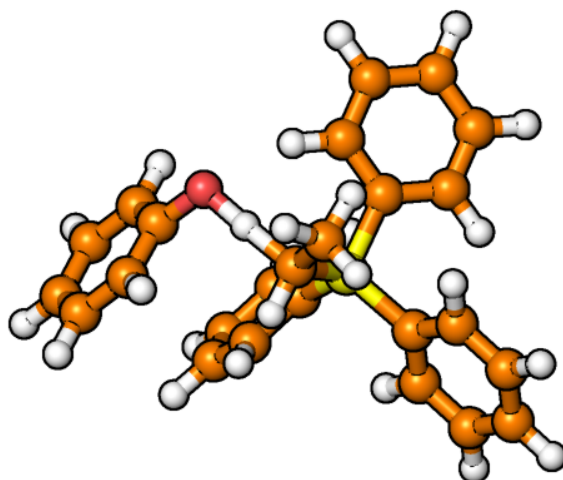
C 3.582528 -0.100417 -1.517516	O 0.051575 -0.214022 0.670757	H -4.171822 0.572128 0.170831
C 2.366401 0.005995 -2.176835	C -1.606572 1.442544 -0.548187	H -3.830719 -0.299989 -1.325595
C 3.582052 -0.245480 -0.130784	H -2.227736 2.107685 0.052918	C -1.476822 -1.749726 -0.826687
H 2.344017 0.119161 -3.253720	H -2.000940 1.457583 -1.563992	H -2.125483 -2.532980 -0.436328
H 4.520292 -0.330448 0.403396	H -0.581787 1.792509 -0.538871	H -1.773883 -1.567246 -1.859108
C 1.163896 -0.029724 -1.476871	P -1.800237 -0.235406 0.153320	H -0.444156 -2.073020 -0.794209
C 2.393302 -0.283456 0.576745	C -2.048714 -0.365004 1.972776	C -1.900860 -1.799182 2.482837
H 0.237794 0.056106 -2.025636	H -1.309792 0.274304 2.446481	H -2.050734 -1.830731 3.562662
H 2.388413 -0.395472 1.652905	H -3.044380 0.016295 2.197044	H -2.634939 -2.469304 2.032170
C 1.151476 -0.175657 -0.077824	C -3.654208 -0.291781 -0.248625	H -0.904779 -2.181409 2.266278
H 4.512418 -0.071457 -2.068592	H -4.110607 -1.190186 0.171358	



1D

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1420.46251694

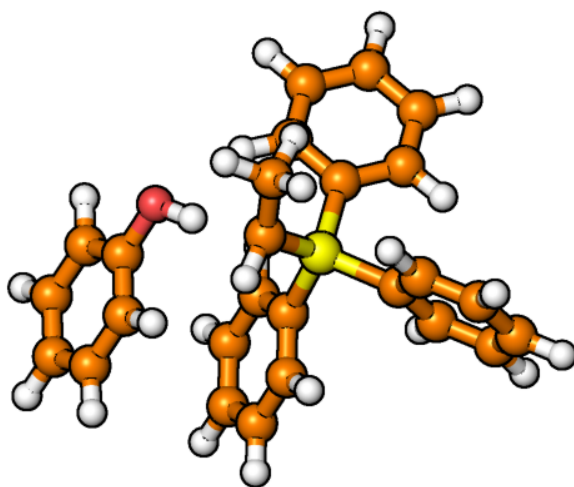
H -4.609711 0.372024 1.014224	H -2.193759 -2.528510 1.445946	C -1.292271 -0.208236 1.551625
H -4.415928 -1.282140 0.425714	H -1.581474 -1.638899 -2.698581	P -1.754501 0.003398 -0.211824
H -5.540920 -0.186882 -0.369532	C -2.280895 -4.596746 -1.222992	H -3.619032 1.277789 -1.079762
C -4.568352 -0.247759 0.120851	C -2.347712 -4.169149 0.095239	H -3.525815 -0.354579 -1.759963
H 2.412154 1.153050 -3.946447	C -2.005512 -3.670289 -2.223605	C -3.481368 0.229049 -0.842185
H 0.415820 2.614449 -3.806657	C -2.132155 -2.829459 0.410428	O -1.886400 1.848402 0.154748
H 2.578655 -0.837439 -2.479751	C -1.794350 -2.337095 -1.899796	H 1.201288 5.200960 2.734096
H -1.346807 2.139335 -2.153747	C -1.840055 -1.884051 -0.575072	C -1.044204 2.667057 0.805234
H 0.754038 -1.387062 -0.939890	H -0.219051 -0.572897 5.259888	H 0.793628 1.594558 0.464583
C 1.618418 0.924683 -3.247369	H 1.167201 -1.559752 3.458909	H -2.662143 3.965388 1.318243
C 0.498897 1.744844 -3.168449	H -2.288604 0.658209 4.675449	C 0.337324 2.459696 0.917227
C 1.713174 -0.190560 -2.423388	H 0.464089 -1.371753 1.121317	C -1.594466 3.809735 1.404209
C -0.506884 1.469240 -2.251511	H -2.923683 0.953375 2.322604	H 2.194045 3.185559 1.685196
C 0.688627 -0.488850 -1.534840	C -0.521072 -0.475570 4.225555	H -1.244879 5.587843 2.538101
C -0.424122 0.346760 -1.425749	C 0.255610 -1.030340 3.215960	C 1.129063 3.367811 1.610194
H -2.443895 -5.637227 -1.471361	C -1.682056 0.214134 3.897865	C -0.794360 4.712581 2.086898
H -2.568418 -4.874884 0.885761	C -0.137672 -0.912128 1.889915	C 0.576787 4.498456 2.198985
H -1.954095 -3.987011 -3.257524	C -2.055249 0.363718 2.568986	



TS_{2→3}D

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1420.43843820

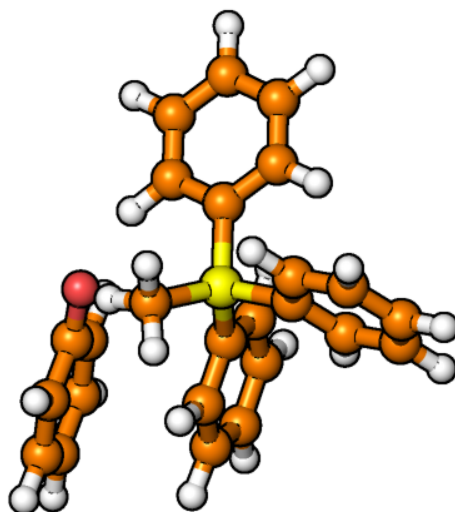
H 4.555888 6.202106 -0.896824	H 1.761199 6.218504 -2.144646	C 2.182677 2.957189 -3.100448
H 5.616113 4.895524 -0.359958	H 4.805999 5.265400 -5.024579	H 2.262813 4.683859 -0.652493
H 4.318092 5.474126 0.678603	C 2.863050 8.026292 -4.800366	P 3.561572 4.028622 -2.652965
C 4.582046 5.253722 -0.357004	C 2.128152 7.691792 -3.667455	H 3.639984 3.281680 -0.449501
H 8.308711 1.674819 -4.725696	C 3.825570 7.150177 -5.287520	C 3.575799 4.260476 -0.926747
H 6.127252 0.571865 -5.111532	C 2.351260 6.487945 -3.012868	O 1.105388 5.051827 -0.493209
H 8.406088 3.811430 -3.477740	C 4.058520 5.943354 -4.639492	H -2.055390 0.932586 0.159031
H 4.055306 1.594120 -4.254759	C 3.328475 5.610242 -3.497039	C 0.299785 4.017973 -0.303632
H 6.342126 4.836337 -2.621821	H -0.796420 0.677304 -4.025165	H -1.135193 4.668848 -1.754958
C 7.399452 2.124032 -4.349257	H 0.517574 0.229317 -1.977848	H 1.502220 3.092951 1.217514
C 6.175130 1.504368 -4.565225	H -0.211900 2.598360 -5.471718	C -0.891968 3.891121 -1.042639
C 7.454888 3.324905 -3.647348	H 2.404279 1.672687 -1.383225	C 0.604942 2.997213 0.619352
C 5.004950 2.080092 -4.083034	H 1.676266 4.063246 -4.874287	H -2.632735 2.724175 -1.458993
C 6.290579 3.901213 -3.161767	C 0.046173 1.307516 -3.774538	H 0.026570 1.132136 1.494418
C 5.052656 3.283303 -3.377896	C 0.787616 1.047937 -2.628427	C -1.723742 2.796167 -0.873729
H 2.683455 8.966690 -5.304653	C 0.371348 2.387815 -4.585439	C -0.232399 1.900603 0.775468
H 1.373399 8.368608 -3.290034	C 1.852668 1.868628 -2.289803	C -1.401418 1.784591 0.029771
H 4.396118 7.403360 -6.171012	C 1.437222 3.213167 -4.251205	



3D

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1420.44592694

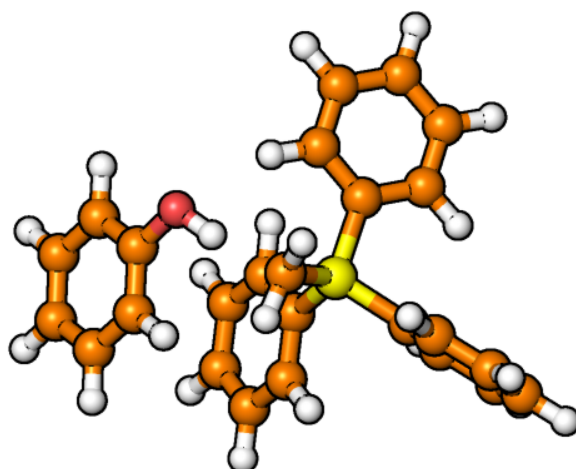
H 4.699558 6.317182 -1.075097	H 2.075746 6.120118 -2.345426	C 2.647747 2.702548 -2.938810
H 5.719203 5.256751 -0.112312	H 5.234463 4.998370 -5.027363	H 2.114366 4.729640 -0.660922
H 4.198120 5.850378 0.536481	C 3.224378 7.716868 -5.103091	P 3.945763 3.917453 -2.590765
C 4.678071 5.481238 -0.373302	C 2.455970 7.457083 -3.973607	H 3.869326 3.412135 -0.323568
H 8.682983 1.580971 -4.754209	C 4.221992 6.825812 -5.478457	C 3.899520 4.307605 -0.940516
H 6.530915 1.268546 -5.935555	C 2.679464 6.312226 -3.220478	O 1.161807 5.060687 -0.586062
H 8.759426 2.883728 -2.651462	C 4.449593 5.677212 -4.730344	H -2.346486 1.193131 -0.252210
H 4.466000 2.262099 -5.025050	C 3.679464 5.407749 -3.596980	C 0.282583 4.042546 -0.475675
H 6.683312 3.864755 -1.731917	H -0.195656 0.107616 -3.316723	H -1.331786 5.272880 -1.145573
C 7.778110 2.019824 -4.355142	H 2.015088 -0.595270 -2.452268	H 1.685242 2.577105 0.225454
C 6.568015 1.844668 -5.020333	H -0.580296 2.468165 -3.942213	C -1.052126 4.281864 -0.813856
C 7.821410 2.751494 -3.174156	H 3.827995 1.054161 -2.214205	C 0.655790 2.767370 -0.041233
C 5.405519 2.405103 -4.508108	H 1.221237 4.121074 -3.696353	H -3.018793 3.463138 -0.996044
C 6.656346 3.308466 -2.658851	C 0.604035 0.829562 -3.222844	H 0.019788 0.767388 0.355937
C 5.441717 3.145824 -3.324098	C 1.843915 0.435565 -2.732543	C -1.988720 3.261655 -0.730013
H 3.048789 8.611720 -5.685556	C 0.387882 2.154320 -3.578155	C -0.288322 1.752785 0.030410
H 1.679756 8.148079 -3.672865	C 2.863756 1.366163 -2.592697	C -1.615004 1.987414 -0.313052
H 4.828945 7.024480 -6.351718	C 1.404542 3.088915 -3.437136	



2C

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1381.19288838

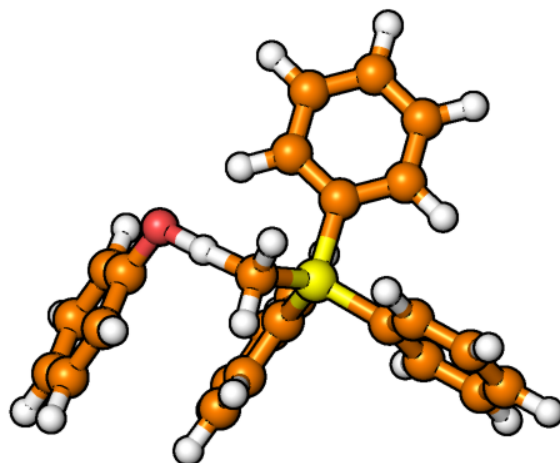
H 8.123728 1.714547 -4.960610	C 2.033769 7.682080 -3.547239	P 3.515142 4.032463 -2.584747
H 5.870121 0.921476 -5.604927	C 3.862871 7.253329 -5.058016	H 4.117434 3.266276 -0.402461
H 8.365589 3.506800 -3.270494	C 2.234926 6.456459 -2.925939	H 4.618558 4.951612 -0.679212
H 3.865649 1.913241 -4.563709	C 4.080235 6.025250 -4.447391	C 3.823672 4.223452 -0.829829
H 6.372442 4.504714 -2.236241	C 3.269569 5.629071 -3.379986	O 1.056772 4.953364 -0.675960
C 7.244741 2.152750 -4.507328	H -0.771791 0.538460 -3.694943	H -2.449586 1.120592 -0.076775
C 5.979706 1.707407 -4.870085	H 0.614130 0.187203 -1.683036	C 0.172909 4.029724 -0.504753
C 7.382036 3.159837 -3.556831	H -0.336449 2.474765 -5.175278	H -1.125972 4.677899 -2.094200
C 4.848743 2.266206 -4.286751	H 2.458471 1.716155 -1.168795	H 1.160610 3.093338 1.166309
C 6.256004 3.720254 -2.971463	H 1.498582 4.034539 -4.659716	C -0.984507 3.925128 -1.328125
C 4.980704 3.277020 -3.334496	C 0.050132 1.207914 -3.482725	C 0.308226 3.027147 0.499644
H 2.674407 9.038808 -5.084110	C 0.834768 1.001105 -2.357210	H -2.758468 2.851585 -1.831420
H 1.236151 8.325154 -3.200019	C 0.292284 2.297486 -4.313473	H -0.477282 1.267750 1.427051
H 4.489221 7.559522 -5.884992	C 1.870529 1.874182 -2.060061	C -1.896091 2.897320 -1.175086
H 1.598052 6.114304 -2.108590	C 1.325171 3.176379 -4.025813	C -0.619219 2.006688 0.645712
H 4.872197 5.382787 -4.803642	C 2.125430 2.961115 -2.901421	C -1.726204 1.916224 -0.195144
C 2.841696 8.082065 -4.606785	H 2.862183 4.572230 -0.408216	



3C

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1381.19512239

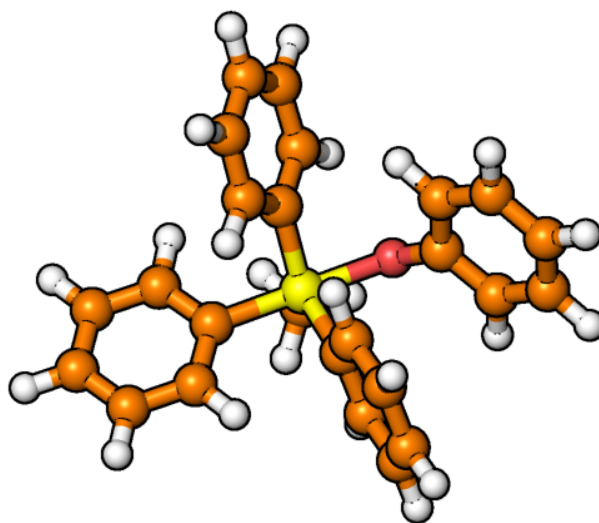
H 8.719798 1.610589 -4.661496	C 2.551425 7.513749 -3.885892	P 3.935720 3.906614 -2.570388
H 6.577025 1.223335 -5.837657	C 4.146311 6.753235 -5.517024	H 3.985660 3.453652 -0.254071
H 8.763986 2.962380 -2.588945	C 2.768405 6.369144 -3.129343	H 4.461398 5.171990 -0.637324
H 4.488949 2.187391 -4.950599	C 4.368324 5.606245 -4.765938	C 3.877013 4.302878 -0.921885
H 6.659820 3.916986 -1.692593	C 3.681547 5.403072 -3.566490	O 1.127394 5.041677 -0.568309
C 7.804682 2.037841 -4.273306	H -0.254190 0.170342 -3.390583	H -2.330447 1.126274 -0.276252
C 6.599960 1.820001 -4.935281	H 1.943080 -0.586996 -2.538340	C 0.262118 4.011702 -0.469181
C 7.829883 2.797202 -3.109269	H -0.600489 2.549926 -3.963010	H -1.368631 5.228800 -1.123618
C 5.423944 2.364402 -4.436453	H 3.780429 1.027453 -2.256911	H 1.684657 2.556702 0.212123
C 6.651985 3.338714 -2.607792	H 1.228445 4.168406 -3.678461	C -1.076086 4.237647 -0.803631
C 5.442994 3.132283 -3.269378	C 0.557096 0.876889 -3.280735	C 0.652156 2.735943 -0.050649
H 3.065849 8.602826 -5.664331	C 1.789679 0.452127 -2.797448	H -3.032208 3.396009 -0.993683
H 1.842425 8.253418 -3.538624	C 0.362486 2.212456 -3.606456	H 0.041746 0.723692 0.324221
H 4.688423 6.900769 -6.441558	C 2.823650 1.362918 -2.634454	C -1.999348 3.204577 -0.730931
H 2.220961 6.222617 -2.210442	C 1.394333 3.126957 -3.444851	C -0.279100 1.708885 0.010414
H 5.085709 4.877201 -5.111315	C 2.630543 2.709152 -2.954517	C -1.609175 1.930446 -0.328813
C 3.237195 7.708900 -5.079201	H 2.084766 4.727763 -0.608763	



TS_{2→3}C

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1381.18588330

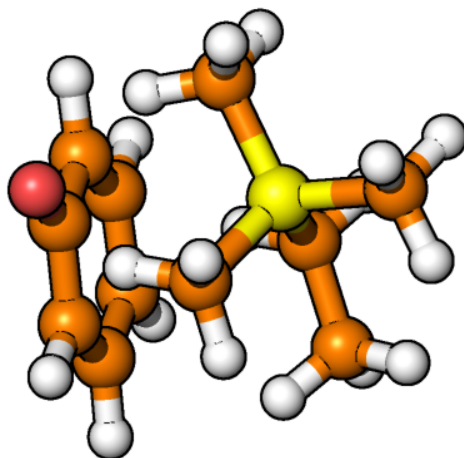
H 8.245756 1.683429 -4.783318	C 2.104599 7.653148 -3.773345	P 3.541401 4.034196 -2.624420
H 6.040049 1.107288 -5.745100	C 3.947922 7.149519 -5.240575	H 3.792246 3.428935 -0.348168
H 8.389629 3.254433 -2.876145	C 2.294817 6.453633 -3.100966	H 4.253720 5.135264 -0.662336
H 3.985755 2.102036 -4.810540	C 4.148601 5.945886 -4.575677	C 3.562702 4.331864 -0.910874
H 6.333769 4.242670 -1.933437	C 3.325798 5.595977 -3.503964	O 1.064665 5.040008 -0.555524
C 7.345600 2.123725 -4.375633	H -0.780530 0.610642 -3.916179	H -1.999458 0.872452 0.235694
C 6.106513 1.800119 -4.917006	H 0.606308 0.171375 -1.916847	C 0.286781 3.995901 -0.331296
C 7.427432 3.006668 -3.303773	H -0.295247 2.566419 -5.351861	H -1.177760 4.575838 -1.784171
C 4.948538 2.361149 -4.392915	H 2.473996 1.659177 -1.360151	H 1.520284 3.134201 1.203848
C 6.271897 3.565939 -2.775254	H 1.571506 4.075294 -4.792232	C -0.910326 3.822475 -1.054463
C 5.025642 3.251068 -3.320400	C 0.053073 1.259394 -3.683725	C 0.620557 3.004820 0.615988
H 2.772022 8.940117 -5.358222	C 0.836160 1.004628 -2.564276	H -2.628938 2.608551 -1.423563
H 1.308700 8.315891 -3.461139	C 0.322531 2.359115 -4.488518	H 0.089582 1.152701 1.545797
H 4.589584 7.418275 -6.068924	C 1.889023 1.848855 -2.247831	C -1.716367 2.715032 -0.849006
H 1.649036 6.174160 -2.275801	C 1.376113 3.209044 -4.176128	C -0.192245 1.895821 0.808877
H 4.943864 5.285604 -4.890201	C 2.164144 2.955529 -3.054315	C -1.364929 1.734217 0.077562
C 2.927046 8.002990 -4.839892	H 2.267768 4.715796 -0.634066	



1C

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1381.20591945

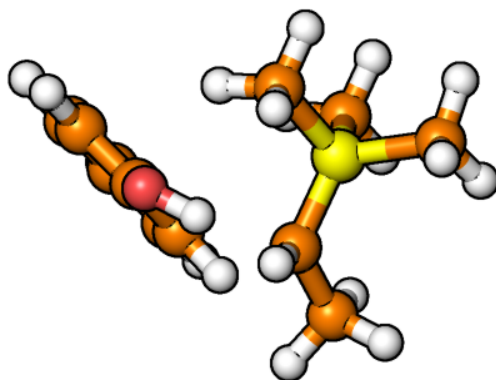
H 1.847916 2.101576 -3.714576	C -2.851868 -3.974537 -0.303765	H -3.966624 1.354644 -0.073308
H -0.580940 2.150774 -4.202885	C -1.498569 -3.466836 -2.216962	H -3.864651 0.045583 -1.295176
H 2.647835 1.145295 -1.574787	C -2.704805 -2.668306 0.138528	H -4.227526 -0.356271 0.368208
H -2.187244 1.268200 -2.570495	C -1.360046 -2.154411 -1.768430	C -3.669239 0.331933 -0.263573
H 1.051077 0.236151 0.047639	C -1.960480 -1.726592 -0.584147	O -1.940853 1.881200 0.700127
C 1.141876 1.696537 -3.002367	H -0.279603 -1.595310 5.267221	H 2.171281 5.093279 1.189516
C -0.220709 1.725329 -3.275685	H 0.943919 -2.402053 3.271556	C -0.880721 2.693406 0.863543
C 1.590734 1.155738 -1.804593	H -2.207263 -0.064122 4.991802	H -0.062418 1.717454 2.596211
C -1.128618 1.218533 -2.355064	H 0.201534 -1.744824 1.022261	H -1.429634 3.892058 -0.818383
C 0.686467 0.637383 -0.885734	H -2.833383 0.736553 2.743429	C 0.059511 2.523143 1.889383
C -0.679316 0.665960 -1.156777	C -0.583927 -1.277679 4.278972	C -0.703598 3.761233 -0.027518
H -2.354437 -5.399781 -1.836397	C 0.102961 -1.730721 3.159116	H 1.861589 3.232416 2.798036
H -3.432472 -4.678513 0.278597	C -1.665644 -0.417036 4.124552	H 0.501103 5.427236 -0.617173
H -1.018329 -3.769755 -3.138454	C -0.301522 -1.340213 1.888740	C 1.146188 3.383653 1.998821
H -3.163370 -2.384655 1.078041	C -2.037845 0.015608 2.859124	C 0.382420 4.614987 0.089217
H -0.770202 -1.467098 -2.356593	C -1.360038 -0.446484 1.730713	C 1.321725 4.429409 1.100183
C -2.246152 -4.380680 -1.489360	P -1.889251 0.074787 0.061388	



2B

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-846.09030633

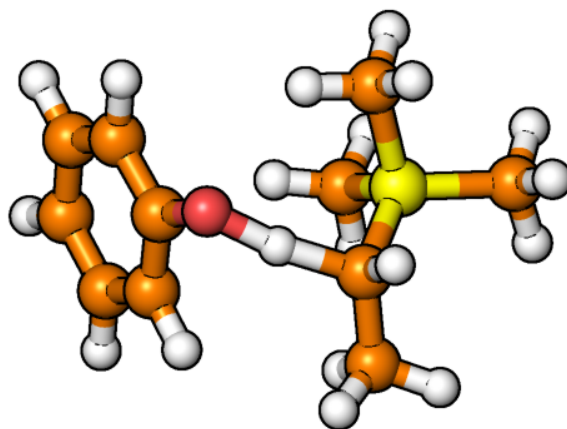
H 4.386725 0.774740 -3.473267	C 4.724736 3.863117 -3.588449	C 1.255697 2.496712 0.220442
H 2.891470 -0.132364 -3.242250	H 1.676244 4.828798 -2.858335	H -0.418274 3.512535 -0.685718
H 3.789745 0.411033 -1.840626	H 2.958652 5.734780 -2.015207	H 2.676286 1.099566 1.050719
C 3.494206 0.685612 -2.851246	H 1.919964 4.615387 -1.075265	C 0.045279 2.543766 -0.540431
H 3.681587 3.200994 0.046861	C 2.404344 4.796771 -2.049514	C 1.789305 1.186746 0.433927
H 2.277924 2.202389 -3.834854	P 3.543605 3.433853 -2.284430	H -1.440308 1.491622 -1.658599
H 1.787975 1.844444 -2.184902	H 4.976830 2.227583 -0.778448	H 1.649541 -0.914116 0.070594
C 2.653518 1.960748 -2.836660	H 5.147313 3.991707 -0.619621	C -0.526273 1.403346 -1.081413
H 5.425230 3.043902 -3.744584	C 4.439792 3.173281 -0.756585	C 1.203405 0.057201 -0.114674
H 5.282661 4.753137 -3.300414	O 1.854543 3.559026 0.626183	C 0.051649 0.145154 -0.897782
H 4.195748 4.061044 -4.520170	H -0.402931 -0.741205 -1.318669	



3B

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-846.08180172

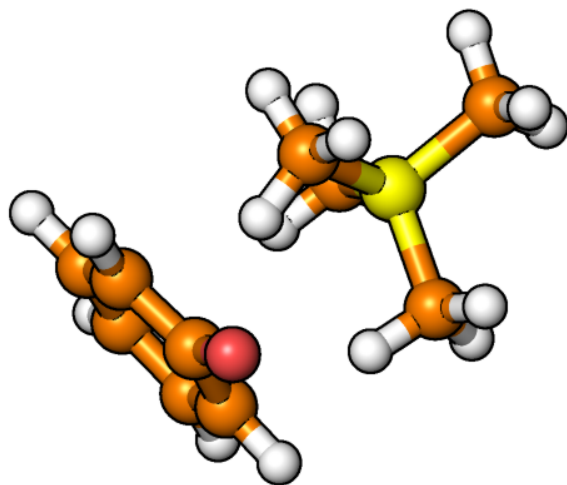
H 6.420039 2.285421 -0.844477	H 4.825435 4.105542 -4.829822	C 1.191723 2.351381 0.065026
H 4.976762 1.308949 -1.076144	C 5.285858 3.970305 -3.849819	H -0.705591 3.336069 0.010330
H 5.314616 2.002671 0.491360	H 2.676138 5.381071 -3.615490	H 2.926195 1.087069 0.143217
C 5.357908 2.206299 -0.581444	H 3.566411 6.041830 -2.231015	C -0.206024 2.376523 0.017559
H 2.826927 3.410116 -0.177913	H 2.133980 5.037255 -1.947911	C 1.847611 1.114434 0.083103
H 3.656931 1.414481 -3.151783	C 2.997642 5.185706 -2.593176	H -2.008661 1.229885 -0.049595
H 2.752515 2.520900 -4.196026	P 4.038403 3.707771 -2.524242	H 1.635933 -1.013272 0.057409
H 2.182348 2.172104 -2.542801	H 4.852572 4.354711 -0.444166	C -0.927144 1.191819 -0.016023
C 3.058582 2.324713 -3.168959	C 4.525786 3.431477 -0.920761	C 1.113561 -0.064898 0.041190
H 5.951043 3.107225 -3.887713	O 1.853753 3.525103 0.089981	C -0.275426 -0.038585 -0.010613
H 5.881372 4.850402 -3.607520	H -0.841366 -0.959618 -0.038486	



TS_{2→3}B

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-846.07605002

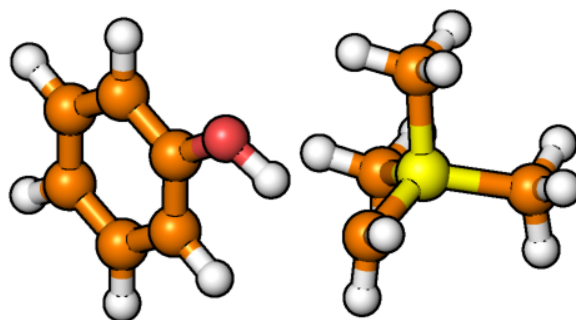
H 6.407728 2.280088 -1.066597	H 4.629110 4.098044 -4.718223	C 1.490755 2.473743 0.147465
H 4.948397 1.299545 -0.905571	C 5.120388 3.969872 -3.753166	H -0.236659 3.602941 -0.434454
H 5.608813 2.113293 0.491793	H 2.302710 5.186030 -3.382893	H 2.997329 1.039693 0.687291
C 5.428597 2.223099 -0.578661	H 3.352255 5.976560 -2.186536	C 0.176940 2.605910 -0.347739
H 3.331355 3.432120 -0.077686	H 2.056288 4.903517 -1.628561	C 2.003743 1.165639 0.277758
H 3.611930 1.336359 -2.977633	C 2.790703 5.071223 -2.416010	H -1.573405 1.628363 -1.092084
H 2.611452 2.386472 -3.998600	P 3.909824 3.656667 -2.426190	H 1.676540 -0.931024 0.008703
H 2.132965 2.043239 -2.315015	H 4.998501 4.373111 -0.504531	C -0.566718 1.493610 -0.714666
C 2.972754 2.217871 -2.984581	C 4.533934 3.434913 -0.820059	C 1.253206 0.060510 -0.100277
H 5.811691 3.129704 -3.816383	O 2.217457 3.542289 0.427598	C -0.034614 0.210097 -0.607314
H 5.688725 4.869159 -3.517632	H -0.617311 -0.653938 -0.896287	



2A

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-806.83160347

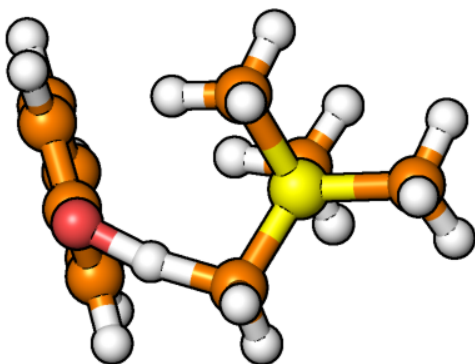
H 3.829638 3.341841 -0.090832	H 2.964964 5.744791 -2.247408	H -0.290128 3.643519 -0.650246
H 3.377154 1.120027 -2.957234	H 1.993042 4.689960 -1.169310	H 2.839872 1.353467 1.184875
H 2.083930 2.070757 -3.724497	C 2.408532 4.809072 -2.186158	C 0.167467 2.685266 -0.433503
H 1.979885 1.658044 -1.997742	P 3.536129 3.437910 -2.415983	C 1.929004 1.396555 0.599114
C 2.655649 1.923056 -2.808571	H 5.044161 2.292927 -0.940981	H -1.373357 1.558244 -1.393552
H 5.318132 2.965524 -3.970136	H 5.262164 4.061168 -0.897003	H 1.749836 -0.726547 0.437093
H 5.181501 4.702599 -3.637123	C 4.531312 3.253097 -0.939746	C -0.439298 1.508986 -0.844332
H 4.025293 3.915452 -4.728236	O 2.031976 3.774904 0.568448	C 1.308460 0.230385 0.180155
C 4.619172 3.788483 -3.823529	H -0.353226 -0.649546 -0.884114	C 0.127563 0.264511 -0.563573
H 1.628237 4.794639 -2.945004	C 1.403553 2.688632 0.284989	



3A

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-806.82975392

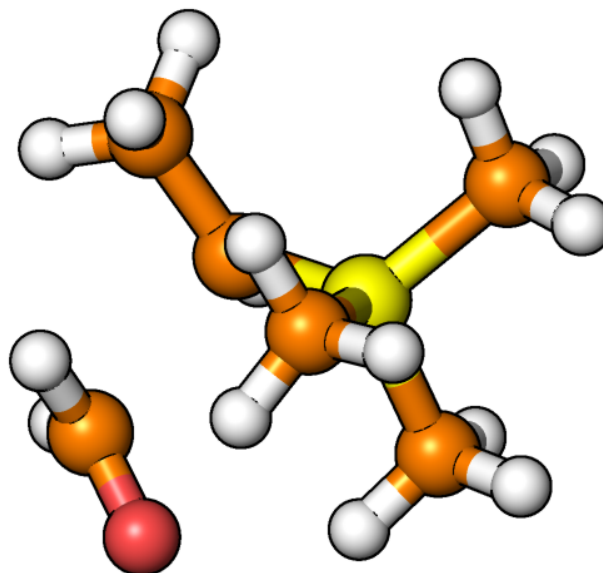
H 2.740821 3.406722 -0.156845	H 3.409477 5.990762 -2.332878	H -0.785516 3.293756 0.145452
H 3.567358 1.338819 -3.074459	H 2.000336 4.972345 -1.997399	H 2.882722 1.102593 0.168971
H 2.636411 2.377846 -4.168991	C 2.849665 5.115482 -2.662856	C -0.271896 2.341686 0.154842
H 2.083402 2.101872 -2.496837	P 3.918177 3.657294 -2.562240	C 1.801794 1.110264 0.160825
C 2.953085 2.237009 -3.136140	H 4.954398 2.486564 -0.787576	H -2.058007 1.168550 0.197346
H 5.798659 3.054022 -3.961827	H 4.909536 4.279720 -0.508626	H 1.620904 -1.020161 0.199276
H 5.742050 4.795634 -3.672652	C 4.424261 3.418757 -0.960236	C -0.975627 1.146507 0.183815
H 4.656989 4.064704 -4.876783	O 1.770684 3.520918 0.106103	C 1.084354 -0.079736 0.182500
C 5.138095 3.919369 -3.908020	H -0.858490 -1.003278 0.214217	C -0.305810 -0.074061 0.192529
H 2.507547 5.278808 -3.684170	C 1.126763 2.336986 0.141016	



TS_{2→3}A

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-806.82266020

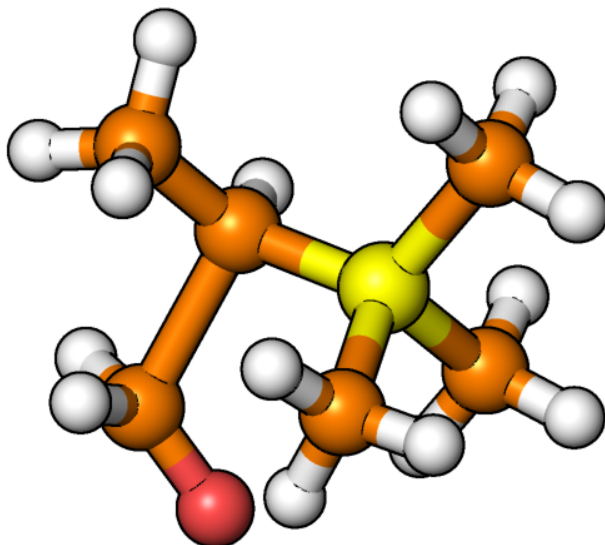
H 3.271194 3.440603 -0.066240	H 3.059862 5.838583 -2.314172	H -0.323106 3.567743 -0.288218
H 3.423355 1.173970 -2.856749	H 1.832020 4.761539 -1.628445	H 2.985838 1.100641 0.834801
H 2.353423 2.127333 -3.907600	C 2.513567 4.907667 -2.466267	C 0.108799 2.581293 -0.172989
H 1.947357 1.881149 -2.188431	P 3.673812 3.526131 -2.467058	C 1.976935 1.194494 0.454467
C 2.756711 2.034507 -2.899634	H 4.942254 2.459822 -0.773142	H -1.649957 1.548395 -0.815750
H 5.500340 2.986600 -3.946254	H 4.999736 4.251265 -0.652728	H 1.671882 -0.916112 0.287010
H 5.382976 4.729673 -3.667573	C 4.380989 3.385155 -0.887824	C -0.629431 1.444104 -0.466771
H 4.262054 3.937224 -4.795720	O 2.161252 3.576880 0.491043	C 1.230934 0.064156 0.149106
C 4.808472 3.823799 -3.858656	H -0.653717 -0.710051 -0.552822	C -0.074686 0.173710 -0.321914
H 1.968518 4.959497 -3.407785	C 1.440762 2.489982 0.284673	



5B-CHH

$E(\text{DLPNO-CCSD(T)}/\text{CBS}(\text{def2-TZVPP}, \text{def2-QZVPP})) = -653.38332352$

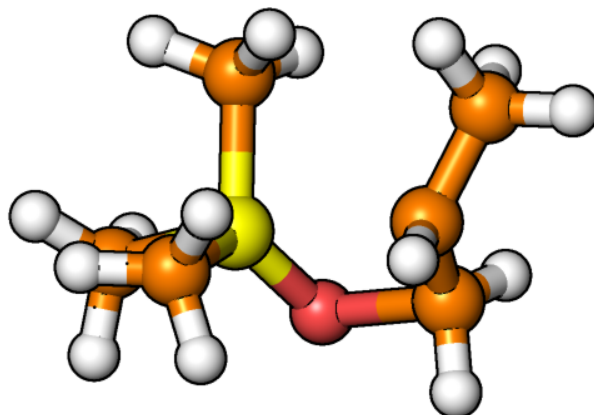
H 2.262287 1.315752 -1.270359	H 3.129782 -1.798694 2.594273	C 2.790755 -0.780822 2.784928
H 1.311122 -0.021907 -1.877164	H 3.317222 -0.385729 3.652705	C 2.554525 1.918157 1.703265
H 3.065704 -0.075666 -1.989402	H 2.638806 2.539970 0.812573	H -0.186007 -0.954525 0.247750
C 2.234615 0.225009 -1.341226	H 1.513154 1.864358 2.019205	C 2.238492 -0.423200 0.021002
H 5.370051 -0.593137 1.073176	H 3.165304 2.353321 2.493552	P 3.107689 0.234783 1.329692
H 5.187985 1.017902 0.365585	H 2.244317 -1.509042 0.032836	O -0.073373 0.115087 1.980988
H 5.350104 0.841691 2.124747	H 0.110920 0.861876 0.094983	C 0.070842 -0.015089 0.762899
H 1.713949 -0.776832 2.959500	C 4.931724 0.393173 1.221684	



TS_{5→6}B-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.38486776

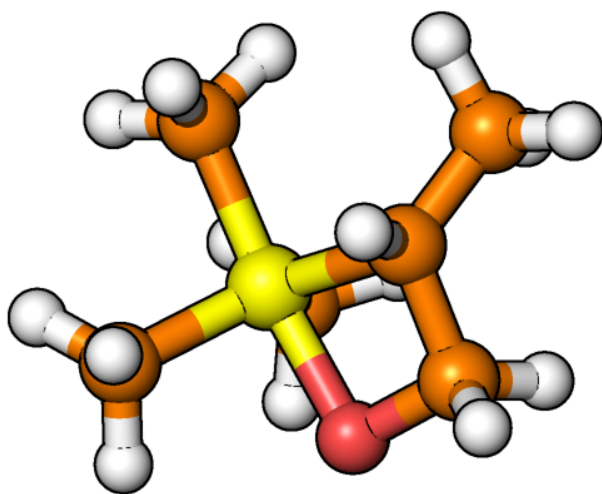
H 1.955890 1.439793 -1.051836	H 2.828848 -1.843653 2.682914	C 2.429935 -0.857430 2.917771
H 1.063197 0.116587 -1.770766	H 2.901553 -0.481326 3.824622	C 2.133798 1.895296 2.021199
H 2.823345 0.060127 -1.725544	H 2.194562 2.579294 1.175396	H -0.492058 -0.804931 0.141178
C 1.936449 0.351830 -1.153894	H 1.094703 1.776911 2.332932	C 1.806041 -0.333534 0.187588
H 4.954530 -0.543106 1.096244	H 2.737238 2.286748 2.839284	P 2.716206 0.255877 1.535926
H 4.728547 1.110054 0.504380	H 1.861731 -1.419530 0.147581	O -0.324946 -0.040810 2.037376
H 4.981397 0.819796 2.237416	H -0.147069 0.982276 0.273180	C -0.116324 0.004171 0.796715
H 1.343189 -0.907610 3.035015	C 4.520266 0.428366 1.329081	



TS_{7→8}B-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.38156447

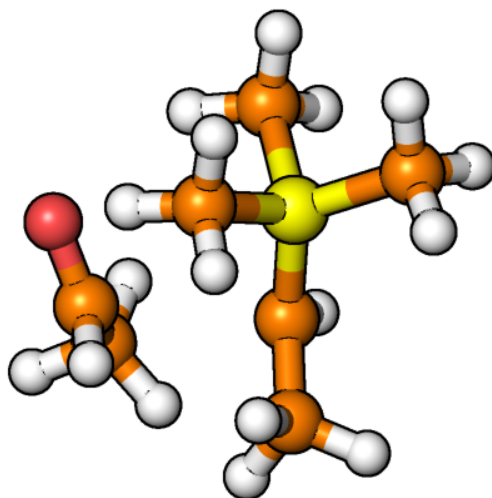
H 3.432770 -0.912179 2.487583	H 0.030042 0.557149 -2.543906	C 0.786799 -0.224883 -2.321577
H 2.043432 -2.039518 2.450389	H 1.652856 -0.098261 -3.010187	C 2.631004 -1.423599 -0.494636
H 2.292651 -0.959324 3.855900	H 3.436831 -1.177516 0.222704	H -0.610826 0.691645 1.972091
C 2.347843 -1.005469 2.736772	H 2.148102 -2.370085 -0.170690	P 1.325676 -0.096232 -0.527251
H 1.414398 2.328292 -0.207343	H 3.061224 -1.571987 -1.510946	C 1.497740 0.055553 2.040943
H 3.018606 1.587860 0.134646	H 1.795447 1.099584 2.271245	C 0.093123 -0.152142 1.830242
H 2.477203 1.842672 -1.588189	H -0.353315 -1.120435 2.136498	O -0.158070 -0.321119 0.076281
H 0.321271 -1.216755 -2.504203	C 2.152853 1.575142 -0.555901	



6B-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.43225152

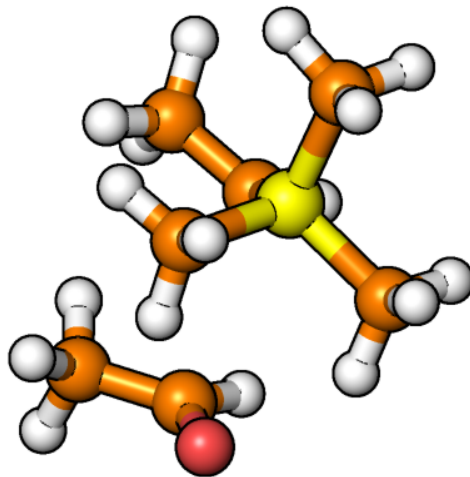
H 3.856390 -0.009651 1.049368	H 0.818203 2.379807 -1.805391	C 0.753654 1.408463 -2.299195
H 2.814340 -1.432550 1.146977	H 1.309114 1.457358 -3.233457	C 1.311925 -1.551691 -1.803575
H 2.805279 -0.240095 2.441646	H 1.996918 -1.734835 -2.629365	H -0.230846 0.698317 1.615200
C 2.873064 -0.362266 1.357801	H 1.551950 -2.242527 -0.993909	P 1.446646 0.154027 -1.161044
H 3.582051 1.420330 -1.413326	H 0.283473 -1.737834 -2.101457	C 1.753742 0.402757 0.671787
H 3.904498 -0.307369 -1.252951	H 1.895285 1.478289 0.814276	C 0.307455 0.002921 0.962949
H 3.336128 0.341162 -2.792251	H 0.248666 -0.997874 1.415234	O -0.192352 0.030349 -0.355840
H -0.296436 1.194542 -2.476194	C 3.237995 0.425940 -1.709028	



5B-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65285753

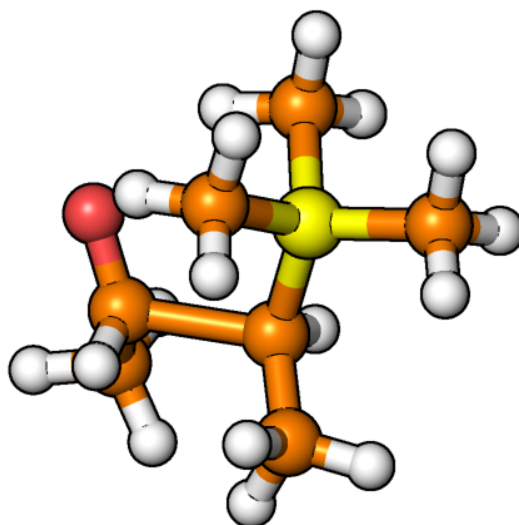
H 2.601962 -2.006567 -1.105299	H 4.815307 -0.566092 1.174457	C 4.354886 0.399362 1.386896
H 0.878094 -2.186545 -0.818500	H 4.608194 1.084268 0.577701	C 2.301868 -0.844014 2.918520
H 2.012534 -2.528936 0.465293	H 4.757737 0.784277 2.325846	C 1.906636 1.845990 1.830375
C 1.812469 -1.841096 -0.361229	H 1.252564 -0.821769 3.207111	H -0.434459 -1.570563 1.282310
H 1.455953 0.336671 -0.631214	H 2.597974 -1.867716 2.691083	C 1.684242 -0.416189 0.115752
H -1.360712 1.078771 0.019475	H 2.920793 -0.478823 3.737417	P 2.523268 0.190823 1.443923
H -2.499415 -0.268510 0.133206	H 1.983265 2.468251 0.938799	O -0.762373 0.094862 2.372172
H -1.023853 -0.460357 -0.824233	H 0.863291 1.767597 2.130878	C -0.763664 -0.519268 1.318744
C -1.436989 -0.006191 0.074008	H 2.492654 2.298904 2.629338	



5B-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65265265

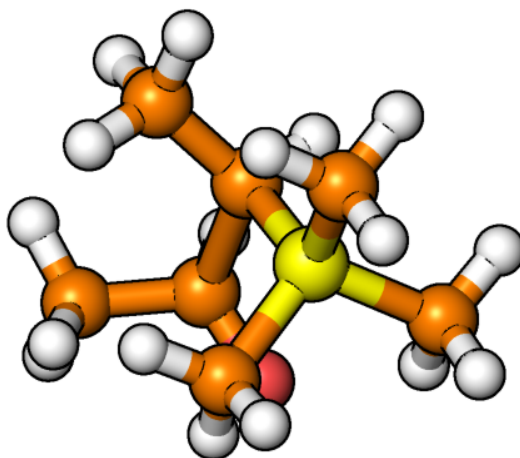
H -1.290876 1.455046 0.441912	H 4.561926 1.246873 0.661572	C 4.335492 0.556123 1.474724
H -2.487262 0.208782 0.056168	H 4.657237 1.003265 2.417403	C 2.305894 -0.939531 2.859710
H -0.940672 0.212011 -0.794412	H 1.245304 -1.007143 3.093521	C 1.807415 1.784866 1.910023
C -1.415254 0.409625 0.163516	H 2.686585 -1.924426 2.590433	H -0.686640 -1.534368 0.928785
H 1.558420 1.330396 -1.101686	H 2.854973 -0.575596 3.727445	C 1.807888 -0.472345 0.081816
H 1.003078 -0.127246 -1.889614	H 1.849770 2.451548 1.048785	P 2.528674 0.180003 1.457729
H 2.720575 0.217343 -1.810008	H 0.769242 1.634644 2.198830	O -0.797051 -0.168082 2.405280
C 1.785700 0.268457 -1.235026	H 2.358769 2.241469 2.731505	C -0.881784 -0.494605 1.236973
H 4.891437 -0.365843 1.305038	H 1.885289 -1.554214 0.032083	



TS_{5→6}B-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65170962

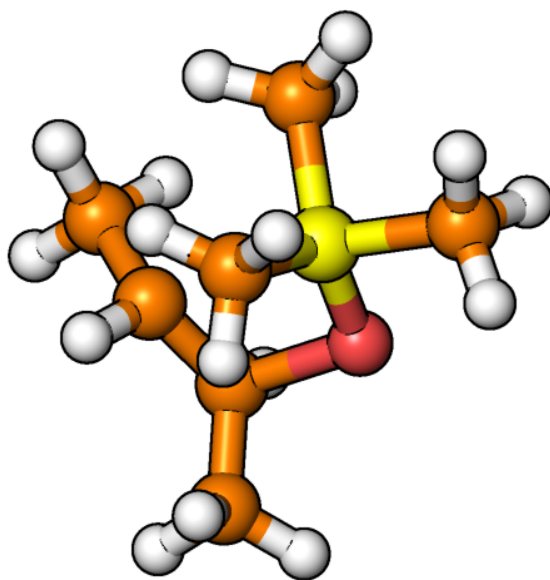
H 3.283238 -1.652718 -0.929855	H 4.914125 -0.736055 1.180834	C 4.556672 0.271647 1.391159
H 1.574346 -1.975475 -1.196637	H 4.863883 0.927697 0.577639	C 2.359405 -0.762819 2.953791
H 2.310136 -2.421623 0.325567	H 5.008359 0.618233 2.321884	C 2.213273 1.945259 1.871562
C 2.299755 -1.650040 -0.448442	H 1.282319 -0.672748 3.110564	H 0.070721 -1.524174 0.907721
H -0.645246 0.979404 -0.740433	H 2.629208 -1.799070 2.753301	C 1.880828 -0.305373 0.114004
H -1.801509 -0.304477 -0.381107	H 2.910454 -0.413523 3.825999	P 2.739982 0.263702 1.519559
H -0.387551 -0.662977 -1.385451	H 2.493026 2.597133 1.043962	O -0.240687 0.291051 1.788464
C -0.740181 -0.086363 -0.527767	H 1.124045 1.890824 1.963023	C -0.000879 -0.423220 0.763501
H 1.856698 0.488799 -0.631998	H 2.667965 2.310050 2.791810	



TS_{5→6}B-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.64782022

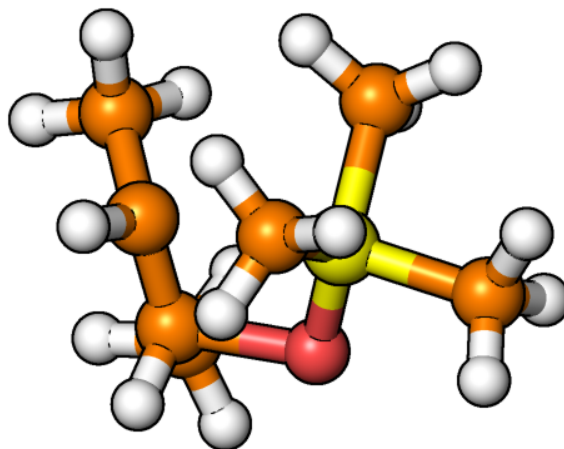
H 2.002176 1.230749 -1.276637	H 4.509248 1.354277 0.490107	C 4.378433 0.638954 1.306612
H 1.646305 -0.314048 -2.034430	H 4.797290 1.069988 2.221787	C 2.497188 -0.877780 2.938953
H 3.286513 0.033553 -1.498320	H 1.435273 -1.115770 3.064047	C 1.835398 1.829731 2.008965
C 2.226082 0.158665 -1.234470	H 3.061746 -1.788371 2.717158	H -0.234037 -1.483506 0.042125
H -0.384583 1.612859 0.046361	H 2.905438 -0.411045 3.840451	C 1.837728 -0.460186 0.108391
H -1.784980 0.560720 -0.163336	H 1.864184 2.529816 1.169306	P 2.602113 0.255369 1.532020
H -0.483599 0.524776 -1.364666	H 0.797694 1.612719 2.277139	O -0.258293 -0.457375 1.820833
C -0.697606 0.619968 -0.294629	H 2.371893 2.269017 2.855203	C -0.074224 -0.503452 0.553098
H 4.927760 -0.273749 1.059649	H 2.070596 -1.530739 0.136994	



TS_{7→8}B-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65549369

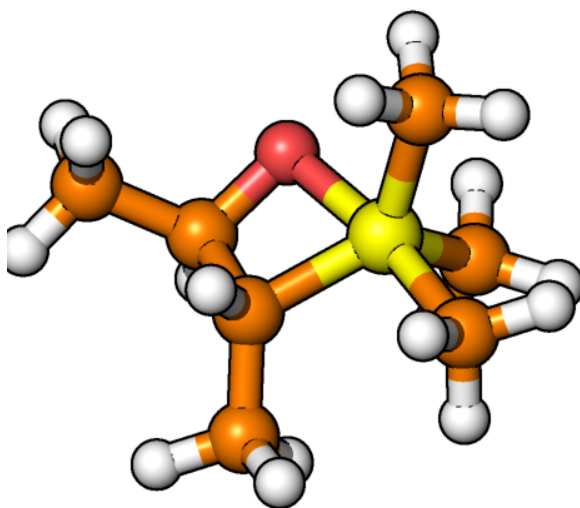
H -0.567338 -1.497111 3.297061	H 1.425995 2.361544 -0.474574	C 2.169859 1.580234 -0.655477
H 0.255741 -2.298429 1.953431	H 2.966252 1.687954 0.078869	C 0.884891 -0.291773 -2.305166
H -1.408019 -1.708637 1.747363	H 2.574854 1.717682 -1.664017	C 2.614805 -1.370584 -0.360741
C -0.440118 -1.491837 2.206794	H 0.419617 -1.271453 -2.445009	H -0.596554 0.669933 1.957939
H 1.294117 2.331517 2.111912	H 0.164973 0.471052 -2.614654	P 1.346946 -0.051760 -0.524689
H 2.940618 1.752267 2.351688	H 1.768010 -0.225469 -2.950946	C 1.492188 0.163541 1.970388
H 1.755672 1.577832 3.637022	H 3.424976 -1.041411 0.289601	C 0.109712 -0.146197 1.791206
C 1.885826 1.514380 2.544219	H 2.150730 -2.251611 0.090801	O -0.111355 -0.215408 0.038103
H 2.095447 -0.664831 2.350363	H 3.010934 -1.652917 -1.343161	



TS_{7→8}B-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65489045

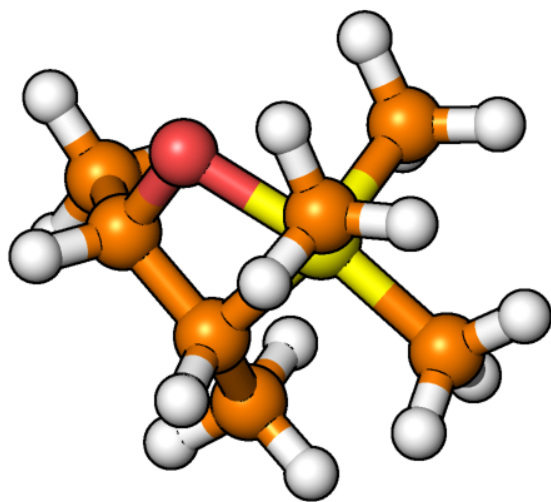
H -0.725985 1.965667 1.732942	H 1.495070 2.395344 -0.513207	H -0.261144 -1.072733 1.948529
H -1.046748 1.047876 3.208995	H 3.002475 1.685085 0.084147	C 2.221004 1.591639 -0.668111
H -1.961780 0.695543 1.728402	H 2.651968 1.707951 -1.668557	C 0.906200 -0.245851 -2.325173
C -0.978461 0.973217 2.115556	H 0.415623 -1.212127 -2.471172	C 2.574942 -1.372229 -0.351646
H 1.562758 2.390608 2.055368	H 0.212557 0.536526 -2.645762	P 1.349702 -0.016996 -0.537424
H 3.056289 1.570649 2.484739	H 1.800035 -0.204916 -2.958231	C 1.470509 0.197253 1.946740
H 1.717551 1.608261 3.623775	H 3.404157 -1.052322 0.279480	C 0.072643 -0.052085 1.758663
C 1.963433 1.500048 2.554151	H 2.086082 -2.222406 0.131993	O -0.121137 -0.152345 0.002354
H 2.031447 -0.672133 2.293171	H 2.950245 -1.695962 -1.329239	



6B-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.69765969

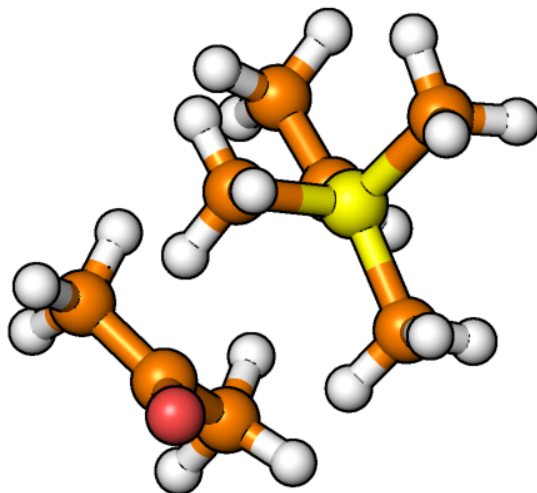
H -0.516101 2.054775 1.349138	H 3.942279 -0.326032 -1.160254	H 0.176457 -0.919952 1.256228
H -0.191800 1.022935 2.757277	H 3.469732 0.274161 -2.750885	C 3.316025 0.401442 -1.678419
H -1.617071 0.731035 1.750290	H -0.155438 1.217396 -2.657334	C 0.891421 1.407783 -2.439377
C -0.569486 1.033533 1.731761	H 0.964008 2.397369 -1.984436	C 1.355287 -1.542701 -1.795586
H 3.778841 0.104436 1.140140	H 1.491302 1.400166 -3.347273	P 1.492879 0.185261 -1.216917
H 2.746115 -1.325740 1.216826	H 2.081210 -1.773960 -2.572948	C 1.701780 0.482230 0.615421
H 2.640974 -0.091469 2.468002	H 1.534437 -2.203520 -0.946212	C 0.236558 0.101463 0.846753
C 2.780399 -0.248725 1.395109	H 0.341429 -1.720334 -2.144356	O -0.189278 0.133999 -0.502003
H 3.664666 1.399606 -1.401232	H 1.824633 1.564212 0.733802	



6B-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.69599981

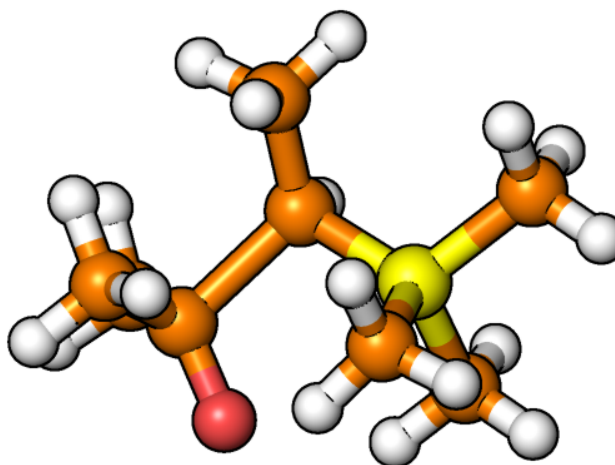
H 0.503258 -1.174576 2.816325	H 3.925781 -0.287261 -1.181843	C 3.241576 0.411031 -1.665785
H 0.663910 -2.066930 1.294261	H 3.344876 0.289445 -2.744981	C 0.732417 1.313612 -2.287690
H -0.922190 -1.512202 1.824360	H -0.306396 1.055515 -2.472615	C 1.380742 -1.604614 -1.723120
C 0.135775 -1.251461 1.790597	H 0.752276 2.298871 -1.818530	H -0.227531 0.848104 1.578652
H 3.871973 0.234086 1.095712	H 1.297668 1.360052 -3.216139	P 1.454500 0.115693 -1.107353
H 2.949711 -1.254321 1.294451	H 1.932405 -1.709405 -2.656352	C 1.751869 0.470832 0.705958
H 2.847217 0.014796 2.508320	H 1.842553 -2.258669 -0.982437	C 0.305288 0.058619 1.034222
C 2.920578 -0.173233 1.434444	H 0.344883 -1.905327 -1.846345	O -0.174092 -0.023028 -0.296001
H 3.559975 1.423797 -1.406379	H 1.845532 1.559198 0.770062	



5B-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-731.92243684

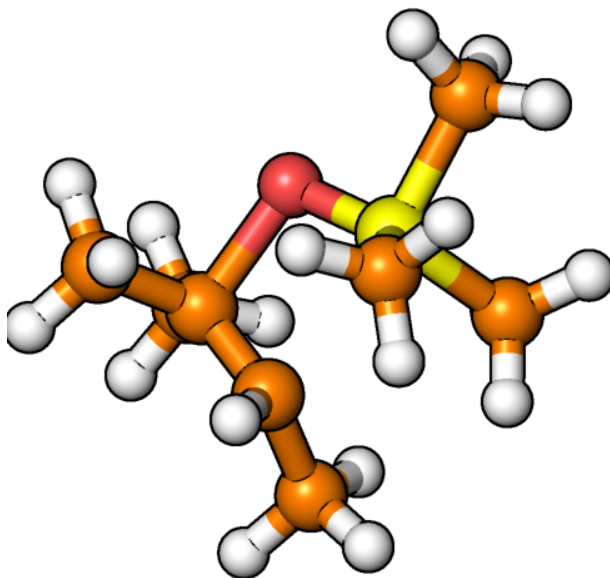
H 1.729246 1.198854 -1.330266	H -0.704978 0.468847 -0.806088	H 2.176837 2.307538 2.474049
H 1.127978 -0.272675 -2.057934	C -1.500429 0.517744 -0.062675	H 2.007055 -1.632886 -0.051131
H 2.856002 0.020766 -1.983244	H 4.857252 -0.313220 1.446575	C 4.273074 0.603367 1.527503
C 1.921313 0.124868 -1.414868	H 4.570913 1.269822 0.716864	C 2.141689 -0.866931 2.765455
H -0.776281 -2.517962 1.470430	H 4.491680 1.087881 2.481320	C 1.700457 1.798940 1.636164
H -0.651862 -2.081404 -0.253645	H 1.066387 -0.922314 2.921231	C 1.917524 -0.551638 -0.064819
H -2.239417 -2.239468 0.504999	H 2.535869 -1.864629 2.573468	P 2.481428 0.184849 1.331501
C -1.205192 -1.921033 0.669696	H 2.623868 -0.465323 3.656057	O -1.032367 -0.095043 2.192777
H -1.575046 1.527640 0.332575	H 1.804494 2.422953 0.748532	C -1.202158 -0.460016 1.046653
H -2.435139 0.247989 -0.561126	H 0.644740 1.647054 1.849349	



TS_{5→6}B-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-731.91350148

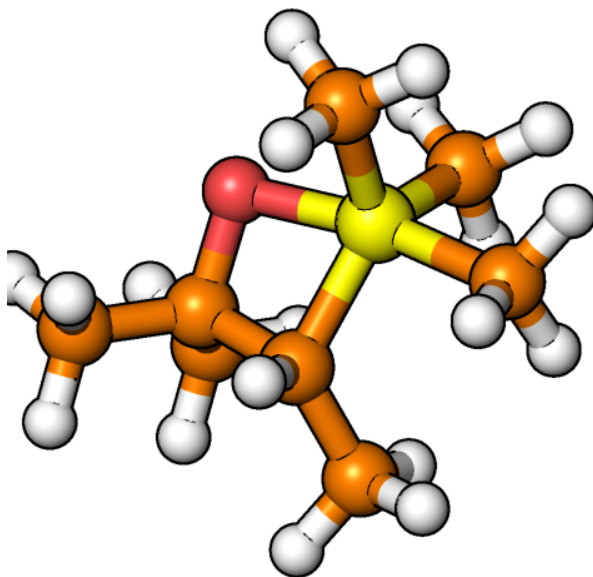
H 1.920965 1.079522 -1.227065	H -0.542417 0.308436 -1.165422	H 2.448844 2.445509 2.792927
H 1.620689 -0.531357 -1.859711	C -0.686154 0.487357 -0.094703	H 2.154182 -1.560590 0.381291
H 3.253435 -0.073622 -1.388581	H 4.962164 -0.190431 1.078687	C 4.408544 0.730002 1.283876
C 2.193784 0.024643 -1.110539	H 4.488928 1.384740 0.412027	C 2.647077 -0.676829 3.121688
H 0.135195 -2.740553 0.969920	H 4.862404 1.233287 2.143680	C 1.885691 1.940961 2.002102
H -0.118885 -2.188596 -0.709430	H 1.600668 -0.926564 3.323775	C 1.860541 -0.508891 0.284003
H -1.454130 -2.154479 0.461767	H 3.224138 -1.589263 2.943370	P 2.651766 0.339604 1.623923
C -0.373442 -2.002735 0.341491	H 3.091172 -0.128414 3.957998	O -0.127407 -0.361770 2.083497
H -0.334322 1.495132 0.145588	H 1.885147 2.573990 1.110246	C -0.026261 -0.574171 0.816066
H -1.764146 0.464732 0.108396	H 0.859652 1.740441 2.320613	



TS_{7→8}B-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-731.91923126

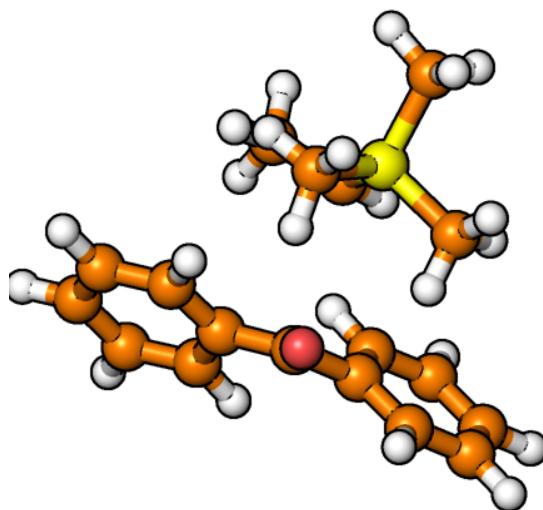
H 3.418984 -0.676397 2.587329	H -1.858493 0.798063 1.585294	H 3.100103 -1.498304 -1.469741
H 2.284522 -1.990682 2.316554	C -0.875465 0.953893 2.038424	H 1.712163 1.057589 2.188717
H 2.158832 -1.004790 3.768369	H 1.407580 2.308346 -0.144062	C 2.137657 1.576900 -0.501045
C 2.364061 -0.961884 2.685643	H 2.993621 1.592934 0.173764	C 0.922695 -0.186092 -2.316905
H -0.551312 -1.606751 3.302413	H 2.450512 1.864992 -1.510934	C 2.660558 -1.378387 -0.473965
H 0.079103 -2.389023 1.848721	H 0.496751 -1.165888 -2.550877	P 1.355205 -0.088042 -0.508953
H -1.541140 -1.673774 1.829905	H 0.177306 0.573821 -2.567926	C 1.474048 0.020404 1.941348
C -0.522168 -1.550560 2.205973	H 1.809308 -0.029408 -2.942281	C 0.061936 -0.214032 1.794910
H -0.456755 1.887938 1.653733	H 3.441707 -1.137754 0.245530	O -0.108286 -0.346958 -0.003209
H -1.010671 1.074545 3.121491	H 2.206600 -2.330456 -0.184323	



6B-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-731.96123821

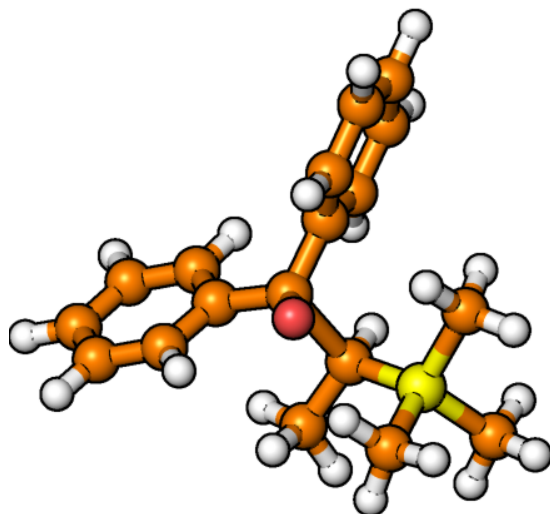
H -0.035885 1.426800 2.744833	H 2.831300 0.141258 2.472439	H 0.314208 -1.957768 -1.735457
H -1.511478 0.992539 1.869790	C 2.907266 -0.088915 1.406768	H 1.843143 1.618153 0.675759
H -0.406109 2.189219 1.186995	H 3.541490 1.391556 -1.504103	C 3.217991 0.369672 -1.717975
C -0.460072 1.257941 1.752167	H 3.900676 -0.309405 -1.205399	C 0.717109 1.258173 -2.374115
H 0.524494 -1.114010 2.777679	H 3.318206 0.201066 -2.791134	C 1.349071 -1.635925 -1.675596
H 0.676273 -1.974994 1.239106	H -0.329283 1.013806 -2.533010	P 1.430320 0.110087 -1.138693
H -0.908980 -1.448745 1.796053	H 0.764877 2.266709 -1.959434	C 1.740997 0.528364 0.653110
C 0.145714 -1.175551 1.755630	H 1.272067 1.242701 -3.310030	C 0.286193 0.152872 1.012336
H 3.859501 0.305473 1.055114	H 1.853634 -1.768154 -2.632028	O -0.193816 0.033278 -0.322444
H 2.936944 -1.174572 1.309123	H 1.863684 -2.253185 -0.938285	



5B-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1114.83778071

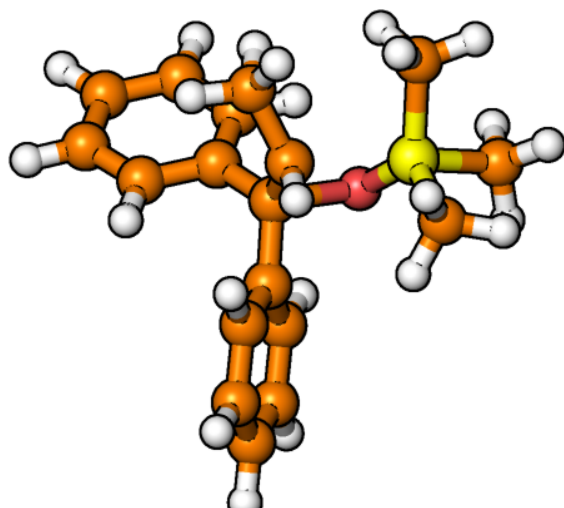
H 2.980535 2.105048 -0.682985	H -0.099556 -5.153741 1.289406	H 3.302232 -1.903773 2.274289
H 2.019216 0.994344 -1.618536	H 0.482093 -3.883604 -0.755655	H 3.920977 -0.922522 3.617733
H 3.774523 0.950891 -1.744252	H -0.626490 -3.939961 3.383359	H 3.533512 2.743657 1.558482
C 2.942597 1.071441 -1.036808	H 0.537522 -1.421621 -0.705409	H 2.285215 1.967971 2.562445
H -1.436069 3.434806 -2.568444	H -0.553180 -1.459343 3.420671	H 3.950215 2.147445 3.171607
H -2.291080 1.113827 -2.487610	C -0.081047 -4.071739 1.309858	H 2.815557 -0.959502 -0.134947
H 0.087808 4.246547 -0.791692	C 0.239575 -3.357904 0.158488	C 5.584953 0.342792 1.649277
H -1.612239 -0.389090 -0.663358	C -0.374443 -3.390353 2.486043	C 3.255687 -0.927324 2.755290
H 0.749090 2.730845 1.049805	C 0.259415 -1.970861 0.180704	C 3.338336 1.959528 2.290241
C -1.137614 2.773587 -1.765560	C -0.341961 -2.002875 2.510595	C 2.941338 0.089031 0.105807
C -1.611736 1.469141 -1.723887	C -0.028927 -1.278740 1.358763	P 3.736895 0.344080 1.559272
C -0.282237 3.230231 -0.765097	H 5.952559 -0.629892 1.321346	O 0.303252 0.728714 2.542896
C -1.220585 0.616559 -0.697498	H 5.972999 1.099708 0.966611	C 0.031000 0.212731 1.466729
C 0.094462 2.385716 0.264534	H 5.957155 0.547734 2.655288	
C -0.355807 1.063592 0.303649	H 2.233732 -0.741026 3.076810	



TS_{5→6}B-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1114.83060421

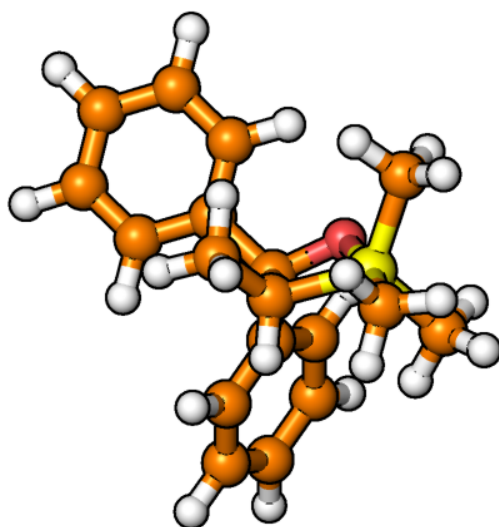
H 4.668519 -1.419840 1.036622	H -2.121726 1.588860 -2.943590	H 1.761086 -0.250438 3.343303
H 3.612314 -2.572668 0.229923	H -3.029167 1.058234 -0.695579	H 3.542011 -0.211442 3.506048
H 3.314932 -2.158383 1.902003	H 0.140808 0.784887 -3.560057	H 2.603768 1.263959 3.822430
C 3.626691 -1.748019 0.940618	H -1.651514 -0.231669 0.918331	H 1.366185 2.162534 0.058076
H 1.431350 -6.555969 -0.138570	H 1.470696 -0.501483 -1.973765	H 0.479378 1.496871 1.440080
H 1.412944 -5.014543 -2.079127	C -1.535384 1.015118 -2.237864	H 1.594044 2.878409 1.673224
H 1.081339 -5.648429 2.142334	C -2.040320 0.718450 -0.976740	C 4.284521 1.725431 1.256613
H 1.074329 -2.614723 -1.748822	C -0.267047 0.563638 -2.581766	C 2.658356 0.357044 3.220975
H 0.734319 -3.201017 2.457040	C -1.279840 -0.010601 -0.071981	C 1.414209 1.953717 1.125200
C 1.286561 -5.493865 0.010659	C 0.487333 -0.172056 -1.673572	C 2.670861 -0.659215 0.476315
C 1.279201 -4.627261 -1.076939	C -0.000765 -0.467396 -0.399250	P 2.740034 0.785478 1.473729
C 1.091962 -4.982312 1.288673	H 2.834552 -0.376335 -0.560501	O 0.368178 -0.968528 1.895365
C 1.090646 -3.263466 -0.886590	H 5.138248 1.076221 1.445890	C 0.725959 -1.254286 0.704592
C 0.904051 -3.618638 1.474840	H 4.345871 2.094629 0.233389	
C 0.911658 -2.737519 0.393685	H 4.321083 2.571124 1.944876	



TS_{7→8}B-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1114.83241993

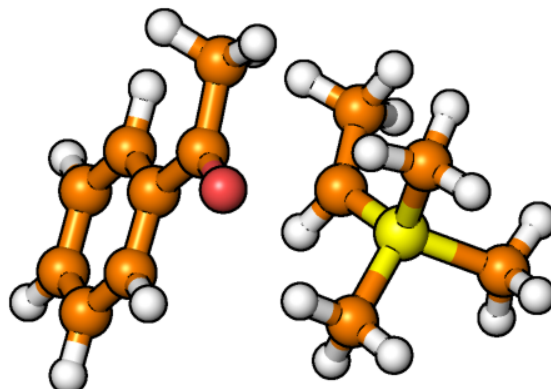
H 2.201721	2.542176	1.408976	C 0.138959	-1.217114	1.567329	H 1.409298	-1.318691	-2.825799
H 3.667185	1.772493	2.001857	H -2.601870	4.211791	2.364493	H 1.476657	0.412186	-3.161208
H 2.254070	1.905519	3.037130	H -1.981624	2.536938	4.086032	H 2.968946	-0.546283	-3.190860
C 2.576855	1.710773	2.007035	H -1.708945	3.981628	0.064979	H 4.027076	-1.290017	0.217293
H 2.632432	-0.468285	1.947187	H -0.489908	0.667771	3.508931	H 2.540272	-2.234565	0.123373
H -1.500428	-4.598610	2.558088	H -0.220544	2.095838	-0.503756	H 3.567424	-2.080396	-1.315695
H 0.456292	-3.745644	3.815568	C -1.941725	3.391644	2.114672	C 3.322200	1.379479	-1.023595
H -2.417461	-3.269678	0.676719	C -1.593936	2.451735	3.079345	C 2.005898	-0.417360	-2.693337
H 1.479514	-1.595091	3.195531	C -1.438612	3.261777	0.826933	C 3.197873	-1.564489	-0.428626
H -1.368693	-1.126379	0.051358	C -0.752314	1.397352	2.754439	P 2.241002	-0.082602	-0.893531
C -1.044340	-3.656729	2.283958	C -0.593261	2.205473	0.501707	C 2.113009	0.366379	1.491984
C 0.053340	-3.180567	2.985242	C -0.239537	1.261031	1.461526	C 0.727232	0.128072	1.222654
C -1.558614	-2.908724	1.227289	H 2.710808	2.272371	-0.902602	O 0.711657	0.007489	-0.571401
C 0.638167	-1.967802	2.629652	H 4.074549	1.377023	-0.241535			
C -0.976286	-1.701441	0.876766	H 3.800087	1.412601	-2.003380			



6B-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1114.87602003

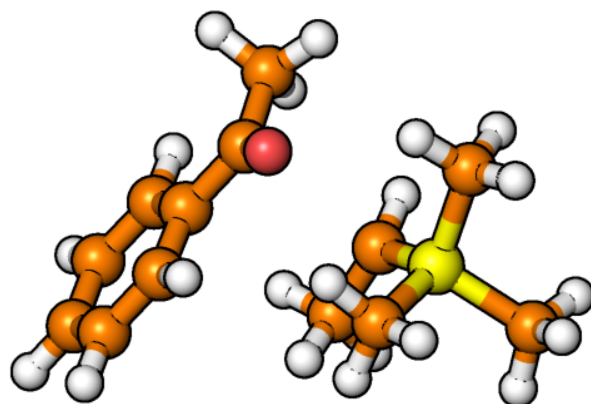
H 1.573354 2.937616 -0.084397	H -2.446736 4.491367 2.745731	H -0.119183 0.485420 -2.685683
H 3.300454 2.564415 -0.005530	H -2.795927 3.565282 0.474239	H 0.750197 1.970788 -2.317541
H 2.358688 2.756051 1.470407	H -0.706792 3.506493 4.210724	H 1.430783 0.852683 -3.509296
C 2.331579 2.367761 0.451864	H -1.392889 1.680576 -0.321879	H 2.549852 -2.047613 -2.094505
H 0.675083 -3.671644 4.487730	H 0.657809 1.628694 3.417970	H 2.105288 -2.128332 -0.377919
H -1.034376 -3.568093 2.695702	C -1.838215 3.669527 2.391992	H 0.833156 -2.102198 -1.583382
H 2.386293 -1.887104 4.648019	C -2.030827 3.150258 1.118024	C 3.481198 0.416255 -1.881318
H -1.011746 -1.695733 1.072174	C -0.860823 3.117092 3.212861	C 0.871249 0.918624 -2.578165
H 2.389561 -0.030726 3.045173	C -1.246284 2.095496 0.663857	C 1.824910 -1.723501 -1.350891
C 0.674039 -2.851012 3.782193	C -0.084186 2.059217 2.759543	P 1.745155 0.095335 -1.202496
C -0.284202 -2.791403 2.774974	C -0.260984 1.541432 1.476128	C 2.029318 0.875820 0.459819
C 1.632680 -1.850427 3.871627	H 2.841151 0.348570 0.961334	C 0.618734 0.414125 0.938987
C -0.281167 -1.741340 1.867158	H 3.680047 1.484956 -1.974168	O 0.143254 -0.045990 -0.310919
C 1.632095 -0.799371 2.959567	H 4.235516 -0.010773 -1.216797	
C 0.676582 -0.731630 1.947800	H 3.604044 -0.033424 -2.867618	



5B-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.38082038

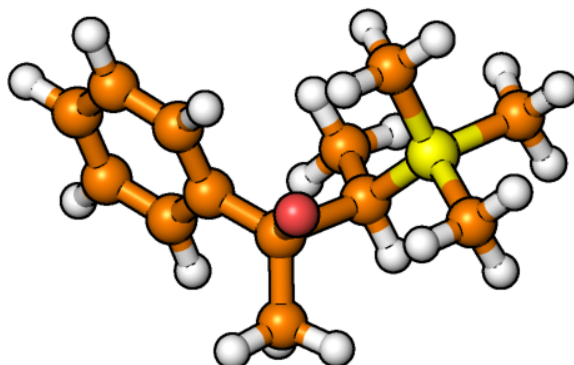
H 0.975153 -0.764521 -1.669107	H -1.241962 -2.000285 -0.843257	H 1.804671 2.449630 0.455204
H 2.710822 -0.561067 -1.788692	C -0.637074 -4.674160 1.135825	H 0.736551 1.914981 1.769574
H 1.693530 0.800381 -1.346052	C -0.511798 -4.022893 2.360024	H 2.294339 2.698366 2.137918
C 1.833058 -0.274522 -1.193523	C -0.907674 -3.938501 -0.012967	C 4.347080 0.824734 1.422976
H 1.924375 -1.678522 0.530955	C -0.646007 -2.645451 2.430681	C 2.303545 -0.350904 3.075800
H -1.455710 1.436966 0.442066	C -1.043037 -2.559140 0.059140	C 1.773082 2.024608 1.458358
H -2.421162 0.071267 -0.150272	C -0.899610 -1.895560 1.279387	C 1.915222 -0.628796 0.266753
H -0.734323 0.226186 -0.640920	H 4.934695 -0.088436 1.516060	P 2.553015 0.380645 1.440385
C -1.427844 0.382060 0.182600	H 4.587127 1.285316 0.463513	O -0.881267 0.139404 2.480919
H -0.529366 -5.749495 1.078734	H 4.617723 1.515640 2.224050	C -1.021199 -0.412330 1.400711
H -0.311152 -4.592605 3.257929	H 1.239016 -0.351602 3.301395	
H -1.010977 -4.440245 -0.966097	H 2.673939 -1.375238 3.066153	
H -0.555064 -2.125209 3.373309	H 2.843322 0.214322 3.834513	



5B-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.38096619

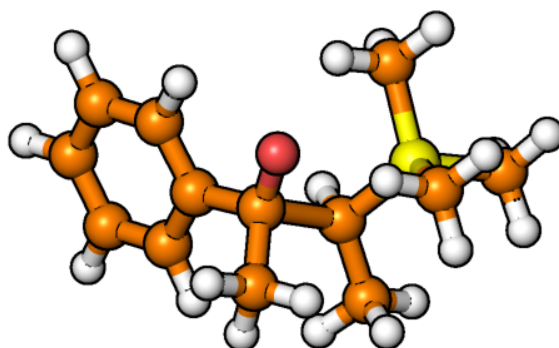
H 3.228468 -2.244228 -0.616273	C -0.677854 -4.799853 1.358168	H 1.736856 2.377071 0.305994
H 1.505391 -2.583034 -0.674775	C -0.446192 -4.044760 2.505283	H 0.724290 1.835350 1.665126
H 2.324325 -2.575648 0.859634	C -1.012534 -4.161859 0.169925	H 2.276667 2.652953 1.972593
C 2.274447 -2.059510 -0.102457	C -0.547670 -2.663982 2.460296	C 4.363974 0.779045 1.286183
H -1.300800 1.249428 0.134035	C -1.105393 -2.776948 0.124482	C 2.359525 -0.395963 2.925543
H -2.480525 -0.036088 -0.174565	C -0.867402 -2.010168 1.266860	C 1.746158 1.965246 1.314856
H -0.855697 -0.153228 -0.861510	H 1.663381 -0.047201 -0.832493	C 1.912954 -0.603632 0.065141
C -1.422707 0.177141 0.004483	H 4.943990 -0.144291 1.286659	P 2.564959 0.350863 1.283329
H -0.599933 -5.878736 1.392302	H 4.598106 1.327144 0.373020	O -0.837301 0.111769 2.304723
H -0.192529 -4.537184 3.434979	H 4.651778 1.379397 2.151699	C -0.981684 -0.521838 1.270381
H -1.196548 -4.742352 -0.724383	H 1.298290 -0.426319 3.161321	
H -0.388817 -2.067652 3.346802	H 2.756071 -1.410365 2.913601	
H -1.355627 -2.295881 -0.809385	H 2.892603 0.179477 3.681505	



TS_{5→6}B-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.37331379

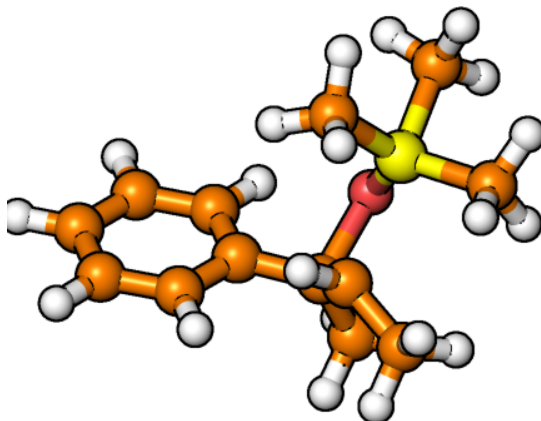
H 1.959630 1.050829 -1.267141	C -1.798785 1.253089 -2.776716	H 0.843310 1.932357 1.989918
H 1.964193 -0.575319 -1.913358	C -1.307178 -0.044339 -2.900912	H 2.418182 2.597583 2.564288
H 3.455699 0.095457 -1.262892	C -1.699850 1.902063 -1.547047	H 2.332230 -1.558697 0.356730
C 2.367773 0.046672 -1.110699	C -0.709920 -0.676747 -1.811709	C 4.414205 0.651282 1.464803
H 0.425372 -2.604306 1.577765	C -1.109817 1.261840 -0.460154	C 2.407059 -0.506112 3.193749
H 0.253404 -2.735356 -0.184215	C -0.589893 -0.031881 -0.574053	C 1.906084 2.045704 1.770343
H -1.172069 -2.442920 0.836052	H 4.930828 -0.309088 1.383403	C 1.957451 -0.533741 0.245469
C -0.108128 -2.211551 0.706768	H 4.631306 1.239610 0.569761	P 2.609813 0.381225 1.627057
H -2.264598 1.747203 -3.624566	H 4.798560 1.187828 2.338282	O -0.184314 -0.080763 1.790827
H -1.391415 -0.569597 -3.848664	H 1.334865 -0.644657 3.351720	C 0.054378 -0.673971 0.666585
H -2.096840 2.907372 -1.430957	H 2.906648 -1.477454 3.126197	
H -0.337784 -1.688126 -1.940071	H 2.855277 0.068063 4.010472	
H -1.067677 1.743525 0.510492	H 2.034744 2.580998 0.825466	



TS_{5→6}B-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.36332485

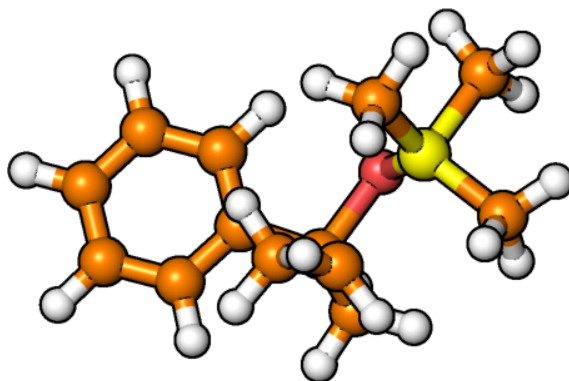
H 2.294383 -2.083686 -1.274379	C -1.937660 0.874756 -2.980236	H 2.078702 2.602234 1.044848
H 2.808776 -2.492240 0.384721	C -2.132036 1.435341 -1.700442	H 0.730391 1.796192 1.976127
H 3.806583 -1.392842 -0.629106	C -1.097644 -0.251020 -3.120547	H 2.232371 2.417990 2.846379
C 2.756820 -1.662945 -0.355545	C -1.487712 0.880205 -0.575594	C 4.383633 0.549081 1.565045
H 0.553837 -2.725153 1.531949	C -0.457699 -0.803739 -1.991927	C 2.279219 -0.736177 3.162183
H 0.206265 -2.901346 -0.229310	C -0.633822 -0.240842 -0.702051	C 1.828301 1.960544 1.917125
H -1.127563 -2.576204 0.932207	H 1.879432 0.338780 -0.605591	C 1.909177 -0.480233 0.147377
C -0.065997 -2.341691 0.691657	H 4.903677 -0.426161 1.455866	P 2.547036 0.292077 1.661233
H -2.441710 1.306606 -3.862902	H 4.630654 1.183362 0.686790	O -0.238724 -0.145582 1.693801
H -2.797131 2.309436 -1.577477	H 4.750562 1.049432 2.488320	C 0.051361 -0.784854 0.589256
H -0.943728 -0.705150 -4.116015	H 1.175512 -0.832948 3.255438	
H -1.636226 1.290564 0.437067	H 2.748234 -1.732964 3.017486	
H 0.188019 -1.688076 -2.128814	H 2.732430 -0.241248 4.048250	



TS_{7→8}B-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.37561924

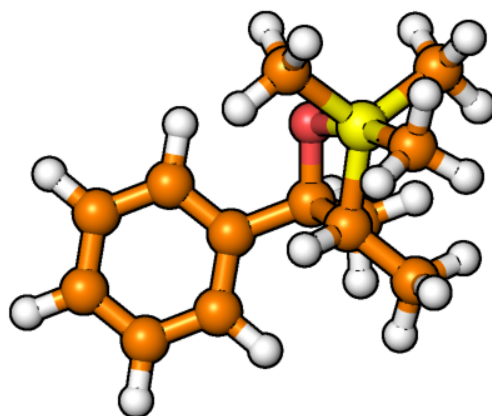
H 3.789974 -0.712085 2.564825	C -1.832565 3.684591 2.722624	H 2.827420 -1.806934 -0.403068
H 2.562463 -1.864203 2.061278	C -2.147252 2.921659 1.598653	H 3.707009 -0.781970 -1.551522
H 2.444268 -1.084555 3.633825	C -0.749093 3.316899 3.514216	H 2.314357 1.217044 2.291359
C 2.711488 -0.909134 2.578710	C -1.385707 1.804744 1.268823	C 2.540088 2.111784 -0.278689
H -0.285887 -1.156996 3.229181	C 0.018291 2.201971 3.178702	C 1.461751 0.464546 -2.296172
H 0.290960 -1.979912 1.769230	C -0.282524 1.432266 2.048917	C 3.238402 -0.805698 -0.562096
H -1.239505 -1.082590 1.737429	H 1.793161 2.728746 0.227674	P 1.867136 0.413938 -0.479522
C -0.222405 -1.088617 2.135494	H 3.440472 2.091578 0.336448	C 1.952480 0.248515 1.950016
H -2.428048 4.556235 2.977863	H 2.764835 2.561144 -1.251855	C 0.526203 0.182245 1.768259
H -2.990647 3.199098 0.972558	H 1.091351 -0.509095 -2.629893	O 0.401194 0.063482 -0.028548
H -0.495738 3.897203 4.396867	H 0.681988 1.206714 -2.487901	
H -1.629981 1.225977 0.385980	H 2.348041 0.723400 -2.887047	
H 0.856107 1.921312 3.808242	H 3.987108 -0.616723 0.205771	



TS_{7→8}B-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.37436070

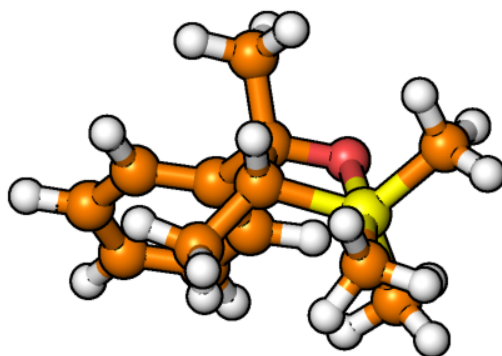
O 0.339522 0.238696 -0.040322	H 2.894608 2.251296 -1.775107	H -2.744065 4.339719 3.378344
C 0.562594 0.379463 1.739987	H 3.424337 2.175072 -0.072808	C 0.033536 -0.996589 2.123033
C 1.978294 0.607986 1.855972	H 1.832389 2.831466 -0.475713	H -0.959662 -1.181612 1.706845
P 1.796068 0.418881 -0.600532	C -0.381855 1.498211 2.123865	H 0.713327 -1.782363 1.781429
C 3.094290 -0.876509 -0.467151	C -0.521221 1.770464 3.493257	H -0.033488 -1.064097 3.215160
C 1.323116 0.161912 -2.379585	C -1.116042 2.268608 1.219427	H 2.529894 -0.276829 2.181828
C 2.572898 2.072808 -0.743865	C -1.365005 2.780258 3.942861	C 2.546039 1.895038 2.427960
H 3.485960 -1.136322 -1.457137	C -1.957389 3.286483 1.670383	H 2.058424 2.790404 2.028963
H 2.652334 -1.773527 -0.024644	C -2.087082 3.548125 3.030449	H 2.461937 1.962072 3.524251
H 3.905353 -0.541410 0.179191	H 0.045972 1.190946 4.215837	H 3.616462 1.981779 2.199879
H 2.200916 0.239550 -3.031356	H -1.037754 2.062122 0.160125	
H 0.589126 0.911077 -2.689296	H -1.454613 2.970931 5.008530	
H 0.873489 -0.826125 -2.512127	H -2.518362 3.873290 0.948258	



6B-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.41795813

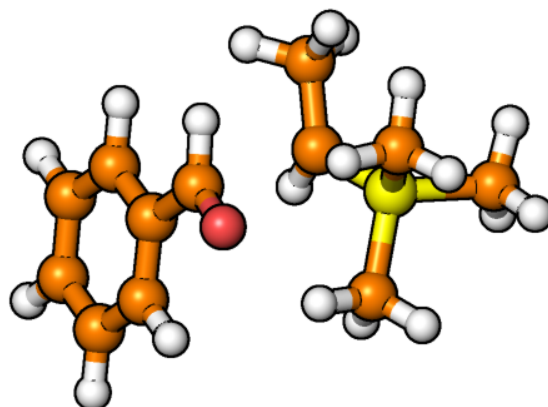
O -0.158923 -0.099484 -0.418809	H -0.197883 0.939856 -2.653030	C -1.625765 1.889991 0.828283
C 0.229263 0.169798 0.916563	H 3.440416 0.232988 -2.741109	C -0.158324 1.904498 2.725015
C 1.714972 0.516436 0.627922	H 3.972571 -0.312546 -1.150634	C -2.324315 2.967578 1.364219
P 1.500088 0.079641 -1.169405	H 3.607735 1.393674 -1.417953	C -0.850867 2.982374 3.260547
C 1.454557 -1.653843 -1.746381	C 2.823556 -0.148895 1.428125	C -1.939878 3.518555 2.580237
C 0.801259 1.263723 -2.375240	H 2.722646 0.089321 2.489273	H -1.912492 1.455743 -0.118039
C 3.302261 0.374965 -1.668384	H 2.811020 -1.235119 1.335431	H 0.688174 1.496808 3.263754
H 1.856197 1.599669 0.661863	H 3.802521 0.204367 1.107921	H -3.171571 3.376966 0.829103
H 0.429572 -1.935318 -1.968944	C 0.015975 -1.073311 1.784304	H -0.541530 3.404711 4.207616
H 1.811912 -2.294072 -0.938573	H -1.045800 -1.317795 1.787923	H -2.481672 4.357928 2.995605
H 2.099645 -1.802294 -2.610808	H 0.558321 -1.924561 1.373121	
H 1.432398 1.379466 -3.253464	H 0.334549 -0.918521 2.815716	
H 0.706916 2.229102 -1.876333	C -0.535562 1.347516 1.501679	



6B-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-923.41857196

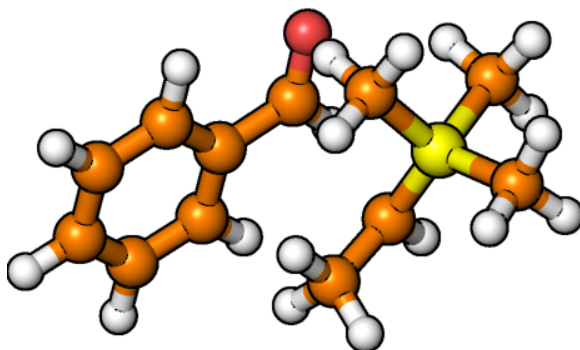
O -0.165972 0.062195 -0.101770	H -0.447545 1.309765 -2.175914	C -0.443023 -2.082442 1.605762
C 0.447787 0.243315 1.161961	H 3.025684 0.195640 -2.971478	C 0.663934 -0.949594 3.402042
C 1.913058 0.384511 0.653941	H 3.740377 -0.548879 -1.541694	C -0.649170 -3.184863 2.428966
P 1.360827 0.110449 -1.104992	H 3.546403 1.204477 -1.615783	C 0.463164 -2.049169 4.226127
C 1.020077 -1.563867 -1.751310	C 3.001570 -0.523800 1.203656	C -0.194410 -3.175176 3.741395
C 0.629658 1.439779 -2.128363	H 3.138318 -0.354710 2.272203	H -0.806622 -2.076188 0.589843
C 3.082666 0.251521 -1.883345	H 2.756799 -1.578529 1.076354	H 1.175305 -0.082414 3.798347
H 2.243673 1.424251 0.731067	H 3.955045 -0.328253 0.715732	H -1.171409 -4.051411 2.043717
H -0.051190 -1.682249 -1.891451	C -0.074683 1.528794 1.809391	H 0.818269 -2.026322 5.248184
H 1.341240 -2.290438 -1.004303	H -1.141024 1.433087 2.011552	H -0.355328 -4.031513 4.383090
H 1.555937 -1.755442 -2.678851	H 0.435215 1.756176 2.746428	
H 1.066873 1.468023 -3.124184	H 0.073073 2.364278 1.124125	
H 0.831216 2.392927 -1.636100	C 0.219486 -0.952360 2.077634	



5B-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11313203

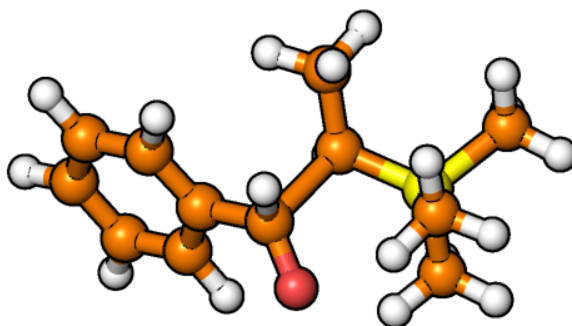
C -0.817685 -0.319283 1.303505	H 2.456139 -1.609543 3.131113	H -1.225513 -1.737217 -0.941543
O -0.811561 0.287675 2.364597	H 1.127400 -0.457669 3.399080	H -1.292019 -4.566173 3.111591
P 2.516662 0.211450 1.574910	H 4.692526 1.070230 2.377832	H -1.609768 -4.173825 -1.143975
C 1.755539 -0.681898 0.366152	H 4.625392 0.926055 0.609008	H -1.628610 -5.591440 0.884832
C 1.902987 1.917582 1.640337	H 4.830918 -0.523625 1.596613	H 1.752377 -1.750068 0.546455
C 2.189520 -0.554235 3.179420	C -1.032148 -1.780056 1.193378	C 1.676089 -0.223483 -1.066761
C 4.344117 0.450228 1.549331	C -1.064273 -2.581342 2.335924	H 2.521205 -0.535856 -1.693776
H -0.807550 0.217272 0.341878	C -1.238601 -2.362314 -0.057570	H 0.775435 -0.615239 -1.551380
H 2.450499 2.494750 2.384747	C -1.272191 -3.947685 2.223667	H 1.614304 0.865929 -1.143483
H 0.844222 1.894186 1.892448	C -1.451312 -3.728615 -0.170559	
H 2.036759 2.389901 0.667311	C -1.463277 -4.525413 0.970475	
H 2.775768 -0.074347 3.961952	H -0.926511 -2.113545 3.300974	



5B-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11344449

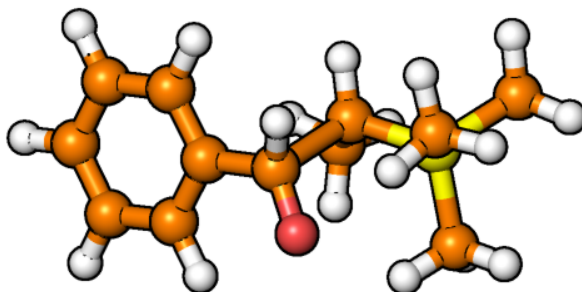
C -0.822664 -0.399655 1.209137	H 2.549057 -1.572582 3.133077	C -1.266131 -2.467979 -0.093974
O -0.785452 0.236433 2.251811	H 1.140617 -0.497627 3.285687	C -1.257414 -4.004669 2.219371
P 2.542357 0.149827 1.454534	H 4.700587 0.966065 2.344579	C -1.502579 -3.833227 -0.172773
C 1.828851 -0.777706 0.238184	H 4.681298 0.882887 0.566850	C -1.494211 -4.605215 0.984475
C 1.888701 1.834974 1.415227	H 4.852191 -0.597073 1.515739	H -0.869213 -2.153442 3.250217
C 2.212318 -0.537055 3.100550	H 1.664308 -0.227818 -0.683314	H -1.255452 -1.861153 -0.991413
C 4.371223 0.380897 1.483671	C 2.108255 -2.255238 0.113614	H -1.256115 -4.605286 3.119695
H -0.835955 0.111200 0.233662	H 3.066891 -2.502501 -0.363034	H -1.688723 -4.296673 -1.132556
H 2.445803 2.477749 2.095744	H 2.098296 -2.751990 1.087061	H -1.673728 -5.670684 0.926149
H 0.839742 1.809024 1.704896	H 1.330358 -2.745210 -0.475394	
H 1.980912 2.227653 0.402617	C -1.028602 -1.860782 1.138927	
H 2.743128 0.027193 3.866325	C -1.033838 -2.638815 2.298175	



TS_{5→6}B-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11181427

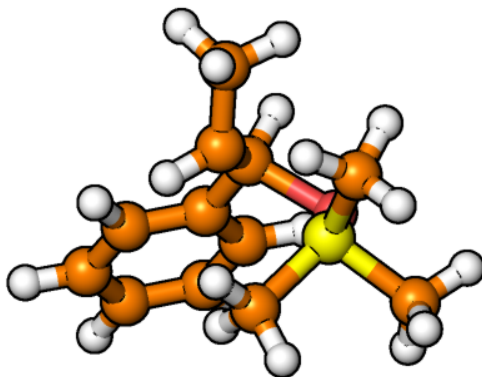
C 0.301035 -0.590845 1.420699	H 3.682864 -0.760671 3.584221	C -0.408318 -4.308875 1.884569
O 0.195341 -0.148257 2.617003	H 2.031521 -0.101823 3.816364	C -1.005260 -3.713490 -0.372278
P 2.939094 0.609336 1.752194	H 5.064232 1.808905 1.828112	C -0.892024 -4.676660 0.627317
C 2.163053 -0.670189 0.817650	H 4.632386 1.344519 0.166020	H 0.315659 -2.689701 3.117480
C 2.017807 2.169411 1.634656	H 5.273892 0.125043 1.285092	H -0.737612 -1.642844 -0.894714
C 3.051876 0.128263 3.491915	C 2.285252 -0.553118 -0.697646	H -0.334923 -5.052301 2.674139
C 4.639963 1.012613 1.207770	H 3.315062 -0.617552 -1.075844	H -1.400901 -3.985089 -1.347360
H 2.520781 -1.633010 1.195424	H 1.723410 -1.365940 -1.168018	H -1.191785 -5.702865 0.434875
H 2.538670 2.957552 2.185917	H 1.855123 0.385633 -1.069079	H -0.031446 0.072264 0.583495
H 1.026588 1.994117 2.062118	C -0.120538 -2.023039 1.130698	
H 1.927921 2.471788 0.587468	C -0.031918 -2.993227 2.134375	
H 3.480369 0.938558 4.089170	C -0.623264 -2.396126 -0.118316	



TS_{5→6}B-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11194915

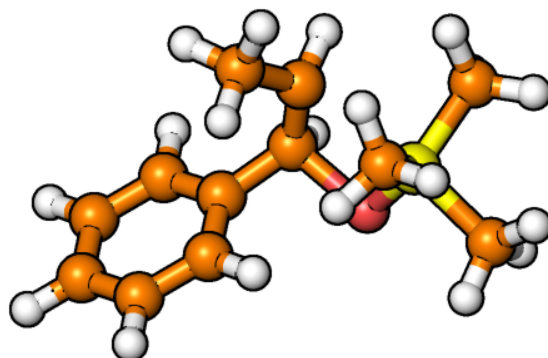
C 0.369731 -0.797988 1.568763	H 2.411302 -0.144243 3.718332	H -0.947926 -5.160949 2.615303
O 0.421608 -0.458242 2.799548	H 5.048569 1.747040 1.231575	H -1.327095 -3.934023 -1.483935
P 2.978763 0.471355 1.501902	H 4.400510 1.191391 -0.332735	H -1.570572 -5.679365 0.268269
C 2.165350 -0.913739 0.771546	H 5.244647 0.049944 0.732605	H -0.002801 -0.045174 0.830160
C 1.956391 1.967006 1.403055	C -0.178562 -2.164447 1.194220	H 2.028754 -0.723624 -0.299118
C 3.351741 0.155953 3.245577	C -0.333987 -3.145790 2.174766	C 2.838939 -2.256858 1.052399
C 4.570670 0.910570 0.710479	C -0.545921 -2.461898 -0.121329	H 2.744293 -2.531215 2.108820
H 2.513815 2.826782 1.785629	C -0.829367 -4.405541 1.842835	H 2.338692 -3.040386 0.477420
H 1.061324 1.798637 2.007718	C -1.041755 -3.718505 -0.457652	H 3.906264 -2.296649 0.789022
H 1.673430 2.160500 0.364680	C -1.180930 -4.698654 0.526045	
H 3.751805 1.060207 3.713527	H -0.074761 -2.893180 3.198327	
H 4.089387 -0.646279 3.331458	H -0.447629 -1.696690 -0.889708	



TS_{7→8}B-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11244721

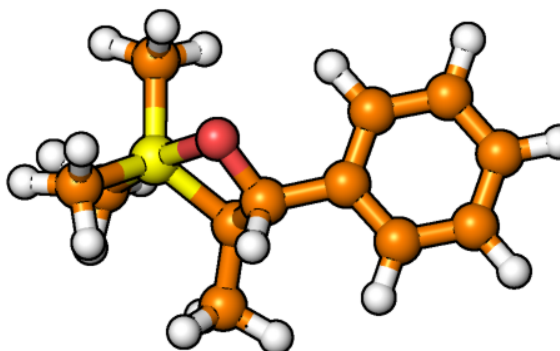
O -0.065408 -0.189319 -0.056554	H 0.499542 0.373638 -2.690706	H 1.062246 -1.835706 3.582502
C 0.014831 -0.140389 1.705126	H 0.685793 -1.363254 -2.405984	H -2.100069 -1.522484 0.703548
C 1.344137 0.318908 1.968606	H 2.812431 1.619659 -1.598922	H 0.251025 -4.068396 4.237966
P 1.453053 -0.063580 -0.464482	H 3.094819 1.639614 0.166498	H -2.941471 -3.741072 1.384343
H -0.781682 0.599939 1.807692	H 1.620801 2.349826 -0.504991	H -1.759687 -5.037591 3.146434
C 2.638292 -1.415543 -0.093989	H 2.014506 -0.402408 2.433492	C 1.534607 1.739235 2.476088
C 1.161829 -0.388442 -2.270058	C -0.450365 -1.519800 2.084772	H 1.260221 1.858557 3.536616
C 2.341797 1.534765 -0.613572	C 0.197157 -2.255938 3.081765	H 2.578188 2.066816 2.391863
H 3.076072 -1.814636 -1.015459	C -1.591509 -2.075060 1.486392	H 0.929414 2.461771 1.913849
H 2.101457 -2.220612 0.415155	C -0.268287 -3.515602 3.460313	
H 3.427796 -1.058632 0.567933	C -2.058323 -3.328463 1.863795	
H 2.107381 -0.375816 -2.824352	C -1.395434 -4.057693 2.852039	



TS_{7→8}B-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.10969626

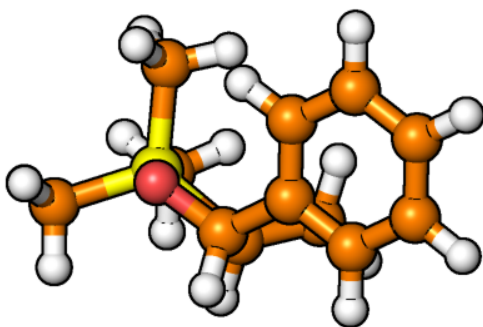
O -0.044754 -0.309615 0.030140	H -0.026173 0.905043 -2.431502	H -0.039425 -2.826870 0.468540
C 0.274385 -0.371192 1.754158	H 0.290356 -0.819711 -2.664853	H -2.016566 -2.734091 5.006940
C 1.696217 -0.227489 1.875927	H 2.342543 2.099256 -1.411580	H -1.055943 -4.867758 1.406543
P 1.355436 0.006672 -0.614451	H 3.057145 1.580473 0.146720	H -2.055293 -4.838129 3.680864
H -0.310276 0.515293 2.001499	H 1.447287 2.313042 0.108744	C 2.568074 -1.351991 2.406105
C 2.654723 -1.264941 -0.845772	C -0.414390 -1.622221 2.209953	H 2.457021 -1.513506 3.490345
C 0.739539 0.128344 -2.356142	C -0.990407 -1.615470 3.486375	H 2.360228 -2.315917 1.930312
C 2.135753 1.656619 -0.430383	C -0.449571 -2.808074 1.471331	H 3.629943 -1.133540 2.234238
H 3.049921 -1.215821 -1.866579	C -1.574583 -2.762949 4.015068	H 2.006974 0.758677 2.224217
H 2.212760 -2.254307 -0.696943	C -1.034501 -3.957029 1.998600	
H 3.464690 -1.142415 -0.128835	C -1.597143 -3.942154 3.272904	
H 1.558353 0.370568 -3.043015	H -0.974865 -0.700790 4.073974	



6B-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.15473882

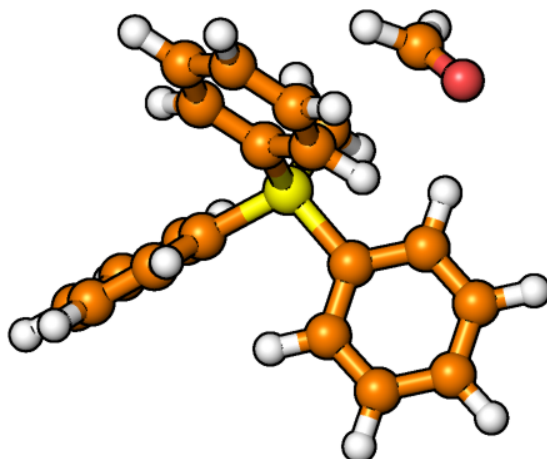
O -0.189928 0.048567 -0.555578	H 0.839671 2.100726 -2.403742	H 0.021683 0.694940 3.437479
C 0.229202 0.294388 0.765442	H -0.211116 0.762877 -2.862614	H -2.579324 4.018898 0.873718
C 1.684232 0.696863 0.457759	H 3.460719 0.019863 -2.834383	H -1.174961 2.498297 4.623022
P 1.494868 0.076439 -1.290487	H 3.965733 -0.287858 -1.172051	H -2.478968 4.171583 3.343083
C 1.448615 -1.726181 -1.575991	H 3.595033 1.358934 -1.688460	H 1.755999 1.786149 0.388787
C 0.822553 1.047137 -2.688085	C -0.572543 1.350420 1.481874	C 2.788489 0.163410 1.351095
C 3.301594 0.311791 -1.795418	C -1.316507 2.288482 0.770396	H 2.646605 0.523266 2.372773
H 0.217190 -0.623815 1.372681	C -0.535469 1.433734 2.873312	H 2.788034 -0.927922 1.383460
H 0.438638 -2.020029 -1.847460	C -1.999242 3.299238 1.437438	H 3.772969 0.494140 1.022688
H 1.702850 -2.229247 -0.641673	C -1.212533 2.446454 3.542166	
H 2.163235 -2.034504 -2.337098	C -1.945863 3.385529 2.824542	
H 1.422212 0.922973 -3.587868	H -1.364554 2.201263 -0.306014	



6B-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.15429410

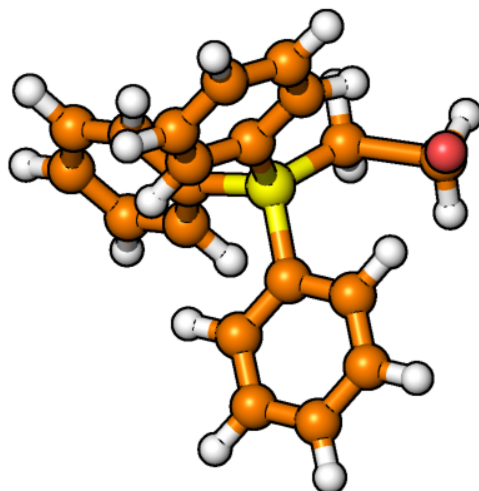
O -0.104117 -0.239613 -0.276390	H 0.547451 2.183849 -1.912223	C -0.422251 1.789453 2.831439
C 0.302290 0.243102 0.981407	H -0.398193 0.820584 -2.507285	C -2.125029 3.173853 1.140645
C 1.769188 0.595305 0.619767	H 3.331461 0.244016 -2.821774	C -1.145039 2.872483 3.313499
P 1.471942 0.098591 -1.155639	H 3.963721 -0.019464 -1.192545	C -1.997674 3.572920 2.465803
C 1.528993 -1.648221 -1.692622	H 3.414654 1.586105 -1.679902	H -1.503310 1.760767 -0.361624
C 0.612237 1.185352 -2.346418	H 2.458666 -0.140742 1.042036	H 0.233457 1.241368 3.498744
C 3.211054 0.518721 -1.773035	C 2.296378 1.993992 0.898054	H -2.798194 3.704177 0.479015
H 0.273342 -0.555707 1.734492	H 2.282635 2.198833 1.969344	H -1.048495 3.167934 4.350270
H 0.517403 -2.007958 -1.856826	H 3.322718 2.103243 0.550610	H -2.564016 4.415883 2.839159
H 1.963583 -2.234840 -0.881618	H 1.686626 2.760275 0.419634	
H 2.142197 -1.779426 -2.582115	C -0.530225 1.393921 1.497920	
H 1.156656 1.253081 -3.286258	C -1.396292 2.090535 0.661058	



5C-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1188.49037674

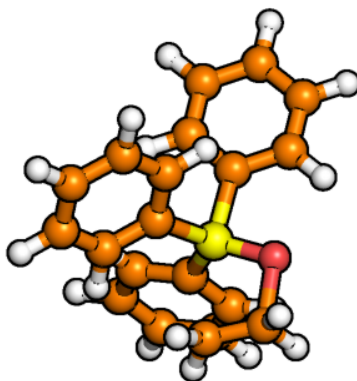
H 2.583113 1.136794 2.001244	H -3.474561 -2.371755 -4.272790	C -0.798494 2.465256 -1.422855
H 1.043564 -1.116727 0.861601	H -1.413157 -3.340112 -3.303971	C -1.797788 -0.362375 1.567665
H -3.556957 -0.959758 0.478947	H -0.277635 -2.193887 -1.420224	C -1.065651 1.925580 -0.162029
H -4.826200 -1.587918 2.485306	H 1.487812 0.174224 -0.371391	C -2.873247 -0.067320 -1.861998
H -3.798964 -1.364941 4.727512	H 1.557430 2.396315 1.087479	C -3.505167 -0.699912 -2.924864
H -1.487606 -0.499119 4.941548	C -3.102763 -0.848472 1.452048	C -2.982904 -1.881341 -3.443152
H -0.219264 0.149153 2.935937	C -3.818750 -1.207332 2.586113	C -1.824899 -2.425318 -2.899217
H -1.578401 2.373716 1.878033	C -3.240188 -1.084212 3.844509	C -1.190580 -1.789079 -1.838459
H -1.703605 4.801012 1.514659	C -1.942353 -0.601613 3.965291	C -1.711925 -0.611157 -1.307275
H -1.230683 5.751759 -0.723229	C -1.219719 -0.240833 2.834922	C 0.797422 -0.176618 0.385734
H -0.642353 4.248762 -2.600723	C -1.393216 2.776498 0.893478	P -0.833028 0.146586 0.119788
H -0.552250 1.812226 -2.249246	C -1.453838 4.148919 0.688717	C 1.726596 1.829314 2.015897
H -3.279818 0.854548 -1.468563	C -1.184303 4.681943 -0.566794	O 1.077750 2.030835 3.019277
H -4.402403 -0.271059 -3.350946	C -0.854105 3.838355 -1.622265	



TS_{5→6}C-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1188.48014226

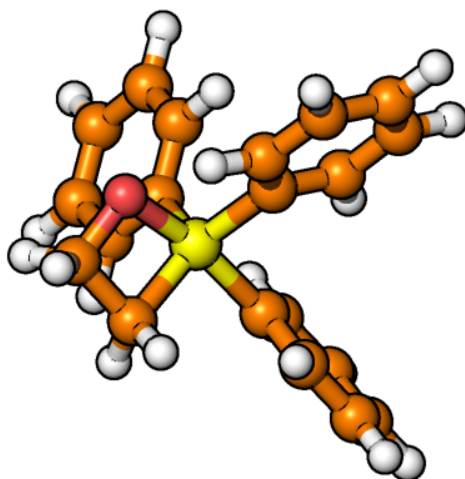
H 2.933723 0.197438 0.232452	H -4.031517 -2.565365 -4.041494	C -0.074945 2.923934 -0.456667
H 0.878966 -1.202813 -0.506955	H -2.991187 -3.742083 -2.124512	C -1.465740 -0.115809 1.443984
H -3.291194 -1.119089 0.891049	H -1.697386 -2.484920 -0.459385	C -1.169081 2.060196 -0.411184
H -4.008230 -1.502823 3.208688	H 1.099711 0.322786 -1.421739	C -2.597221 0.083440 -2.484383
H -2.611996 -0.703605 5.089341	H 1.857041 -0.409715 1.571661	C -3.317767 -0.634538 -3.432139
H -0.500842 0.507820 4.629913	C -2.668644 -0.775294 1.703312	C -3.469325 -2.009016 -3.303437
H 0.221695 0.927177 2.312706	C -3.077097 -0.987823 3.014151	C -2.885708 -2.670013 -2.226208
H -3.319767 1.912585 -0.321729	C -2.293235 -0.535970 4.068865	C -2.161158 -1.958134 -1.282685
H -3.680458 4.340900 -0.474786	C -1.105715 0.141263 3.811580	C -2.021656 -0.569083 -1.392825
H -1.741549 5.875484 -0.614174	C -0.686331 0.360894 2.506441	C 0.761634 -0.120043 -0.486198
H 0.559715 4.964323 -0.555883	C -2.469698 2.577430 -0.399403	P -0.911606 0.287032 -0.231240
H 0.930021 2.539126 -0.354871	C -2.673639 3.945187 -0.479483	C 2.091160 0.443702 0.905545
H -2.478127 1.150712 -2.602107	C -1.581349 4.806716 -0.554774	O 1.953621 1.619635 1.329240
H -3.758654 -0.115781 -4.272930	C -0.290623 4.296574 -0.532038	



TS_{7→8}C-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1188.49813015

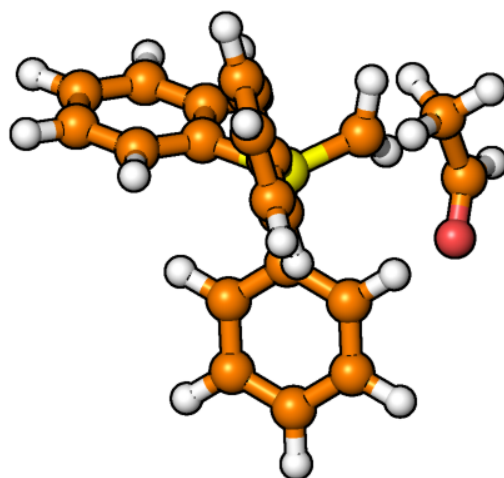
H 2.484101 1.014362 2.085436	H 1.334504 2.833399 -0.189790	H 1.504075 0.502439 -6.478850
H -0.041620 -0.599148 1.482258	H 5.015859 0.772881 -0.964375	C 2.843765 0.182038 -4.828971
H 5.709761 -2.832940 0.798029	H 6.245918 2.878301 -0.719919	C 2.964439 0.088409 -3.450522
H 4.493327 -0.695311 0.737788	H 5.040335 4.981845 -0.214376	C 1.849920 0.239015 -2.620409
H 1.652743 -2.388160 -1.984674	C 3.110755 4.035382 -0.175919	C 0.608467 0.487049 -3.206211
H 2.793388 -4.563587 -1.821112	C 2.410539 2.844318 -0.300282	C 0.486003 0.581294 -4.589422
H 4.848868 -4.788696 -0.457187	C 3.088244 1.651478 -0.566270	C 1.600571 0.429845 -5.403520
C 4.818996 -2.738670 0.191117	C 4.474262 1.677453 -0.730710	H 2.321947 -0.808109 2.080522
C 4.149492 -1.526164 0.140216	C 5.170771 2.871966 -0.597215	H 0.096164 1.196081 1.490466
C 3.008673 -1.383250 -0.652396	C 4.494619 4.053618 -0.316843	P 2.078649 0.169544 -0.789030
C 2.531815 -2.486841 -1.362702	H 3.717718 0.060650 -5.455414	C 1.974669 0.142104 1.700395
C 3.182733 -3.712396 -1.278539	H 3.936298 -0.111828 -3.019885	C 0.610160 0.254073 1.335918
C 4.334388 -3.838688 -0.513332	H -0.257426 0.600438 -2.572287	O 0.570536 0.262623 -0.387978
H 2.574281 4.951750 0.032106	H -0.484645 0.771618 -5.028624	



6C-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1188.53119765

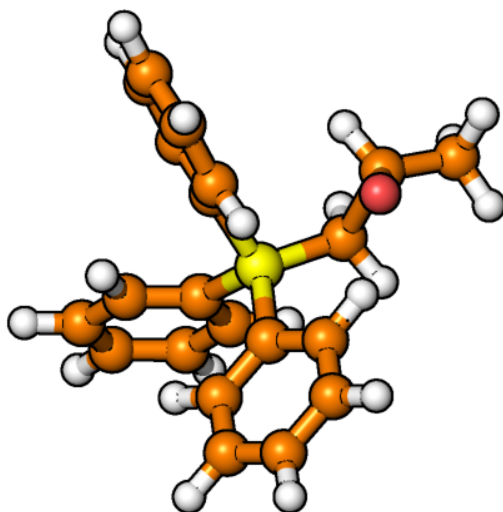
H 1.962635 1.366279 1.905938	H 4.239137 -1.634708 -1.039132	H 1.899729 4.286745 -4.428543
H -0.443766 0.965350 1.850881	H 3.833206 2.264110 0.690052	C 2.883708 2.551791 -3.628136
H 1.832502 -4.625036 -0.060751	H 6.259735 2.388637 0.984805	C 2.901472 1.606906 -2.613019
H 2.230737 -2.372938 0.831885	H 7.703841 0.505943 0.260098	C 1.918326 1.608704 -1.617595
H 1.148510 -0.678618 -2.954797	C 6.048248 -0.677174 -0.429806	C 0.928140 2.591827 -1.655706
H 0.793741 -2.940265 -3.858849	C 4.665466 -0.751316 -0.586110	C 0.932812 3.560326 -2.653687
H 1.125061 -4.925388 -2.415002	C 3.835997 0.293503 -0.179664	C 1.904305 3.539587 -3.645273
C 1.686785 -3.763273 -0.698699	C 4.442940 1.420921 0.386021	H 2.207659 -0.374064 2.083083
C 1.903915 -2.487216 -0.192752	C 5.818715 1.502333 0.546546	H -0.190279 -0.767255 1.547888
C 1.718450 -1.365479 -1.001119	C 6.630074 0.447379 0.138501	P 1.933291 0.306368 -0.314872
C 1.311817 -1.540470 -2.323245	H 3.642062 2.523521 -4.399837	C 1.668839 0.389744 1.524078
C 1.105856 -2.817154 -2.830254	H 3.684376 0.863173 -2.596933	C 0.168815 0.240440 1.309022
C 1.290847 -3.931940 -2.020091	H 0.148650 2.576405 -0.910916	O 0.148620 0.494777 -0.085510
H 6.668446 -1.501725 -0.757835	H 0.165887 4.324120 -2.660361	



5C-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.76235625

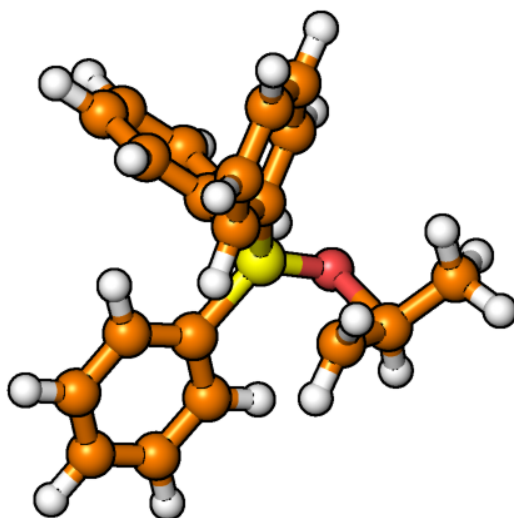
H 3.033427 0.470296 2.443350	H 0.282676 1.014214 -2.050892	C 0.099530 3.100639 -1.600420
H 1.389541 -1.859137 1.163465	H -2.743301 0.464716 -1.196119	C 0.023890 1.747893 -1.298817
H 2.200596 3.138708 1.101313	H -4.040049 -0.609480 -2.996846	C -1.339235 -0.742058 1.860889
H 2.738850 1.662672 0.256766	H -3.391621 -2.848946 -3.825752	C -0.391805 1.329753 -0.031431
H 3.885561 2.565509 1.239622	H -1.434649 -4.007734 -2.849738	C -2.458857 -0.516919 -1.551069
C 2.837521 2.260436 1.162387	H -0.121311 -2.910808 -1.049783	C -3.188991 -1.120815 -2.566515
H -3.124108 -1.384174 0.843782	H 1.968536 -0.661214 -0.113809	C -2.823874 -2.380584 -3.032532
H -4.410545 -1.736976 2.907196	C -2.662542 -1.184907 1.799046	C -1.724616 -3.031645 -2.484286
H -3.369882 -1.301696 5.111260	C -3.388745 -1.386805 2.965824	C -0.992159 -2.423650 -1.471060
H -1.025637 -0.508056 5.230281	C -2.802677 -1.145124 4.203080	C -1.356555 -1.167740 -0.991669
H 0.264083 -0.148037 3.163380	C -1.486172 -0.703068 4.271020	C 1.230999 -0.932316 0.629510
H -1.047966 1.973525 1.910766	C -0.753383 -0.502876 3.108187	P -0.347934 -0.442404 0.370463
H -0.947370 4.368786 1.363149	C -0.741504 2.283380 0.922891	C 2.488030 1.426220 2.359169
H -0.199988 5.102320 -0.881329	C -0.676718 3.636801 0.614252	O 1.700413 1.761117 3.213803
H 0.427942 3.416212 -2.581823	C -0.253893 4.047843 -0.644215	



TS_{5→6}C-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.74992720

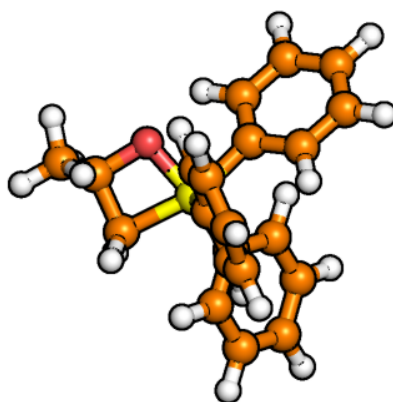
H 1.976853 2.272877 0.081609	H -0.116471 2.119973 -2.743932	C -0.278171 4.198873 -2.263383
H 1.053808 -0.697534 0.682998	H -2.836511 1.389210 -2.116345	C -0.338726 2.843910 -1.971643
H 3.955380 1.678720 1.644130	H -3.920305 0.184204 -3.972528	C -1.680819 0.312047 1.135481
H 3.722418 0.539100 0.304803	H -3.105121 -2.054208 -4.642213	C -0.689029 2.417193 -0.687524
H 3.166026 0.129952 1.948802	H -1.203519 -3.085955 -3.440325	C -2.483184 0.407700 -2.399507
C 3.276523 0.934328 1.220104	H -0.120792 -1.879813 -1.575064	C -3.091281 -0.270469 -3.447069
H -3.412001 -0.275581 -0.010807	H 1.571860 0.027877 -0.884542	C -2.632751 -1.529300 -3.822697
H -4.801987 -0.720451 1.964695	C -2.999423 -0.123689 0.975738	C -1.564595 -2.109286 -3.148500
H -3.871933 -0.397157 4.236418	C -3.784140 -0.377382 2.091840	C -0.955038 -1.432872 -2.098804
H -1.541542 0.389000 4.515769	C -3.259414 -0.195936 3.367274	C -1.409820 -0.171033 -1.717041
H -0.134156 0.875050 2.528352	C -1.949188 0.240795 3.524515	C 1.011093 0.174882 0.036142
H -1.193508 3.035600 1.307710	C -1.148966 0.494185 2.416434	P -0.632975 0.652197 -0.292802
H -1.109163 5.438225 0.780632	C -0.963285 3.357126 0.304756	C 1.929818 1.614680 0.975354
H -0.511833 6.191315 -1.499546	C -0.902418 4.712575 0.005967	O 1.286415 2.037260 1.983941
H -0.005590 4.523861 -3.258382	C -0.561863 5.134230 -1.273250	



TS_{7→8}C-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.76340682

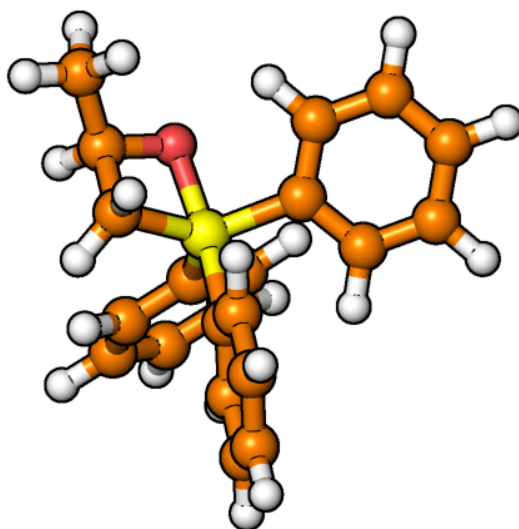
H -0.401394 1.699209 1.613396	C 2.631349 -3.134851 -0.892735	H -0.498544 1.610398 -2.479890
H -0.906665 -0.545170 2.751282	C 3.841672 -3.237781 -0.219578	H -0.621750 1.841778 -4.935960
H -0.108083 -1.348535 1.396710	H 2.155176 5.564859 0.325836	H 1.314553 1.199542 -6.341123
H -1.604401 -0.438660 1.125660	H 0.929060 3.434004 0.143246	C 2.520614 0.612222 -4.661876
C -0.672567 -0.462131 1.687350	H 4.548538 1.464209 -1.040093	C 2.584947 0.487956 -3.280898
H 1.972222 1.683305 2.179064	H 5.773972 3.575590 -0.811306	C 1.501162 0.848634 -2.475531
H 5.356157 -2.175693 0.875591	H 4.590064 5.641155 -0.128782	C 0.347840 1.338004 -3.091707
H 4.202644 -0.006965 0.733621	C 2.682955 4.664171 0.041312	C 0.281855 1.463816 -4.475225
H 1.079524 -1.817744 -1.572363	C 1.990792 3.466396 -0.061308	C 1.366979 1.103200 -5.264395
H 2.172658 -4.014457 -1.324318	C 2.657429 2.295233 -0.428111	H 1.944935 -0.141265 2.194167
H 4.332114 -4.197494 -0.126386	C 4.021822 2.349004 -0.714784	P 1.662911 0.796375 -0.629401
C 4.417323 -2.100742 0.343384	C 4.713930 3.547944 -0.595704	C 1.533569 0.774687 1.790849
C 3.781320 -0.872874 0.244165	C 4.049402 4.708288 -0.216473	C 0.149838 0.775922 1.465545
C 2.578532 -0.758648 -0.454963	H 3.369343 0.322696 -5.267776	O 0.140273 0.868232 -0.295981
C 2.009174 -1.898479 -1.025069	H 3.485872 0.093048 -2.831257	



7C-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.79278823

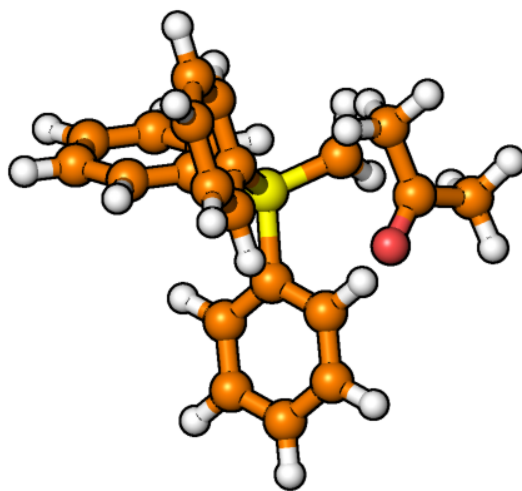
H -0.738933 -0.277120 1.565998	C 4.193117 -3.350618 -0.943282	H -0.253298 -0.933970 -1.976350
H 1.993634 0.591589 2.404339	C 4.986875 -3.455834 0.189592	H -0.415026 -1.232974 -4.413579
H 0.446920 2.542055 1.697744	H 2.328017 4.919521 -0.757318	H 1.441916 -0.501697 -5.883037
H -0.553010 1.767835 2.934751	H 1.169371 2.742244 -0.783233	C 2.649258 0.193202 -4.244995
H -1.248302 2.166054 1.357627	H 4.771761 0.813703 0.490360	C 2.741266 0.345034 -2.867291
C -0.348282 1.815437 1.863623	H 5.926337 2.977128 0.516095	C 1.702245 -0.057123 -2.025749
H 5.459164 -2.589027 2.099528	H 4.714570 5.047334 -0.101876	C 0.566845 -0.624043 -2.606522
H 3.817269 -0.791834 1.903543	C 2.862087 4.022425 -0.472962	C 0.474262 -0.788382 -3.985071
H 2.695600 -2.234850 -1.972421	C 2.206391 2.798965 -0.483150	C 1.514768 -0.379315 -4.810093
H 4.275492 -4.083983 -1.735243	C 2.878137 1.629367 -0.120950	H 1.438680 -1.071189 2.113611
H 5.696578 -4.266980 0.287368	C 4.223091 1.707668 0.235125	P 1.908885 0.071946 -0.153912
C 4.852568 -2.515109 1.206114	C 4.880364 2.933469 0.242534	C 1.429151 -0.053007 1.732632
C 3.927095 -1.489092 1.085413	C 4.201970 4.094387 -0.107071	C 0.052061 0.445292 1.351032
C 3.145071 -1.343556 -0.068075	H 3.464837 0.520639 -4.876881	O 0.258481 0.454097 -0.086356
C 3.289297 -2.300173 -1.074521	H 3.636849 0.781484 -2.446485	



6C-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.79609506

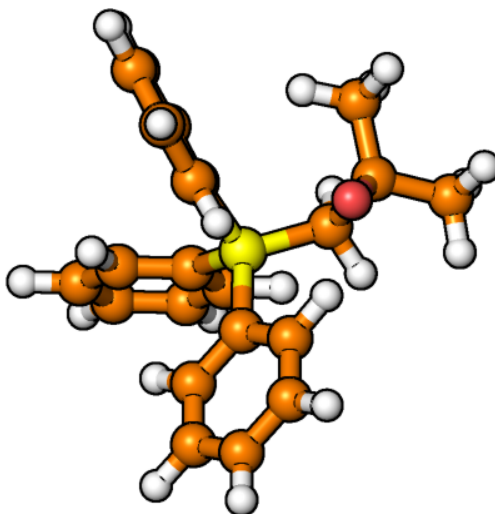
H -0.154424 -0.864847 1.495104	C 1.223896 -2.848696 -2.891650	H 0.088460 2.497159 -0.929703
H 1.926128 1.317287 1.889106	C 1.435049 -3.965631 -2.091014	H 0.071052 4.263219 -2.659818
H -0.428123 2.162864 1.841110	H 6.721248 -1.400874 -0.776176	H 1.821791 4.295378 -4.411655
H -0.717161 0.945732 3.098026	H 4.298353 -1.594142 -1.076404	C 2.848248 2.581317 -3.619552
H -1.776380 1.029179 1.682014	H 3.777247 2.267917 0.703065	C 2.884151 1.626698 -2.613964
C -0.745589 1.133369 2.022047	H 6.197512 2.453053 1.015797	C 1.892619 1.589178 -1.627638
H 1.979033 -4.662169 -0.133459	H 7.696074 0.619425 0.276293	C 0.874381 2.543323 -1.665923
H 2.299315 -2.408180 0.785684	C 6.077139 -0.597679 -0.441300	C 0.860010 3.522161 -2.653646
H 1.202706 -0.708549 -2.994159	C 4.697845 -0.706221 -0.608016	C 1.840791 3.540462 -3.636086
H 0.925978 -2.970680 -3.924604	C 3.837648 0.310283 -0.193261	H 2.205523 -0.418813 2.052882
H 1.304043 -4.959540 -2.497752	C 4.411052 1.445563 0.391433	P 1.933748 0.272756 -0.338195
C 1.812798 -3.798682 -0.763995	C 5.783112 1.561424 0.562571	C 1.657332 0.337950 1.493462
C 1.985869 -2.521964 -0.243161	C 6.625093 0.534070 0.146166	C 0.155824 0.166153 1.280082
C 1.773681 -1.398072 -1.041856	H 3.614444 2.583052 -4.384014	O 0.147419 0.405519 -0.122383
C 1.385711 -1.571557 -2.369634	H 3.688869 0.906695 -2.597935	



5C-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.03224832

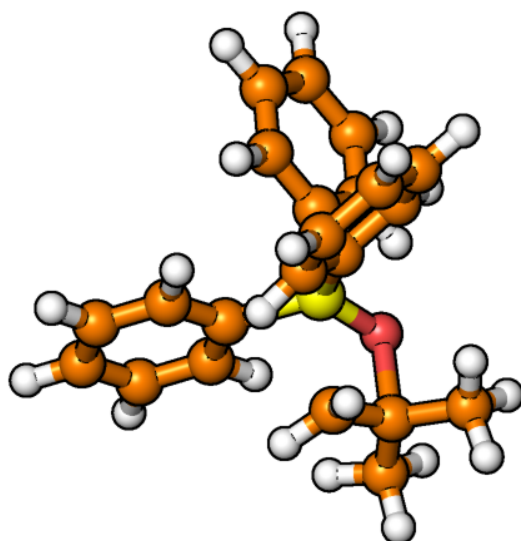
H 0.836963 -1.638850 0.551898	H -0.572085 5.472531 -1.208931	C -0.647793 4.416620 -0.984279
H 1.777300 3.604317 0.785798	H 0.049629 3.794152 -2.919939	C -0.297123 3.473637 -1.946476
H 2.181886 1.971622 0.208465	H -0.143678 1.389649 -2.417562	C -0.399466 2.119807 -1.661027
H 3.430450 2.951347 0.972082	H -3.307205 0.966659 -1.413821	C -1.793606 -0.379132 1.481959
C 2.364714 2.713977 0.987674	H -4.737846 0.034324 -3.192957	C -0.839040 1.695540 -0.403164
H 3.803070 0.986445 2.588812	H -4.215962 -2.177120 -4.172109	C -3.078344 -0.003314 -1.835050
H 2.391176 0.061676 2.069224	H -2.252768 -3.451377 -3.368182	C -3.883874 -0.527243 -2.837296
H 2.503689 0.618199 3.761599	H -0.804498 -2.496560 -1.590923	C -3.590082 -1.771469 -3.388040
C 2.726665 0.869743 2.727272	H 1.423953 -0.360157 -0.638154	C -2.487337 -2.487271 -2.936922
H -3.599505 -1.081134 0.546435	C -3.106171 -0.855339 1.479644	C -1.679083 -1.958764 -1.936654
H -4.795073 -1.431768 2.664908	C -3.781441 -1.054359 2.677775	C -1.970874 -0.718785 -1.374329
H -3.685004 -0.923780 4.818708	C -3.156395 -0.772237 3.886734	C 0.706547 -0.656952 0.116423
H -1.359613 -0.066010 4.832740	C -1.850059 -0.295126 3.896259	P -0.858090 -0.085812 -0.046937
H -0.156908 0.268615 2.710295	C -1.168418 -0.104192 2.702163	C 1.978354 2.113072 2.316274
H -1.512079 2.331429 1.536496	C -1.186749 2.643896 0.555813	O 1.084183 2.572892 2.994784
H -1.358135 4.726615 1.018990	C -1.094123 3.999622 0.263204	



TS_{5→6}C-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.01349794

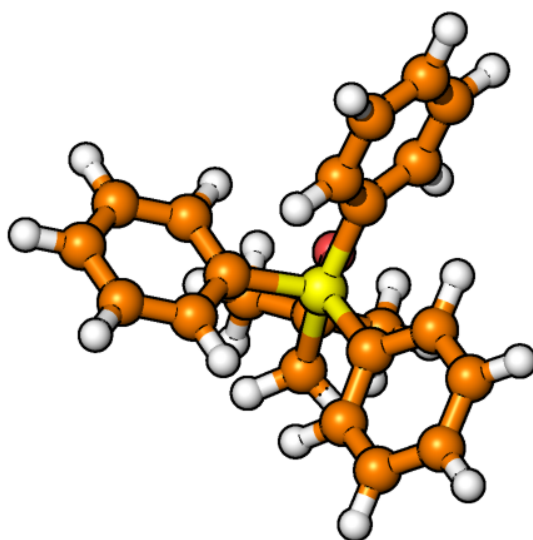
H 0.767257 -1.087050 1.067483	H -0.996300 5.827111 -1.051638	C -1.009514 4.771268 -0.814768
H 1.588947 2.590036 -0.078997	H -0.580290 4.154459 -2.829068	C -0.776489 3.833302 -1.815059
H 2.901305 1.422624 -0.356614	H -0.600776 1.754967 -2.289747	C -0.789183 2.479839 -1.509843
H 3.058222 2.679468 0.882651	H -3.221948 0.925832 -1.509416	C -1.911505 -0.072343 1.655893
C 2.358293 1.990818 0.401917	H -4.322542 -0.314721 -3.330589	C -1.035834 2.057938 -0.200698
H 3.550857 0.763423 2.618517	H -3.417827 -2.497243 -4.068899	C -2.828368 -0.030845 -1.822643
H 3.309838 -0.453670 1.351826	H -1.409239 -3.435436 -2.969104	C -3.446226 -0.728948 -2.850686
H 2.332024 -0.492868 2.840360	H -0.309689 -2.195346 -1.139632	C -2.937284 -1.956108 -3.264822
C 2.801913 0.157168 2.102070	H 1.275487 -0.313652 -0.463724	C -1.809149 -2.483390 -2.648113
H -3.606184 -0.830838 0.554630	C -3.193185 -0.616455 1.529025	C -1.189343 -1.786716 -1.617503
H -4.928339 -1.326359 2.562423	C -3.939625 -0.899881 2.664266	C -1.693707 -0.556319 -1.197703
H -3.996891 -0.865480 4.809598	C -3.413927 -0.641389 3.925812	C 0.757856 -0.170034 0.482748
H -1.730573 0.105413 5.030514	C -2.139857 -0.099472 4.050024	P -0.908092 0.300439 0.201588
H -0.386466 0.639083 3.001310	C -1.377190 0.184895 2.923267	C 1.752573 1.111778 1.508331
H -1.408049 2.684962 1.820811	C -1.260694 3.000905 0.801320	O 1.017663 1.724286 2.359901
H -1.419233 5.081800 1.270215	C -1.252444 4.353894 0.488148	



TS_{7→8}C-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.02854657

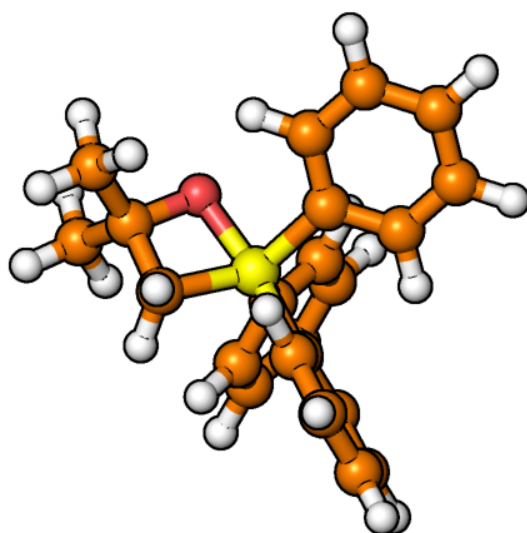
H 0.310446	2.348684	1.514600	C 2.933303	-1.355827	-0.626304	H 3.995666	0.026906	-2.920984
H -0.429174	1.424186	2.820458	C 2.388622	-2.429588	-1.334097	H -0.234305	0.572101	-2.627198
H -1.184396	1.438817	1.218506	C 2.973615	-3.688439	-1.267604	H -0.384463	0.697315	-5.092775
C -0.231026	1.433624	1.745191	C 4.129988	-3.881518	-0.522692	H 1.661759	0.483937	-6.471175
H -0.290161	-1.266972	2.642999	H 2.597735	5.069884	-0.390922	C 2.954975	0.242783	-4.770649
H 0.481756	-1.917900	1.194477	H 1.341562	2.955465	-0.553365	C 3.030626	0.176831	-3.387295
H -1.085646	-1.099471	1.068553	H 5.035109	0.781854	-0.673696	C 1.884648	0.294421	-2.595610
C -0.122243	-1.096463	1.576285	H 6.278884	2.884838	-0.514508	C 0.656784	0.483048	-3.229571
H 2.425169	1.166112	2.001436	H 5.076355	5.044603	-0.357781	C 0.577388	0.551504	-4.618038
H 5.578064	-2.958393	0.769645	C 3.132582	4.130400	-0.439982	C 1.723754	0.431520	-5.392051
H 4.477121	-0.763012	0.745020	C 2.422616	2.940910	-0.525879	H 2.448604	-0.654985	2.011605
H 1.506813	-2.278926	-1.941449	C 3.095913	1.717888	-0.587140	P 2.057218	0.239043	-0.740139
H 2.530472	-4.513944	-1.808703	C 4.491046	1.710775	-0.593667	C 1.998905	0.246863	1.619978
H 4.594784	-4.857582	-0.481871	C 5.196837	2.904590	-0.509060	C 0.590026	0.218952	1.404924
C 4.682857	-2.814078	0.179209	C 4.523095	4.117601	-0.425127	O 0.538196	0.340911	-0.415698
C 4.076272	-1.566839	0.146451	H 3.854529	0.147412	-5.364854			



7C-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.05806713

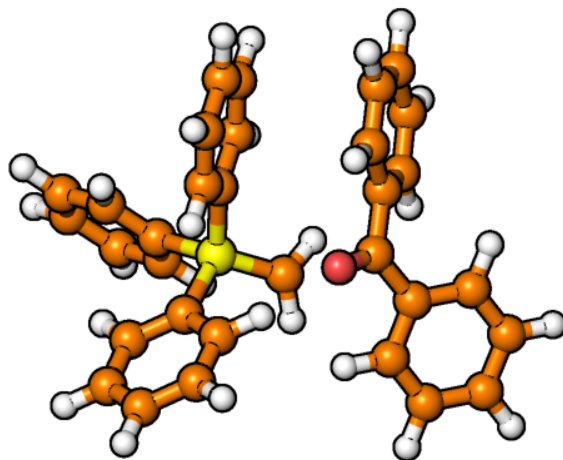
H 2.012355 0.710062 2.373879	C 3.136862 -1.356060 -0.066447	H 3.705674 0.702706 -2.408807
H -1.129572 -0.783798 2.768132	C 3.210960 -2.348885 -1.044691	H -0.267202 -0.831877 -2.020943
H -0.643621 -1.672228 1.316758	C 4.094199 -3.416990 -0.916535	H -0.399055 -1.103312 -4.462909
H -1.928062 -0.459438 1.221222	C 4.938848 -3.500463 0.181025	H 1.516158 -0.450527 -5.893497
C -0.973938 -0.702648 1.691157	H 2.273613 4.921819 -0.765157	C 2.725558 0.173619 -4.228613
H 0.371590 2.492746 1.631003	H 1.148586 2.727447 -0.789912	C 2.797970 0.312045 -2.848758
H -0.560636 1.734358 2.925979	H 4.783314 0.853148 0.475494	C 1.726444 -0.045132 -2.027018
H -1.313655 2.029997 1.352502	H 5.907170 3.033245 0.489586	C 0.577297 -0.554530 -2.633481
C -0.386016 1.741595 1.848906	H 4.661684 5.085105 -0.121397	C 0.502355 -0.704264 -4.015344
H 5.522208 -2.578832 2.033781	C 2.822722 4.032915 -0.483347	C 1.575280 -0.339564 -4.818618
H 3.905630 -0.753982 1.853628	C 2.185579 2.799375 -0.491519	H 1.573008 -1.001272 2.193327
H 2.577702 -2.296680 -1.916314	C 2.875908 1.640408 -0.130798	P 1.922582 0.071882 -0.147763
H 4.122543 -4.179886 -1.683581	C 4.220738 1.738724 0.220418	C 1.485743 -0.011460 1.751890
H 5.634580 -4.323887 0.274494	C 4.860174 2.974048 0.222133	C 0.062408 0.365566 1.380334
C 4.874861 -2.521740 1.168289	C 4.163133 4.124893 -0.124119	O 0.273871 0.390357 -0.068554
C 3.966701 -1.479404 1.055160	H 3.567751 0.465047 -4.843059	



6C-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.06059342

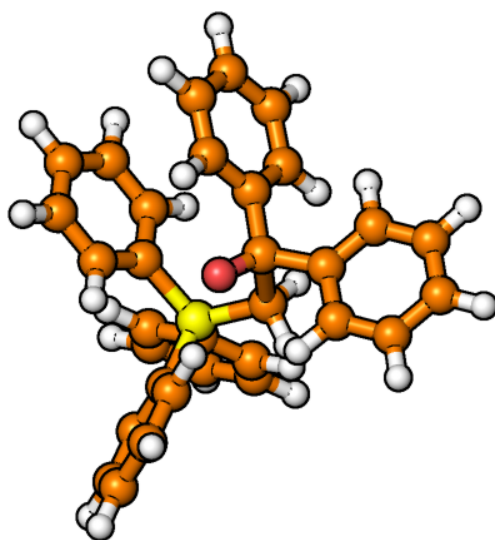
H 1.999475 1.161008 1.968670	C 1.787526 -1.465095 -1.064967	H 3.667275 0.870434 -2.561304
H -0.533834 -1.177911 2.854837	C 1.288331 -1.612829 -2.358060	H 0.043437 2.413047 -0.898508
H -0.046718 -1.947952 1.333892	C 1.153464 -2.877163 -2.918112	H 0.030295 4.205552 -2.596682
H -1.594380 -1.110924 1.438425	C 1.500871 -4.008240 -2.188129	H 1.793085 4.274962 -4.335769
C -0.554648 -1.087321 1.766757	H 6.752503 -1.325684 -0.795427	C 2.823125 2.554151 -3.562952
H -0.135471 2.347890 1.570952	H 4.341327 -1.589183 -1.107963	C 2.858473 1.585388 -2.570706
H -0.619204 1.395087 2.981970	H 3.688585 2.193675 0.792793	C 1.861484 1.527859 -1.590793
H -1.654870 1.444589 1.546859	H 6.098784 2.450373 1.114367	C 0.837172 2.475368 -1.624060
C -0.619896 1.424053 1.890393	H 7.659420 0.690968 0.322937	C 0.823783 3.469709 -2.596500
H 2.263675 -4.741899 -0.318452	C 6.082003 -0.556104 -0.434245	C 1.811113 3.508684 -3.571795
H 2.540389 -2.507281 0.660742	C 4.706996 -0.705741 -0.605484	H 2.077074 -0.598295 2.023196
H 0.996603 -0.740077 -2.925217	C 3.810749 0.264190 -0.156356	P 1.901865 0.192573 -0.317187
H 0.769189 -2.978070 -3.924607	C 4.348118 1.399988 0.461088	C 1.619200 0.249144 1.513643
H 1.389580 -4.992415 -2.623354	C 5.715459 1.558181 0.635778	C 0.100069 0.212305 1.309314
C 1.990784 -3.867666 -0.894793	C 6.592054 0.573473 0.189618	O 0.122012 0.291652 -0.121659
C 2.139134 -2.602933 -0.339246	H 3.593346 2.570340 -4.322773	



5C-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1649.94746840

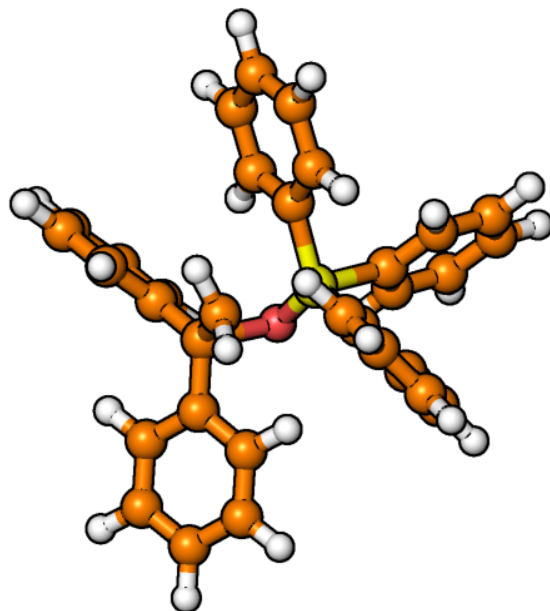
H 3.163179 1.056510 -4.644808	C 5.015186 0.366930 1.206660	C -1.260688 -0.064357 3.675468
H 1.922092 2.839619 -3.459651	C 3.663926 0.313865 1.551163	C -0.652844 -0.444662 2.486932
H 4.127665 -0.831834 -3.367643	H -2.622169 -3.099848 1.717171	C -1.241775 0.452333 -0.755405
H 1.658006 2.728155 -0.993469	H -3.682444 -2.429316 3.832587	C -1.460712 1.379901 -1.768083
H 3.895642 -0.905168 -0.912283	H -2.820628 -0.481651 5.092864	C -1.015203 1.125116 -3.057734
C 3.055669 1.019154 -3.568408	H -0.880275 0.791072 4.217889	C -0.339574 -0.058931 -3.334806
C 2.360309 2.022577 -2.902476	H 0.189508 0.114887 2.107204	C -0.126908 -0.989176 -2.329638
C 3.602642 -0.039192 -2.850809	H -1.588777 0.661686 0.245221	C -1.139795 -1.541651 1.768550
C 2.214557 1.969620 -1.525014	H -1.979443 2.302545 -1.544028	C -0.579325 -0.741400 -1.030328
C 3.477729 -0.080116 -1.469270	H -1.185658 1.848454 -3.844270	C -2.523656 -3.213435 -1.051908
C 2.786025 0.927493 -0.794106	H 0.024211 -0.256278 -4.333874	C -3.253736 -4.301010 -1.511885
H 1.654886 -2.671088 1.451456	H 0.384096 -1.915351 -2.556340	C -2.763245 -5.592710 -1.339405
H 6.353797 -1.122091 3.940167	H -2.906602 -2.210925 -1.191563	C -1.539309 -5.791667 -0.711386
H 3.957330 -1.226451 4.559650	H -4.203114 -4.143515 -2.006616	C -0.807786 -4.700383 -0.254822
H 7.027397 -0.080414 1.798478	H -3.331748 -6.439822 -1.699817	C -1.296277 -3.406703 -0.414153
H 2.248678 -0.289326 3.036146	H -1.152382 -6.794189 -0.582381	C 1.349683 -2.193046 0.532211
H 5.315651 0.822898 0.274484	H 0.156193 -4.838677 0.219515	P -0.282035 -2.007932 0.238090
C 5.603197 -0.718561 3.273420	H 2.021009 -2.251170 -0.311479	C 2.608028 0.923638 0.688638
C 4.255768 -0.774369 3.623205	C -2.238205 -2.248549 2.259480	O 1.639821 1.468103 1.193216
C 5.981311 -0.139502 2.068939	C -2.837219 -1.869038 3.455390	
C 3.294988 -0.251026 2.773938	C -2.351364 -0.777013 4.163735	



TS_{5→6}C-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1649.93409148

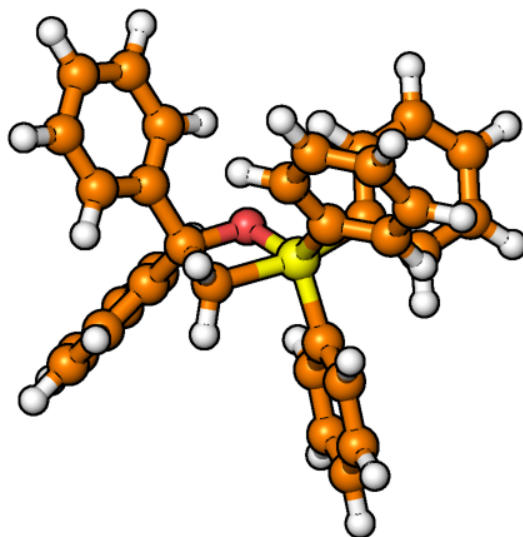
H 3.041292 1.223922 -4.585708	C 4.766525 -0.472888 0.903886	C -1.530802 -0.000075 3.786284
H 2.108176 2.912440 -3.028433	C 3.510579 -0.247557 1.462692	C -0.788832 -0.290001 2.647907
H 3.609677 -1.034703 -3.734169	H -2.791498 -2.721288 1.351982	C -1.283680 0.809813 -0.636518
H 1.750209 2.323202 -0.636085	H -4.082723 -2.195034 3.376884	C -1.553497 1.748796 -1.624043
H 3.261698 -1.588609 -1.377795	H -3.281471 -0.455528 4.944301	C -1.212559 1.490808 -2.945061
C 2.886880 0.979827 -3.542585	H -1.180138 0.764180 4.467162	C -0.595315 0.291542 -3.284414
C 2.366600 1.925034 -2.667195	H 0.124705 0.254368 2.408826	C -0.329721 -0.651333 -2.304979
C 3.204741 -0.286731 -3.064012	H -1.527034 1.024363 0.392340	C -1.247272 -1.273034 1.764985
C 2.167525 1.607829 -1.329464	H -2.019887 2.686930 -1.355555	C -0.677865 -0.397308 -0.975951
C 3.004935 -0.597719 -1.724745	H -1.414760 2.228530 -3.710137	C -2.010104 -3.248679 -1.212470
C 2.483561 0.344161 -0.835048	H -0.305031 0.097458 -4.307306	C -2.493216 -4.470885 -1.660008
H 1.544326 -1.956822 1.733802	H 0.159096 -1.576882 -2.573804	C -1.861618 -5.651443 -1.282705
H 6.578322 -1.070688 3.713392	H -2.499228 -2.333118 -1.513371	C -0.745824 -5.608497 -0.454705
H 4.356600 -0.642590 4.733904	H -3.360334 -4.501188 -2.306048	C -0.260461 -4.387283 -0.004517
H 6.833342 -0.928323 1.253093	H -2.237040 -6.602489 -1.636194	C -0.888069 -3.199503 -0.381453
H 2.426293 -0.080629 3.291911	H -0.251239 -6.524443 -0.160828	C 1.432573 -1.667973 0.693577
H 4.906759 -0.399265 -0.163715	H 0.608342 -4.352690 0.638632	P -0.274319 -1.624509 0.286371
C 5.725313 -0.841671 3.087921	H 1.977411 -2.346829 0.046153	C 2.248820 0.116426 0.663860
C 4.476892 -0.602939 3.658474	C -2.436606 -1.956816 2.027756	O 1.470042 0.950539 1.233197
C 5.865015 -0.766466 1.709762	C -3.164860 -1.660352 3.172233	
C 3.389507 -0.301948 2.853732	C -2.712781 -0.682743 4.052070	



TS_{7→8}C-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1649.94193320

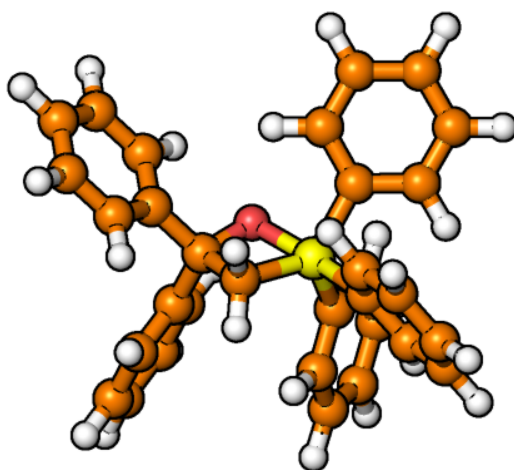
H -2.147633 -4.043240 2.443473	C 0.658125 1.437243 1.693463	C 5.031196 1.403883 -0.639240
H -2.622242 -1.787141 3.352329	H 3.187261 0.584549 1.864777	C 5.773518 2.565569 -0.466720
H -0.151855 -4.385121 1.009126	H 6.040974 -3.351478 0.367642	C 5.135948 3.784220 -0.263189
H -1.134429 0.094038 2.830544	H 4.939043 -1.164855 0.553733	H 4.185822 0.393840 -5.517468
H 1.335147 -2.510375 0.496389	H 2.056809 -2.364341 -2.377711	H 4.420779 0.089071 -3.097777
C -1.490412 -3.213980 2.217505	H 3.078218 -4.601014 -2.463738	H 0.182891 0.391469 -2.625487
C -1.756345 -1.950331 2.724156	H 5.098196 -5.097256 -1.117026	H -0.062620 0.697523 -5.066068
C -0.368761 -3.405221 1.414064	C 5.164387 -3.140134 -0.230408	H 1.940236 0.699921 -6.522837
C -0.914583 -0.882863 2.426665	C 4.556781 -1.896420 -0.142040	C 3.304411 0.394042 -4.889381
C 0.474356 -2.345057 1.125876	C 3.438041 -1.596391 -0.921701	C 3.433147 0.223250 -3.518970
C 0.212750 -1.064473 1.625499	C 2.919671 -2.582258 -1.764373	C 2.312595 0.219851 -2.683378
H -0.635882 4.980158 2.615392	C 3.503362 -3.842588 -1.819834	C 1.055044 0.393988 -3.260665
H 1.245622 3.973192 3.873914	C 4.634566 -4.121229 -1.063972	C 0.921975 0.565143 -4.636158
H -1.700768 3.701802 0.777148	H 3.238709 4.779901 -0.098392	C 2.043780 0.565923 -5.453998
H 2.061328 1.725616 3.285693	H 1.920610 2.730723 -0.418496	H 2.837744 -1.192737 1.795839
H -0.866873 1.453224 0.193271	H 5.545633 0.469173 -0.805213	P 2.561400 0.006368 -0.843883
C -0.278681 3.990438 2.363130	H 6.854271 2.516571 -0.495178	C 2.563897 -0.201740 1.465329
C 0.776717 3.427155 3.066020	H 5.717207 4.685980 -0.124674	C 1.159167 0.063549 1.353592
C -0.876926 3.271230 1.331136	C 3.746806 3.836425 -0.247656	O 1.049776 0.136970 -0.471583
C 1.241273 2.158691 2.732004	C 2.999485 2.680245 -0.425671	
C -0.416973 2.005051 1.004680	C 3.636931 1.450339 -0.607867	



7C-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1649.96959256

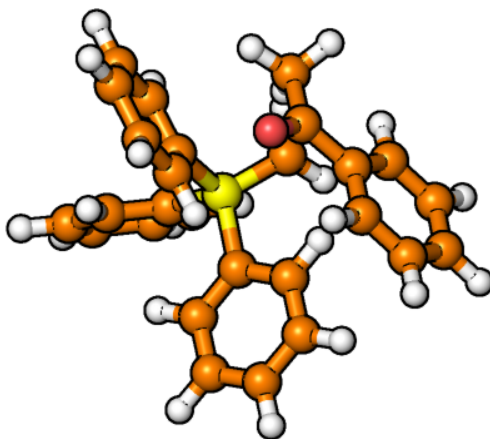
H -5.124436 0.760389 0.136510	C 0.151804 0.156342 3.090797	C 3.197785 1.532597 -1.838364
H -4.397113 -1.487991 0.882986	H 1.066964 -2.002904 1.859851	C 3.988027 2.616887 -2.216484
H -3.481082 2.611807 0.051363	H 4.864572 -1.896863 3.706871	C 4.446715 3.514883 -1.263955
H -2.053684 -1.878004 1.522423	H 2.756659 -1.037227 2.795816	H -0.830881 -0.204797 -3.956417
H -1.132494 2.212722 0.705235	H 4.499127 -0.928743 -1.121062	H 0.036228 0.724842 -1.845104
C -4.096449 0.589385 0.427079	H 6.571741 -1.891032 -0.222492	H 2.671546 -2.632668 -1.451874
C -3.688062 -0.671290 0.846074	H 6.777340 -2.360517 2.201643	H 1.829135 -3.541153 -3.576586
C -3.173023 1.627589 0.379412	C 4.778690 -1.712215 2.644127	H 0.072005 -2.336792 -4.838190
C -2.364990 -0.890571 1.209806	C 3.583322 -1.225549 2.125175	C -0.057120 -0.732901 -3.414993
C -1.852077 1.408027 0.749323	C 3.458555 -0.957644 0.761986	C 0.430613 -0.207848 -2.225102
C -1.435215 0.144939 1.164463	C 4.558249 -1.178143 -0.071279	C 1.425188 -0.880292 -1.513647
H 0.501123 0.756154 6.907835	C 5.736730 -1.703216 0.439741	C 1.916477 -2.089426 -2.002941
H 1.179334 2.515383 5.301812	C 5.852490 -1.966976 1.801188	C 1.434638 -2.606714 -3.200136
H -0.408234 -1.388880 6.061201	H 4.464749 4.011682 0.827409	C 0.447775 -1.930891 -3.908760
H 0.958791 2.122854 2.870400	H 3.080913 2.099341 1.488045	H 0.036930 -1.940989 0.421913
H -0.626855 -1.767812 3.640586	H 2.858671 0.847316 -2.601200	P 1.904977 -0.203176 0.114279
C 0.400656 0.589958 5.843338	H 4.242981 2.754506 -3.259684	C 0.660864 -1.356027 1.090489
C 0.780993 1.575910 4.941371	H 5.061509 4.356154 -1.556337	C 0.002066 -0.081450 1.596793
C -0.109074 -0.613988 5.367666	C 4.109955 3.320976 0.073125	O 0.866161 0.854889 0.875548
C 0.655976 1.361248 3.573112	C 3.322373 2.240756 0.442841	
C -0.231836 -0.827338 4.001181	C 2.847011 1.327129 -0.505128	



6C-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1649.97694626

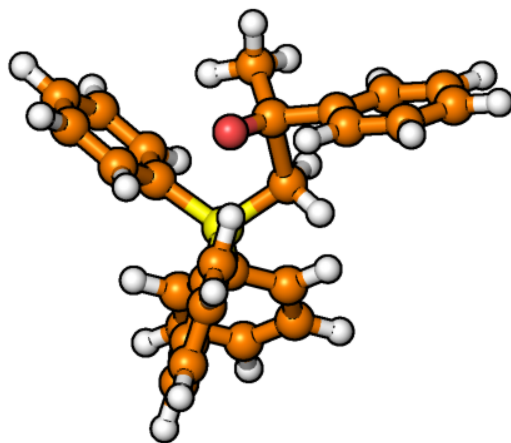
H 1.955457 1.077478 1.959111	C -1.804640 1.431553 1.457832	C 4.409984 1.350110 0.475774
H -1.400154 -5.165001 2.314616	C -0.682304 0.892856 2.083389	C 5.779884 1.520958 0.614283
H -0.107564 -3.920726 4.023983	H 2.271479 -4.785056 -0.446998	C 6.655696 0.579542 0.081404
H -1.961504 -4.065506 0.165750	H 2.620975 -2.581455 0.572510	H 3.327899 2.770629 -4.256675
H 0.609993 -1.611339 3.590087	H 1.007933 -0.700872 -2.925842	H 3.494352 0.902550 -2.672194
H -1.204064 -1.747286 -0.271105	H 0.705596 -2.912206 -3.967594	H 0.197214 2.481927 -0.446576
C -1.085893 -4.147253 2.124342	H 1.320871 -4.966036 -2.728050	H 0.112218 4.428767 -1.961340
C -0.359347 -3.448958 3.083007	C 2.010144 -3.893139 -1.000303	H 1.656777 4.564186 -3.892802
C -1.402625 -3.528307 0.920940	C 2.205184 -2.645525 -0.423355	C 2.650835 2.720453 -3.414215
C 0.047267 -2.143973 2.834193	C 1.850353 -1.486855 -1.112721	C 2.735683 1.657913 -2.526274
C -0.991204 -2.224656 0.673572	C 1.306137 -1.592100 -2.391338	C 1.851370 1.561117 -1.447926
C -0.258819 -1.522639 1.625203	C 1.126161 -2.840650 -2.973165	C 0.898366 2.562860 -1.261740
H -3.002485 3.356530 3.981370	C 1.472762 -3.994065 -2.277889	C 0.843805 3.649153 -2.128215
H -1.009577 2.406632 5.105263	H 6.813838 -1.256930 -1.016562	C 1.710782 3.725872 -3.210634
H -3.502659 2.726463 1.638063	H 4.395011 -1.549375 -1.256460	H 2.271762 -0.660473 2.040763
H 0.461498 0.847529 3.902004	H 3.749463 2.111017 0.874968	P 1.973716 0.134901 -0.300520
H -2.010375 1.158442 0.432888	H 6.165574 2.390019 1.131763	C 1.706153 0.111956 1.524491
C -2.356376 2.668130 3.452930	H 7.724978 0.708547 0.185457	C 0.194606 -0.093478 1.326999
C -1.238705 2.134147 4.083270	C 6.143526 -0.521535 -0.590032	O 0.166144 0.177704 -0.066329
C -2.635536 2.313753 2.137352	C 4.766333 -0.686833 -0.722583	
C -0.408230 1.252531 3.400923	C 3.872512 0.241028 -0.188379	



5C-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.49297141

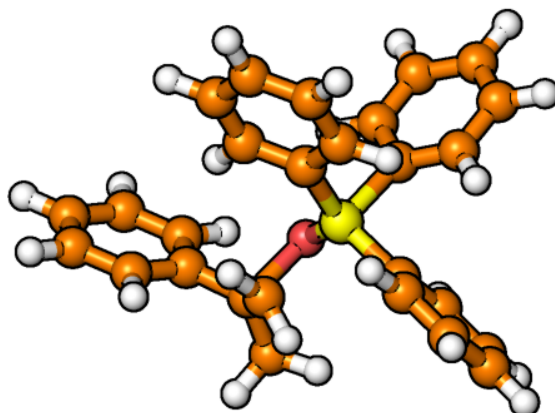
H 0.885863 -2.313526 -0.680240	H -0.274270 -2.061948 4.033341	C -0.322760 3.327610 0.614107
H 2.916302 -3.032386 4.573464	H 0.553626 -1.390821 1.806497	C -0.090804 3.997865 -0.580390
H 3.456530 -2.954212 2.161076	H -0.719476 1.440408 1.545406	C -0.093876 3.296570 -1.782367
H 2.237842 -0.963833 5.755008	H -0.293727 3.861374 1.553385	C -0.331391 1.928991 -1.789375
H 3.306603 -0.834684 0.931143	H 0.098845 5.062994 -0.575009	C -1.399986 -1.100725 0.982495
H 2.115198 1.183261 4.505523	H 0.088169 3.815003 -2.714514	C -0.559799 1.249387 -0.589732
C 2.862821 -2.094113 4.036457	H -0.341859 1.388830 -2.727037	C -3.160451 0.117286 -1.954044
C 3.171513 -2.050365 2.682333	H -3.144652 1.048233 -1.403331	C -4.199769 -0.141188 -2.839767
C 2.480930 -0.930623 4.701114	H -4.988813 0.587792 -2.972793	C -4.223928 -1.332861 -3.557133
C 3.100008 -0.847835 1.990134	H -5.032904 -1.532847 -4.247576	C -3.201752 -2.261911 -3.393090
C 2.411625 0.268870 4.011565	H -3.214056 -3.186712 -3.954902	C -2.158561 -1.997971 -2.514027
C 2.721503 0.323146 2.649954	H -1.344617 -2.703581 -2.398974	C -2.132901 -0.812651 -1.781274
H 2.725981 2.678630 0.089622	H 1.370625 -0.841779 -1.682413	C 0.767666 -1.258288 -0.886560
H 2.295461 0.953710 -0.065509	C -2.773186 -1.154780 1.231767	P -0.727335 -0.556672 -0.615395
H 3.959080 1.409278 0.285960	C -3.242330 -1.528337 2.484540	C 2.614601 1.637854 1.942414
C 2.915786 1.678069 0.466054	C -2.346782 -1.855215 3.497381	O 2.282952 2.638777 2.549035
H -3.477035 -0.915539 0.448333	C -0.979233 -1.810224 3.253517	
H -4.308069 -1.568396 2.668157	C -0.506302 -1.432870 2.003032	
H -2.715687 -2.146331 4.472161	C -0.557447 1.958119 0.610316	



TS_{5→6}C-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.47257204

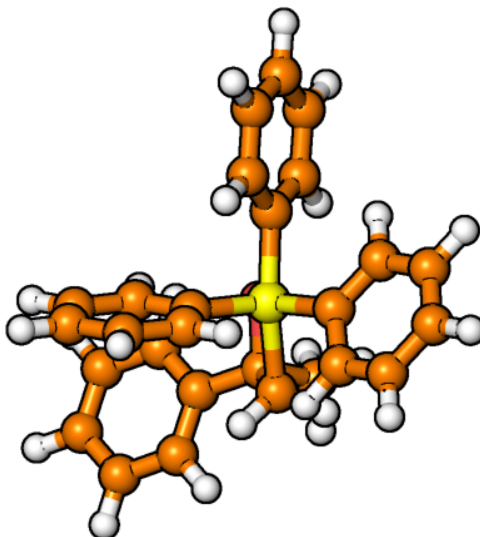
H 0.552014 -1.656265 0.910479	H -1.813101 -0.418147 4.863793	C -0.720306 4.005819 0.560231
H 4.899993 -3.644329 3.408699	H -0.382936 0.038694 2.878947	C -0.410473 4.456402 -0.717264
H 5.000706 -3.118456 0.988884	H -1.109292 2.301816 1.798262	C -0.295168 3.551063 -1.766927
H 3.420345 -2.315422 4.886779	H -0.795201 4.705932 1.380887	C -0.491695 2.197062 -1.537054
H 3.626549 -1.313647 0.057827	H -0.252686 5.512001 -0.895545	C -1.980131 -0.338682 1.484558
H 2.044982 -0.468713 3.922390	H -0.046495 3.897436 -2.760920	C -0.806227 1.742373 -0.253724
C 4.295640 -2.844882 2.999694	H -0.391954 1.496861 -2.355001	C -2.805365 -0.031148 -2.016384
C 4.350064 -2.549298 1.641243	H -3.079251 0.957547 -1.675883	C -3.480215 -0.604392 -3.085078
C 3.462498 -2.099454 3.826188	H -4.280524 -0.060666 -3.568787	C -3.125290 -1.872418 -3.534725
C 3.572118 -1.523449 1.117976	H -3.649271 -2.315475 -4.370954	C -2.095062 -2.566965 -2.912198
C 2.688165 -1.072853 3.297881	H -1.815093 -3.551563 -3.260701	C -1.418604 -1.996287 -1.840782
C 2.725013 -0.774805 1.937786	H -0.615538 -2.535496 -1.357605	C -1.767658 -0.724708 -1.386473
H 1.827441 1.973690 -0.014544	H 1.178196 -0.929062 -0.597343	C 0.672122 -0.736002 0.345408
H 2.951416 0.678749 -0.463466	C -3.328957 -0.666197 1.319442	P -0.912950 -0.033379 0.061354
H 3.332472 1.768576 0.876680	C -4.123636 -0.904956 2.431974	C 1.826716 0.360385 1.424436
C 2.525137 1.234906 0.370985	C -3.579137 -0.817135 3.708884	O 1.169546 1.002544 2.315268
H -3.758583 -0.749262 0.332102	C -2.238157 -0.489519 3.871215	
H -5.165238 -1.165201 2.300028	C -1.428404 -0.252575 2.766816	
H -4.199732 -1.008086 4.574565	C -0.913223 2.651519 0.797961	



TS_{7→8}C-CPHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.48615800

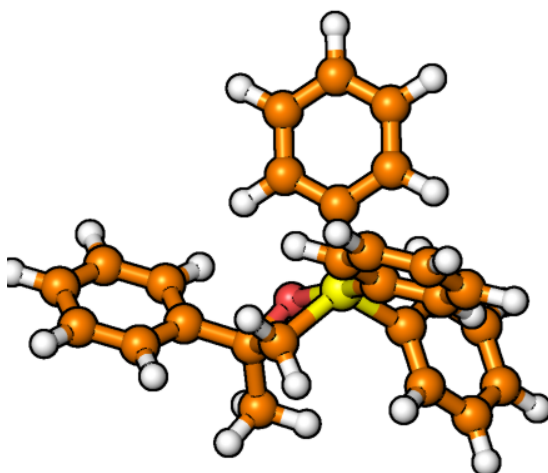
H -1.046819 -1.319612 1.337167	H 2.595628 -4.749052 -1.138527	H 3.551569 -0.561062 -5.212218
H -0.248494 -1.494442 2.905619	H 4.868182 -4.900752 -0.167038	H 3.711063 -0.925002 -2.795293
H 0.512756 -2.158538 1.452750	C 4.986949 -2.796161 0.256816	H 0.125668 1.336399 -2.206635
C -0.081516 -1.331884 1.838409	C 4.337016 -1.572250 0.199213	H -0.034411 1.708647 -4.637323
H -2.285791 4.252360 3.100648	C 3.066787 -1.477490 -0.370308	H 1.679414 0.760798 -6.155781
H -0.297790 3.593195 4.424283	C 2.447248 -2.629719 -0.855864	C 2.800322 -0.137836 -4.558014
H -2.912335 2.934666 1.097694	C 3.089483 -3.859704 -0.770184	C 2.889539 -0.340281 -3.185316
H 1.051934 1.647995 3.739920	C 4.363989 -3.945292 -0.223947	C 1.929705 0.184454 -2.317610
H -1.547905 0.996932 0.416805	H 2.686339 4.802956 0.696968	C 0.877905 0.925743 -2.863740
C -1.694302 3.395481 2.806380	H 1.459556 2.678459 0.557188	C 0.789152 1.133023 -4.234254
C -0.578676 3.027488 3.545651	H 4.906124 0.812303 -1.185699	C 1.750222 0.601643 -5.087588
C -2.046291 2.653648 1.682577	H 6.149243 2.917707 -0.978244	H 2.503906 -0.954926 2.217230
C 0.185298 1.931056 3.159573	H 5.048991 4.930234 -0.042931	P 2.125098 0.069164 -0.468143
C -1.287416 1.556782 1.302861	C 3.180407 3.925368 0.301473	C 2.066053 -0.027889 1.874303
C -0.154515 1.186345 2.031248	C 2.484234 2.727648 0.219265	C 0.654289 -0.024738 1.664032
H 2.525112 0.861102 2.280789	C 3.106111 1.587090 -0.291990	O 0.599746 0.078786 -0.144363
H 5.976591 -2.856771 0.689391	C 4.424534 1.671058 -0.740937	
H 4.806495 -0.693233 0.616872	C 5.123738 2.867382 -0.637254	
H 1.464436 -2.561806 -1.302823	C 4.505318 3.997686 -0.115922	



7C-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.51529289

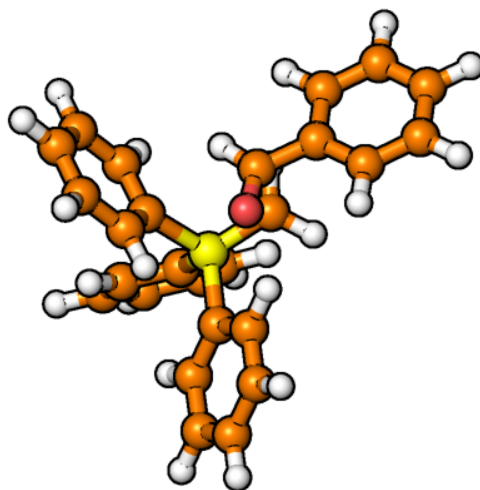
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H -1.810982 5.054137 3.125341	H 5.700382 -4.283375 0.217952	H 3.572752 0.777350 -2.418956
H -0.424743 3.657529 4.630486	C 4.917455 -2.500930 1.131079	H -0.298060 -0.979636 -1.943124
H -2.335182 4.243998 0.843106	C 3.983934 -1.479491 1.038529	H -0.481103 -1.233326 -4.382127
H 0.438949 1.487251 3.855478	C 3.127790 -1.376007 -0.065193	H 1.356654 -0.463120 -5.856014
H -1.461134 2.064377 0.073551	C 3.206694 -2.362424 -1.049011	C 2.574430 0.209973 -4.216880
C -1.436228 4.096917 2.787972	C 4.117312 -3.409761 -0.941153	C 2.677013 0.339632 -2.837579
C -0.658221 3.313181 3.631478	C 4.983808 -3.476360 0.140332	C 1.649338 -0.083058 -1.992026
C -1.728949 3.641446 1.507085	H 2.108178 4.916832 -0.320843	C 0.513131 -0.648864 -2.574026
C -0.170388 2.087591 3.192571	H 1.007849 2.720769 -0.418990	C 0.408986 -0.789593 -3.954444
C -1.243431 2.414457 1.072886	H 4.782001 0.800744 0.223960	C 1.438703 -0.359337 -4.781950
C -0.450130 1.628878 1.907738	H 5.882138 2.991294 0.310429	H 1.588145 -1.065123 2.224630
H -1.108283 -0.866270 2.870194	H 4.555657 5.066981 0.048696	P 1.884197 0.022426 -0.118150
H -0.617201 -1.779760 1.430931	C 2.696540 4.017229 -0.197224	C 1.480868 -0.075408 1.787818
H -1.932077 -0.593376 1.329385	C 2.072406 2.778107 -0.248806	C 0.043673 0.274589 1.440028
C -0.968506 -0.811561 1.790217	C 2.809743 1.604724 -0.082191	O 0.222783 0.283889 -0.008425
H 5.584703 -2.543780 1.982113	C 4.186836 1.695461 0.117618	
H 3.927426 -0.750963 1.834695	C 4.811523 2.937145 0.161570	
H 2.556585 -2.320886 -1.908837	C 4.068611 4.101614 0.010228	



6C-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.51790974

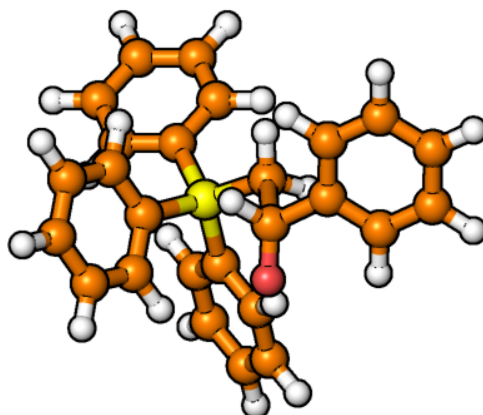
H 1.967460 0.960701 2.073446	H 0.706332 -3.031858 -3.896536	H 3.116916 2.643728 -4.239013
H -2.823581 3.748815 3.800147	H 1.538195 -5.056863 -2.738357	H 3.324369 0.777790 -2.657348
H -0.967377 2.674214 5.040121	C 2.188802 -3.973683 -1.001522	H 0.136094 2.404444 -0.308991
H -3.310510 3.046404 1.474988	C 2.300241 -2.727388 -0.397573	H 0.016443 4.346036 -1.820615
H 0.387449 0.924139 3.964545	C 1.829226 -1.584604 -1.042958	H 1.484103 4.459023 -3.813449
H -1.931804 1.288008 0.398688	C 1.248078 -1.706124 -2.304025	C 2.473107 2.603521 -3.370314
C -2.228942 2.977813 3.328341	C 1.153559 -2.950298 -2.914635	C 2.580202 1.541699 -2.483896
C -1.186818 2.374487 4.023578	C 1.619703 -4.087695 -2.264615	C 1.737070 1.456815 -1.372332
C -2.499999 2.583376 2.023028	H 6.779022 -1.131827 -1.073913	C 0.805446 2.470239 -1.151351
C -0.421642 1.387698 3.413241	H 4.374070 -1.529316 -1.261006	C 0.730593 3.556883 -2.015944
C -1.732693 1.596002 1.415332	H 3.617344 2.043526 0.979860	C 1.554535 3.621234 -3.132162
C -0.682132 0.991708 2.102376	H 6.021874 2.427658 1.182097	H 2.170800 -0.791309 2.097269
H -0.364270 -1.592964 2.959908	H 7.632095 0.843366 0.155442	P 1.889621 0.037400 -0.218094
H 0.161050 -2.276918 1.406154	C 6.087823 -0.439324 -0.610366	C 1.644832 0.030801 1.613050
H -1.452830 -1.574374 1.565791	C 4.716546 -0.664945 -0.711343	C 0.124420 -0.112420 1.441117
C -0.412556 -1.478516 1.875862	C 3.793726 0.204624 -0.129239	O 0.098301 0.011848 0.020056
H 2.552661 -4.853445 -0.487300	C 4.299619 1.321526 0.546873	
H 2.764703 -2.648750 0.576364	C 5.663443 1.553324 0.653947	
H 0.859946 -0.830131 -2.804481	C 6.567457 0.667175 0.075857	



5C-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1419.22045645

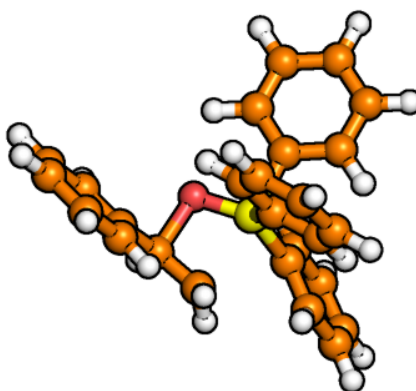
H 0.574577 -1.910471 0.461106	H -1.322862 2.054024 1.599378	C -0.324437 4.258617 -0.768492
H 6.173095 -2.177725 1.802834	H -0.887972 4.454422 1.295345	C -0.152984 3.381380 -1.834718
H 5.584838 -0.911362 -0.238982	H -0.120918 5.313560 -0.897191	C -0.417219 2.028327 -1.669902
H 4.805918 -1.937531 3.849110	H 0.182688 3.751373 -2.794523	C -2.020655 -0.589433 1.269088
H 3.607476 0.586582 -0.230399	H -0.295232 1.351487 -2.505333	C -0.843795 1.538911 -0.432050
H 2.833320 -0.416580 3.845693	H -3.297383 1.070331 -1.628644	C -3.125610 0.106381 -2.089180
C 5.314739 -1.518597 1.804172	H -4.702611 0.350659 -3.521875	C -3.916722 -0.297680 -3.156614
C 4.984954 -0.806068 0.655266	H -4.307903 -1.843605 -4.595374	C -3.694479 -1.532081 -3.760143
C 4.543812 -1.383826 2.957214	H -2.498989 -3.315823 -3.767464	C -2.678088 -2.358783 -3.295601
C 3.881540 0.035111 0.660365	H -1.075164 -2.575855 -1.871759	C -1.884461 -1.950754 -2.229838
C 3.443955 -0.540598 2.961750	H 1.264336 -0.681668 -0.731640	C -2.105029 -0.720759 -1.615163
C 3.104606 0.170092 1.809710	C -3.394875 -0.827843 1.196039	C 0.498495 -0.944354 -0.016001
H 1.760118 1.593782 0.841126	C -4.126680 -1.065850 2.352425	P -1.014501 -0.256184 -0.203359
H -3.893564 -0.841534 0.238504	C -3.494735 -1.065885 3.590714	C 1.941806 1.082713 1.800838
H -5.189559 -1.256315 2.284119	C -2.127074 -0.829306 3.669500	O 1.253699 1.321341 2.772132
H -4.066210 -1.251403 4.490697	C -1.389281 -0.593050 2.516659	
H -1.629632 -0.823692 4.630330	C -1.014177 2.422702 0.632656	
H -0.330177 -0.395413 2.579968	C -0.757600 3.777570 0.461737	



TS_{5→6}C-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1419.21107904

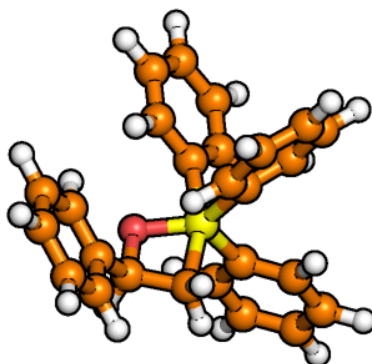
H 0.584947 -1.563468 0.881430	H -1.311297 2.255883 1.807946	C -0.550584 4.500251 -0.610546
H 6.204049 -2.263445 1.605246	H -1.023745 4.677642 1.476535	C -0.373101 3.629780 -1.681221
H 5.633745 -1.071630 -0.490761	H -0.409701 5.563964 -0.750753	C -0.549915 2.265732 -1.500024
H 4.692322 -2.101018 3.559525	H -0.092206 4.011555 -2.653500	C -2.068661 -0.385898 1.414901
H 3.550394 0.253702 -0.629380	H -0.408744 1.592564 -2.334809	C -0.911133 1.765617 -0.245742
H 2.605608 -0.741317 3.401864	H -3.146176 1.012747 -1.739538	C -2.864647 0.033089 -2.099666
C 5.291291 -1.685526 1.540133	H -4.312689 0.038405 -3.678121	C -3.519645 -0.515302 -3.193702
C 4.968949 -1.017149 0.362423	H -3.662211 -2.194588 -4.523729	C -3.153744 -1.771204 -3.667994
C 4.439540 -1.593912 2.636792	H -1.843191 -3.453512 -3.414500	C -2.131875 -2.478785 -3.045916
C 3.797446 -0.274349 0.285372	H -0.676285 -2.478943 -1.466526	C -1.475082 -1.932794 -1.949910
C 3.270695 -0.846515 2.555175	H 1.137902 -0.801451 -0.651856	C -1.836642 -0.674259 -1.469982
C 2.934340 -0.188642 1.375551	C -3.416752 -0.708398 1.236056	C 0.603285 -0.657224 0.283553
H 1.717633 1.358990 0.479272	C -4.214475 -0.980576 2.338714	P -1.001593 -0.023538 0.007233
H -3.843113 -0.759811 0.244902	C -3.673528 -0.929584 3.619187	C 1.653362 0.618783 1.302293
H -5.255819 -1.236368 2.196438	C -2.333116 -0.606415 3.795392	O 1.082896 0.970604 2.380098
H -4.296706 -1.144937 4.477214	C -1.520097 -0.337860 2.700591	
H -1.911418 -0.562003 4.790865	C -1.077507 2.639554 0.827745	
H -0.476888 -0.050096 2.829638	C -0.900366 4.004394 0.639337	



TS_{7→8}C-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1419.22039468

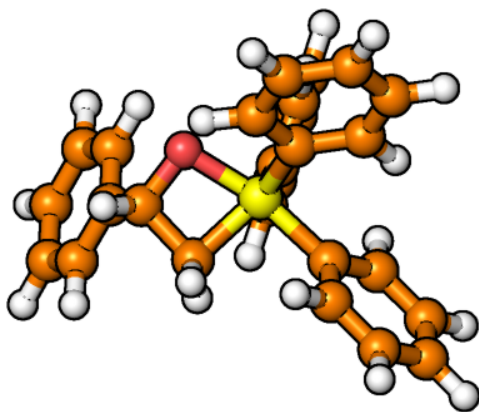
H -2.239079 4.348973 2.993103	C 4.180090 -1.755969 0.419368	H -0.227978 0.389298 -2.223799
H 0.142340 4.202481 3.656921	C 3.055304 -1.548789 -0.381526	H -0.403333 0.691349 -4.671416
H -3.286404 2.468692 1.763275	C 2.609576 -2.586539 -1.202456	H 1.637254 0.657825 -6.073884
H 1.460006 2.204870 3.099878	C 3.274712 -3.806968 -1.220537	C 2.953049 0.336114 -4.404447
H -1.947156 0.479020 1.182091	C 4.413137 -3.992369 -0.447111	C 3.043064 0.167218 -3.030847
C -1.657374 3.471407 2.743494	H 2.441899 4.804056 0.362786	C 1.899832 0.182148 -2.226508
C -0.321401 3.388967 3.114573	H 1.271189 2.666241 0.027871	C 0.660387 0.374544 -2.836166
C -2.245492 2.414473 2.053970	H 5.047906 0.654631 -0.272539	C 0.567073 0.544399 -4.214963
C 0.425279 2.260096 2.797217	H 6.208732 2.786269 0.059289	C 1.710359 0.525539 -5.002342
C -1.496540 1.291962 1.736242	H 4.920839 4.875836 0.392572	H 2.336390 -1.165993 2.282166
C -0.149228 1.200524 2.097556	C 3.014917 3.895615 0.231744	H 0.013437 -0.920106 1.789920
H 2.558935 0.629622 2.439059	C 2.351175 2.690848 0.045107	P 2.097663 0.002410 -0.384891
H 5.747317 -3.099732 0.982465	C 3.073854 1.505544 -0.115492	C 2.011204 -0.180742 1.980608
H 4.502664 -0.984310 1.101905	C 4.468755 1.552858 -0.119437	C 0.618447 -0.022650 1.733905
H 1.743663 -2.439138 -1.832732	C 5.126798 2.762293 0.064301	O 0.571911 0.049210 -0.043802
H 2.907897 -4.606950 -1.849857	C 4.404501 3.936460 0.247238	
H 4.940274 -4.936787 -0.471852	H 3.850451 0.320520 -5.009157	
C 4.867185 -2.959603 0.368855	H 4.016650 0.018632 -2.582459	



7C-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1419.24771706

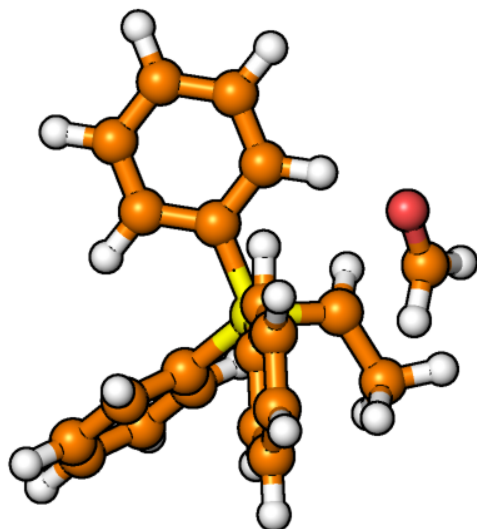
H 0.540742 0.682373 6.931485	C 4.703460 -1.740696 2.646678	H 0.141146 0.808085 -1.973000
H 1.460655 2.365418 5.365558	C 3.521872 -1.229207 2.119977	H 2.565359 -2.673957 -1.374101
H -0.633124 -1.309384 6.037815	C 3.413082 -0.953262 0.757197	H 1.768145 -3.596126 -3.511342
H 1.211667 2.051235 2.923368	C 4.514309 -1.194725 -0.068371	H 0.132782 -2.337347 -4.879502
H -0.861351 -1.620621 3.604107	C 5.678628 -1.743434 0.449985	C 0.027025 -0.691288 -3.503499
C 0.432188 0.548876 5.863128	C 5.779134 -2.012758 1.811604	C 0.491767 -0.159702 -2.306771
C 0.949183 1.491414 4.983436	H 4.486286 4.008837 0.808774	C 1.417267 -0.862605 -1.534893
C -0.226383 -0.569615 5.360822	H 3.048024 2.135008 1.460164	C 1.863441 -2.108913 -1.971935
C 0.812924 1.318893 3.609597	H 2.911941 0.823211 -2.613252	C 1.407088 -2.633066 -3.175766
C -0.357300 -0.742987 3.989593	H 4.348002 2.691669 -3.262880	C 0.488376 -1.926838 -3.944174
C 0.163805 0.197813 3.100018	H 5.152811 4.304774 -1.563071	H -0.061328 -1.838504 0.387101
H 0.980121 -2.001921 1.809970	C 4.137516 3.314027 0.055469	P 1.876723 -0.173120 0.095407
H -1.023878 0.151488 1.319637	C 3.318207 2.255958 0.420121	C 0.598288 -1.307803 1.068503
H 4.776714 -1.931410 3.709281	C 2.848663 1.336916 -0.525317	C 0.013321 -0.020339 1.615674
H 2.693369 -1.029760 2.784830	C 3.241011 1.514214 -1.851508	O 0.843774 0.901591 0.854580
H 4.466925 -0.944733 -1.118580	C 4.062411 2.576493 -2.224957	
H 6.514608 -1.946071 -0.206649	C 4.513537 3.480552 -1.274584	
H 6.693232 -2.425068 2.217885	H -0.690417 -0.137107 -4.094524	



6C-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1419.25485706

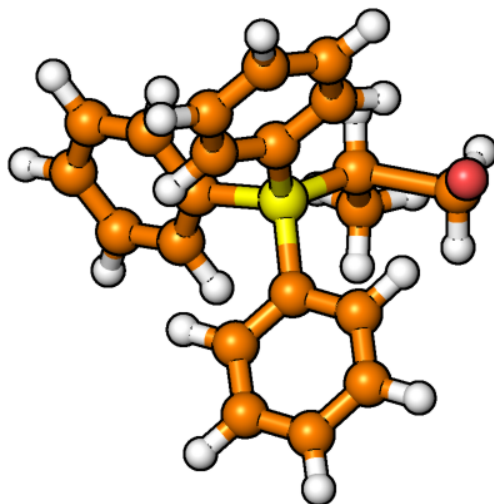
H -1.839405 -4.679005 2.623108	C 1.811881 -3.827887 -0.856751	H 3.667748 0.848318 -2.637330
H -0.629404 -3.312991 4.298657	C 2.039447 -2.564940 -0.327479	H 0.174706 2.530892 -0.833667
H -2.142404 -3.809906 0.322107	C 1.772565 -1.424858 -1.084259	H 0.186313 4.345765 -2.512604
H 0.273208 -1.107691 3.675094	C 1.281193 -1.565948 -2.380989	H 1.890170 4.356500 -4.309906
H -1.214048 -1.594202 -0.294980	C 1.065174 -2.830885 -2.913354	C 2.867384 2.581930 -3.592743
C -1.447395 -3.708063 2.351033	C 1.326280 -3.964675 -2.151798	C 2.891743 1.599340 -2.614174
C -0.766594 -2.941326 3.291434	H 6.731900 -1.442194 -0.862696	C 1.924042 1.573920 -1.604608
C -1.618197 -3.218332 1.061453	H 4.307393 -1.622490 -1.152168	C 0.943858 2.567104 -1.588413
C -0.257810 -1.697976 2.937368	H 3.804454 2.176113 0.764826	C 0.944170 3.573790 -2.547771
C -1.107414 -1.974704 0.709992	H 6.225569 2.346717 1.067442	C 1.899047 3.580081 -3.555712
C -0.417234 -1.206886 1.642190	H 7.716728 0.538262 0.254691	H 2.185498 -0.483587 2.036047
H 1.950169 1.260365 1.876769	C 6.091381 -0.650716 -0.494883	P 1.954839 0.228824 -0.350331
H -0.416173 0.924949 1.772745	C 4.711060 -0.752294 -0.655274	C 1.661215 0.289789 1.477769
H 2.007034 -4.703941 -0.253181	C 3.854716 0.248876 -0.197203	C 0.152284 0.142547 1.256124
H 2.412086 -2.474127 0.683190	C 4.433730 1.363163 0.421465	O 0.148366 0.383515 -0.138787
H 1.053647 -0.687831 -2.968934	C 5.807142 1.471573 0.586694	
H 0.684536 -2.929710 -3.921178	C 6.644798 0.458711 0.128858	
H 1.148284 -4.949104 -2.563692	H 3.612576 2.574909 -4.377570	



5D-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.74459418

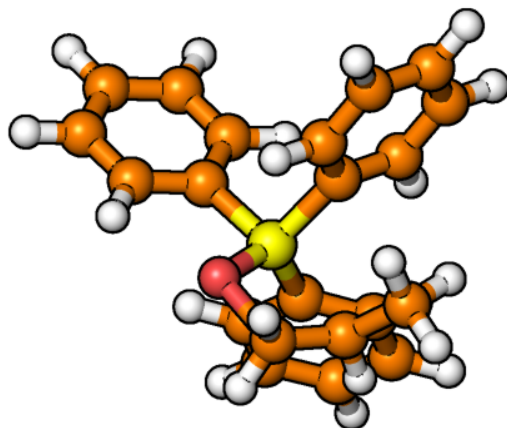
H 2.632476 0.062549 1.242232	H -3.944893 -0.110880 -0.153120	C 0.053753 4.167466 -0.539249
H 0.758084 -2.455911 -0.973741	H -5.544902 -1.120117 -1.733660	C 0.074062 2.806958 -0.258463
H 0.360526 -2.190046 0.715660	H -4.735908 -2.127046 -3.844384	C -1.639955 -0.040742 1.385971
H 1.997317 -1.921291 0.152270	H -2.317684 -2.116195 -4.370644	C -0.990187 1.995491 -0.664458
C 0.944876 -1.794085 -0.119188	H -0.712406 -1.097757 -2.776822	C -3.586812 -0.544089 -1.077155
H -2.216778 -2.080238 1.004112	H 1.249410 0.193277 -1.085417	C -4.488204 -1.114199 -1.966759
H -2.915802 -2.521993 3.321679	H 1.125836 -0.380478 2.240565	C -4.032989 -1.679245 -3.154378
H -2.767971 -0.731034 5.025218	C -2.136102 -1.297200 1.745489	C -2.674673 -1.673180 -3.450338
H -1.887427 1.496827 4.397194	C -2.537007 -1.545045 3.051996	C -1.773213 -1.102590 -2.559659
H -1.144215 1.928462 2.096036	C -2.453160 -0.538943 4.008034	C -2.221128 -0.530034 -1.370103
H -2.893160 1.949391 -1.672493	C -1.962049 0.713197 3.655437	C 0.633546 -0.340260 -0.371518
H -2.919056 4.357270 -2.153593	C -1.552665 0.962614 2.352371	P -0.955352 0.229403 -0.276030
H -1.031282 5.789912 -1.435233	C -2.068943 2.565687 -1.345681	C 1.779139 0.412277 1.844800
H 0.879834 4.787309 -0.217417	C -2.081606 3.926398 -1.621116	O 1.668242 1.572479 2.191532
H 0.900451 2.385484 0.292726	C -1.020175 4.729624 -1.219276	



TS_{5→6}D-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.73941679

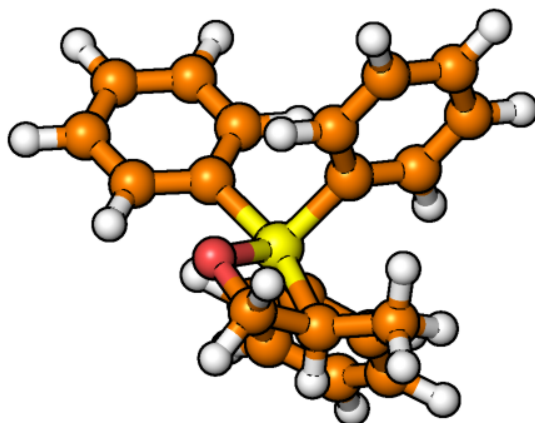
H 0.598249 -2.139760 -1.475391	H -2.343524 1.153134 -2.666546	C -0.314171 4.291696 -0.531444
H 0.591074 -2.162368 0.290016	H -3.615520 -0.072892 -4.371153	C -0.091570 2.920390 -0.451186
H 2.079239 -1.821629 -0.573544	H -4.042258 -2.497933 -4.106303	C -1.475182 -0.133381 1.446062
C 0.999594 -1.649270 -0.584162	H -3.167800 -3.687830 -2.116929	C -1.181238 2.051079 -0.410767
H 2.894038 0.243796 0.157977	H -1.898125 -2.469596 -0.408619	C -2.531613 0.097629 -2.533119
H -3.332769 -1.084651 0.908007	H 1.062024 0.377337 -1.411425	C -3.246028 -0.597382 -3.500089
H -4.025312 -1.483416 3.229133	H 1.870085 -0.411314 1.517644	C -3.484773 -1.958700 -3.352122
H -2.585397 -0.741245 5.100485	C -2.689850 -0.767589 1.714907	C -2.995654 -2.626256 -2.234708
H -0.457811 0.435841 4.626261	C -3.085266 -0.987395 3.028275	C -2.280668 -1.935658 -1.266312
H 0.238117 0.872956 2.306174	C -2.277164 -0.566999 4.077890	C -2.053664 -0.559429 -1.395648
H -3.331664 1.891777 -0.347709	C -1.080208 0.089452 3.812287	C 0.735081 -0.157541 -0.519630
H -3.704391 4.318094 -0.504967	C -0.674083 0.316142 2.503937	P -0.932135 0.276592 -0.231635
H -1.772384 5.863145 -0.628525	C -2.484657 2.561716 -0.413216	C 2.069370 0.462644 0.864743
H 0.532989 4.963655 -0.551112	C -2.695361 3.928101 -0.498044	O 1.928425 1.624694 1.318710
H 0.914695 2.542140 -0.342424	C -1.607170 4.795365 -0.565231	



TS_{7→8}D-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.75486072

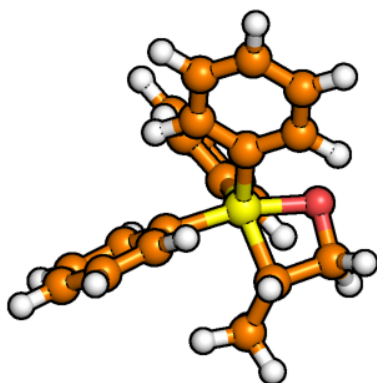
H 0.003785 -0.681540 1.455078	C 4.286479 -3.842676 -0.540458	H -0.569330 0.442312 -4.987944
H 2.517589 1.200592 3.595401	H 2.623005 5.008014 -0.234030	H 1.430348 0.451602 -6.447659
H 2.209186 2.243418 2.211708	H 1.365246 2.898836 -0.439475	C 2.810864 0.348041 -4.803466
H 3.706127 1.340959 2.307349	H 5.058906 0.730980 -0.666205	C 2.950606 0.288136 -3.425035
C 2.631537 1.281472 2.507345	H 6.303790 2.827944 -0.437059	C 1.829871 0.280917 -2.590033
H 5.611429 -2.904508 0.869061	H 5.101719 4.982146 -0.218562	C 0.562502 0.337234 -3.169534
H 4.426560 -0.754526 0.837200	C 3.157349 4.071069 -0.320114	C 0.420731 0.398557 -4.552986
H 1.691178 -2.304453 -2.073513	C 2.447178 2.885580 -0.436014	C 1.541656 0.403491 -5.372370
H 2.797232 -4.496303 -1.942282	C 3.120148 1.664483 -0.547623	H 2.338231 -0.843665 2.032290
H 4.787347 -4.800640 -0.498211	C 4.516108 1.657332 -0.554727	H 0.061837 1.116044 1.589017
C 4.750550 -2.776399 0.226280	C 5.221852 2.848008 -0.432741	P 2.085488 0.205569 -0.762653
C 4.097823 -1.554191 0.191807	C 4.548269 4.057729 -0.313454	C 1.979459 0.143178 1.765797
C 2.995267 -1.363014 -0.645527	H 3.689978 0.352824 -5.434407	C 0.617662 0.208317 1.375682
C 2.539556 -2.435653 -1.416577	H 3.943240 0.246227 -2.996477	O 0.582113 0.314383 -0.343981
C 3.171824 -3.671809 -1.350324	H -0.306806 0.333119 -2.530076	



7D-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.78744212

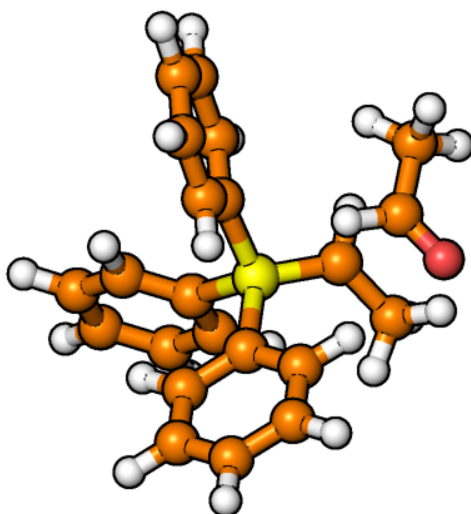
H -0.628639 -0.283518 1.670973	C 4.873068 -3.554981 0.183117	H -0.357235 -0.963881 -4.532231
H 1.701289 1.016619 3.722438	H 2.181084 4.969063 -0.576683	H 1.613489 -0.419450 -5.932634
H 2.151154 2.080293 2.389051	H 1.101832 2.751678 -0.623828	C 2.829939 0.133544 -4.247521
H 3.253864 0.823918 2.923993	H 4.874365 0.902708 0.209780	C 2.886982 0.267933 -2.866973
C 2.201936 1.052900 2.750374	H 5.951443 3.109153 0.240393	C 1.785748 -0.029978 -2.059972
H 5.627000 -2.552289 1.928791	H 4.613623 5.157229 -0.142791	C 0.619866 -0.474428 -2.686888
H 4.086115 -0.664478 1.741579	C 2.771651 4.079939 -0.398593	C 0.558413 -0.616656 -4.070544
H 2.428564 -2.362274 -1.824767	C 2.161810 2.832666 -0.419794	C 1.661977 -0.312876 -4.856775
H 3.899325 -4.305074 -1.576284	C 2.908092 1.674728 -0.192034	H 1.630316 -0.934651 2.140799
H 5.537342 -4.403465 0.280762	C 4.275843 1.787144 0.047714	H -0.165125 1.433268 1.593162
C 4.922583 -2.516532 1.107922	C 4.886544 3.036574 0.061535	P 1.979854 0.096540 -0.177739
C 4.056595 -1.439094 0.991046	C 4.137078 4.186080 -0.156403	C 1.555470 0.088136 1.770878
C 3.156517 -1.345997 -0.076900	H 3.697339 0.376900 -4.847662	C 0.142670 0.414927 1.344175
C 3.117001 -2.397260 -0.994634	H 3.808125 0.609544 -2.414644	O 0.313651 0.299736 -0.084645
C 3.957800 -3.497391 -0.858486	H -0.247404 -0.709147 -2.089594	



6D-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1227.79129923

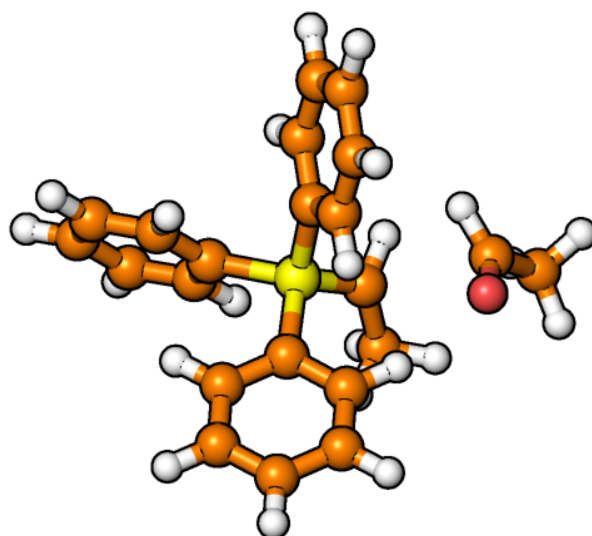
H -0.116983 -1.178013 4.125079	C 0.492131 4.800522 5.069784	H 2.611788 -0.408692 1.366218
H -1.281207 -1.305428 0.900235	C 0.486750 4.246719 6.344901	H 4.746313 -0.154165 0.171905
H 0.268620 -0.629398 0.398899	H -3.332133 3.986828 1.234420	H 5.806593 2.076997 -0.014682
H -1.190951 0.356818 0.317669	H -1.850511 2.827578 2.798806	C 4.220689 3.077701 1.033474
C -0.671365 -0.399477 0.903092	H 1.173044 2.605567 -0.226411	C 2.989634 2.939343 1.661718
H 0.831538 -1.684063 2.712224	H -0.304325 3.773914 -1.785880	C 2.388668 1.686176 1.777721
H 0.552780 2.425707 7.479695	H -2.571524 4.479407 -1.075799	C 3.042343 0.574307 1.247827
H 0.736916 0.978720 5.489630	C -2.343109 3.687177 0.911797	C 4.257338 0.716506 0.588692
H 0.513314 4.426798 2.971919	C -1.499247 3.027528 1.793721	C 4.852726 1.968030 0.484255
H 0.443926 5.873904 4.941885	C -0.208410 2.631938 1.420119	H -1.390610 0.349058 2.786138
H 0.432731 4.886560 7.215964	C 0.193701 2.909309 0.113810	P 0.765109 1.492393 2.610432
C 0.553331 2.867428 6.491861	C -0.647266 3.570571 -0.779357	C -0.439362 0.065716 2.331630
C 0.636955 2.045692 5.373845	C -1.917591 3.964442 -0.384424	C 0.413609 -0.816375 3.236768
C 0.625794 2.587959 4.086211	H 4.682640 4.054051 0.968825	O 1.420090 0.120439 3.572071
C 0.546645 3.978577 3.952817	H 2.501720 3.814040 2.065780	



5D-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.01421910

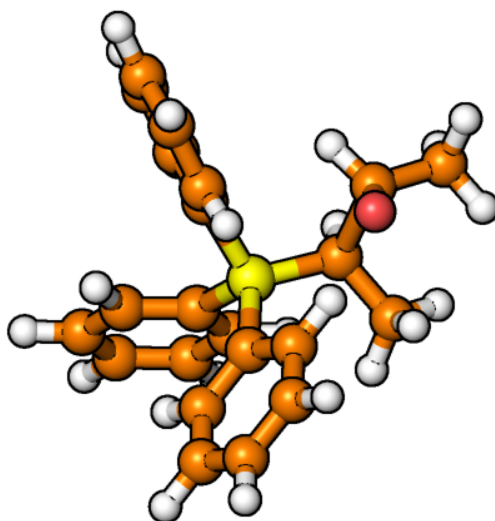
O 2.027027 1.200209 2.853243	C -1.829105 2.813287 0.591993	H -2.442253 4.794820 1.131103
C 1.557389 1.970264 2.043606	C -1.118008 -0.202686 2.658822	H -2.186182 2.373207 1.512588
P -0.900632 0.250106 -0.074046	C -1.787167 -0.539633 3.828828	H -0.081440 0.097510 2.702866
C 0.752385 0.042614 0.075414	C -3.120177 -0.932436 3.787093	H -1.260979 -0.494527 4.772942
C -1.851018 -0.580721 -1.419696	C -3.784880 -0.997718 2.567476	H -3.638388 -1.192336 4.700863
C -1.400466 -1.829781 -1.848401	C -3.118855 -0.670555 1.393498	H -4.820238 -1.309414 2.528234
C -2.066545 -2.510763 -2.858978	H 0.486740 2.235765 2.074053	H -3.638646 -0.738655 0.449058
C -3.183113 -1.940791 -3.462928	H 1.329236 0.672044 -0.589558	C 2.375230 2.746462 1.048654
C -3.630993 -0.690234 -3.051855	H -0.516433 -2.258723 -1.393846	H 1.795460 2.973345 0.155684
C -2.969364 -0.013761 -2.033077	H -1.711547 -3.480772 -3.181498	H 2.660585 3.696798 1.512774
C -1.224344 2.008995 -0.373372	H -3.697530 -2.466411 -4.256541	H 3.283561 2.203854 0.792599
C -1.782584 -0.264401 1.429833	H -4.493655 -0.240432 -3.526030	C 1.430574 -1.162653 0.671294
C -0.775541 2.588077 -1.563850	H -3.321376 0.960029 -1.719447	H 1.948667 -1.775779 -0.074082
C -0.908626 3.954369 -1.771407	H -0.323919 1.969188 -2.327792	H 2.172559 -0.862174 1.420219
C -1.506320 4.752901 -0.801288	H -0.552171 4.395063 -2.693027	H 0.722607 -1.818769 1.180559
C -1.970638 4.179332 0.376585	H -1.614221 5.816638 -0.966156	



5D-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.01497259

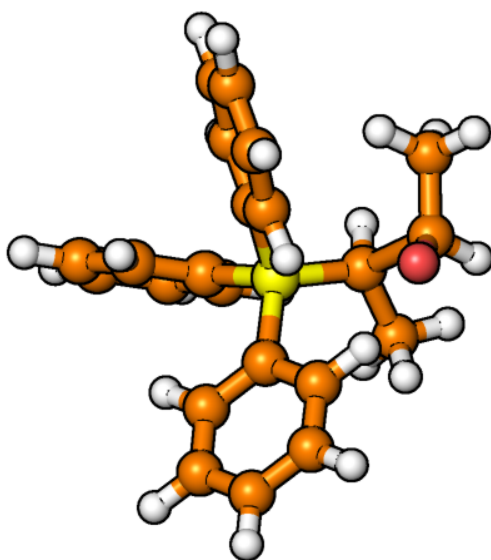
O 1.080302 2.172456 2.951359	C -1.364287 2.732848 0.777628	H -1.634802 4.763672 1.398042
C 1.792631 2.078716 1.978048	C -1.213365 -0.193469 2.713865	H -1.579088 2.333547 1.757388
P -0.860432 0.089133 -0.013381	C -1.890019 -0.549948 3.872537	H -0.239254 0.267410 2.773947
C 0.765787 -0.267313 0.161968	C -3.147310 -1.139384 3.795428	H -1.432342 -0.364878 4.835133
C -1.854530 -0.611609 -1.402665	C -3.727334 -1.372231 2.553908	H -3.672124 -1.419032 4.699581
C -1.390916 -1.780333 -2.004166	C -3.055540 -1.014152 1.391445	H -4.702194 -1.837002 2.487957
C -2.094847 -2.362338 -3.052324	H 1.490009 2.535856 1.019730	H -3.511216 -1.208198 0.432163
C -3.264094 -1.770368 -3.516519	H 1.407707 0.314557 -0.489366	C 3.145460 1.430162 1.988475
C -3.728137 -0.596574 -2.930028	H -0.467774 -2.222673 -1.652614	H 3.259301 0.778368 1.123191
C -3.027902 -0.021184 -1.877266	H -1.728196 -3.271422 -3.510701	H 3.907012 2.213041 1.911364
C -1.037373 1.876128 -0.272810	H -3.809335 -2.217278 -4.337382	H 3.298374 0.871541 2.909733
C -1.794330 -0.419394 1.461974	H -4.633443 -0.129310 -3.295273	C 1.297008 -1.567643 0.711035
C -0.736722 2.411631 -1.528313	H -3.391777 0.892921 -1.426596	H 1.587686 -2.296997 -0.055691
C -0.747429 3.786581 -1.723803	H -0.498086 1.752849 -2.352529	H 2.183157 -1.403407 1.334019
C -1.073739 4.636317 -0.672006	H -0.506675 4.193479 -2.697077	H 0.560025 -2.059684 1.348921
C -1.384730 4.107171 0.575553	H -1.086739 5.707393 -0.825147	



TS_{5→6}D-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.00469833

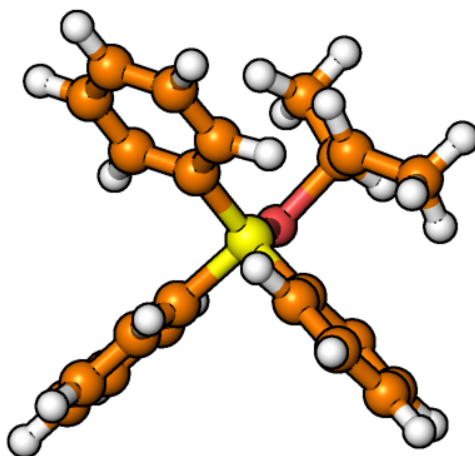
O 1.108999 1.501735 2.529093	C -1.399081 2.864250 0.951800	H -1.691745 4.887197 1.582692
C 1.624875 1.385521 1.376540	C -1.414589 -0.001797 2.839889	H -1.534027 2.462064 1.943165
P -0.876434 0.240924 0.140173	C -2.169760 -0.399635 3.935754	H -0.472445 0.533227 2.962718
C 0.817661 -0.132122 0.373373	C -3.363514 -1.090679 3.759257	H -1.816345 -0.171126 4.932455
C -1.616555 -0.533441 -1.332068	C -3.810101 -1.389479 2.477077	H -3.942904 -1.401124 4.618829
C -0.999888 -1.649215 -1.896890	C -3.068167 -0.993654 1.372063	H -4.734320 -1.933095 2.334331
C -1.565973 -2.278194 -2.999969	H 1.371646 2.143775 0.609089	H -3.420041 -1.238344 0.381136
C -2.749070 -1.794885 -3.545536	H 1.307503 -0.069332 -0.597598	C 3.102596 1.011296 1.291631
C -3.368338 -0.680028 -2.987785	H -0.074889 -2.018574 -1.477061	H 3.436216 0.834902 0.266526
C -2.806126 -0.051531 -1.885703	H -1.080919 -3.142256 -3.433316	H 3.677453 1.844895 1.703303
C -1.110046 2.018093 -0.118088	H -3.186662 -2.281967 -4.406535	H 3.315718 0.134418 1.903162
C -1.872126 -0.293498 1.550015	H -4.286561 -0.299199 -3.413872	C 1.128046 -1.401608 1.154663
C -0.891074 2.558421 -1.388595	H -3.284971 0.819102 -1.459540	H 0.441833 -2.235350 0.982177
C -0.968694 3.929248 -1.586828	H -0.662614 1.909693 -2.223024	H 2.128953 -1.748830 0.899681
C -1.261857 4.769748 -0.517909	H -0.796829 4.340465 -2.572484	H 1.119127 -1.185243 2.225571
C -1.474804 4.235894 0.747099	H -1.320775 5.839295 -0.671721	



TS_{5→6}D-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.00337973

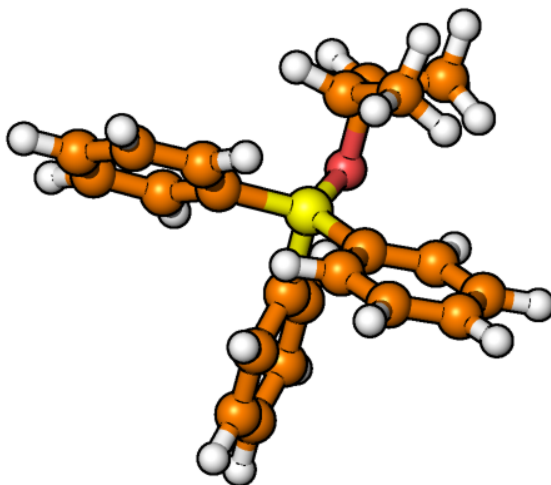
O 0.917411 1.746736 2.345938	C -1.497130 2.908949 0.882856	H -1.581167 2.534002 1.888900
C 1.636412 1.309941 1.390541	C -1.426468 0.070579 2.829632	H -0.507238 0.653261 2.922288
P -0.950809 0.275307 0.111825	C -2.139645 -0.342958 3.947769	H -1.779453 -0.075772 4.932397
C 0.762415 -0.067923 0.302526	C -3.298863 -1.098143 3.810024	H -3.845134 -1.419508 4.687090
C -1.710531 -0.528238 -1.335329	C -3.752368 -1.447678 2.543284	H -4.648726 -2.042531 2.429568
C -1.049774 -1.577418 -1.972298	C -3.053193 -1.037593 1.415979	H -3.410458 -1.324125 0.438565
C -1.629606 -2.208308 -3.067665	H 1.221953 0.035573 -0.681132	C 1.090011 -1.398857 0.968752
C -2.871118 -1.794062 -3.532931	H -0.079724 -1.893692 -1.618504	H 0.643943 -2.281073 0.498728
C -3.534446 -0.743774 -2.904391	H -1.108610 -3.019685 -3.557655	H 2.172357 -1.536197 0.959953
C -2.957615 -0.112516 -1.812131	H -3.319967 -2.282990 -4.387065	H 0.776596 -1.391781 2.012249
C -1.231004 2.039021 -0.173843	H -4.497810 -0.414205 -3.268952	C 2.131866 2.323733 0.357904
C -1.892618 -0.271173 1.554426	H -3.469345 0.711485 -1.334345	H 2.811270 3.008463 0.872613
C -1.072509 2.546600 -1.466256	H -0.860162 1.880091 -2.290655	H 2.676399 1.854846 -0.465481
C -1.183352 3.909827 -1.699500	H -1.055392 4.295885 -2.701774	H 1.311459 2.916893 -0.040929
C -1.455825 4.773707 -0.644147	H -1.541551 5.837197 -0.824957	H 2.455302 0.603857 1.650317
C -1.613672 4.271568 0.641738	H -1.812863 4.941651 1.466708	



TS_{7→8}D-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.02025631

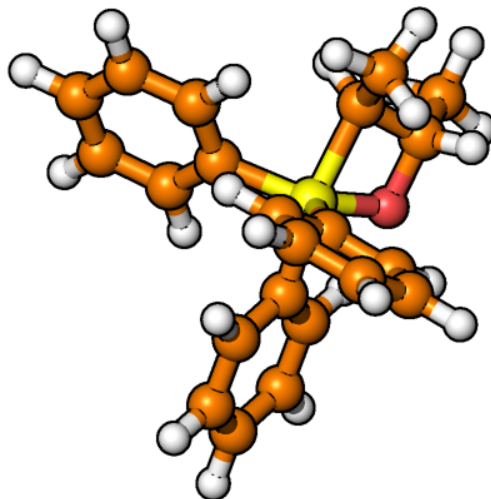
O 0.584265 0.380300 -0.422070	C 4.647819 4.035953 -0.250388	C 4.570010 -2.796929 0.708309
C 0.454423 0.265041 1.327119	C 5.293141 2.804992 -0.231180	H 4.531627 -4.873144 0.151293
C 1.797835 0.314216 1.795748	C 4.565386 1.626298 -0.337991	H 2.646984 -4.585862 -1.431019
P 2.118476 0.220673 -0.663943	C 3.174990 1.666753 -0.455541	H 1.678315 -2.355123 -1.805058
H 2.172738 -0.627837 2.180231	C 2.531919 2.907827 -0.483888	H 4.324138 -0.718464 1.139832
C 2.067817 0.142412 -5.316315	C 3.264218 4.081599 -0.381979	H 5.385664 -2.916355 1.409274
C 0.869506 0.246736 -4.622699	H 5.217861 4.951330 -0.166590	C 2.309451 1.536553 2.515658
C 0.863224 0.267727 -3.230697	H 6.370544 2.758704 -0.138703	H 3.395299 1.636885 2.430998
C 2.057725 0.185959 -2.515229	H 5.088476 0.681802 -0.342302	H 1.882476 2.451675 2.102547
C 3.257114 0.083128 -3.225393	H 1.455264 2.947102 -0.586333	H 2.072802 1.525254 3.587046
C 3.265644 0.060385 -4.611960	H 2.752186 5.034692 -0.404814	C -0.339976 -1.004487 1.464401
H 2.071790 0.125949 -6.398565	C 4.089620 -3.897145 0.002302	H -1.215784 -1.012785 0.818114
H -0.065991 0.311793 -5.163289	C 3.034295 -3.735767 -0.885490	H 0.281093 -1.868797 1.227821
H -0.067184 0.348044 -2.689488	C 2.479152 -2.477691 -1.088924	H -0.670686 -1.103142 2.501285
H 4.196250 0.018730 -2.690979	C 2.949644 -1.370843 -0.377450	H -0.138718 1.168238 1.442544
H 4.204549 -0.020695 -5.144019	C 3.989876 -1.549191 0.538028	



TS_{7→8}D-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.01861563

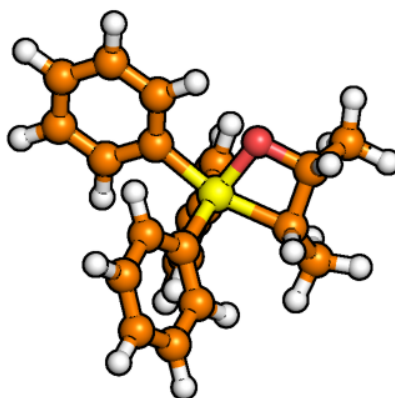
O 0.562014 0.386037 -0.422465	C 4.611756 4.047915 -0.236772	C 4.556733 -2.785529 0.720733
C 0.429595 0.384877 1.335406	C 5.255041 2.817874 -0.161079	H 4.575967 -4.849013 0.117604
C 1.778370 0.314031 1.795750	C 4.533246 1.636613 -0.275465	H 2.731256 -4.562302 -1.511556
P 2.096132 0.222087 -0.662656	C 3.150072 1.672244 -0.460239	H 1.730449 -2.344598 -1.865289
H 2.077359 -0.671125 2.131886	C 2.510030 2.912707 -0.551398	H 4.257724 -0.722811 1.189916
C 2.045950 0.139253 -5.315615	C 3.236528 4.089448 -0.437922	H 5.353462 -2.904728 1.443230
C 0.844816 0.201614 -4.621851	H 5.177280 4.965311 -0.145012	C 2.417691 1.444866 2.561420
C 0.838155 0.225416 -3.229813	H 6.326924 2.774586 -0.017707	H 3.495492 1.288490 2.651062
C 2.034946 0.187951 -2.514602	H 5.055622 0.692978 -0.233557	H 2.289362 2.412291 2.074907
C 3.237149 0.126493 -3.224936	H 1.441759 2.949799 -0.718437	H 2.027445 1.545983 3.582401
C 3.246121 0.101664 -4.611458	H 2.726652 5.041310 -0.509222	C -0.420586 1.602464 1.566122
H 2.050318 0.121405 -6.397855	C 4.119165 -3.878546 -0.022856	H -1.334036 1.570888 0.975841
H -0.092511 0.232133 -5.162347	C 3.086317 -3.717466 -0.936647	H -0.691435 1.647213 2.624387
H -0.094286 0.273845 -2.688169	C 2.512420 -2.466056 -1.128756	H 0.120327 2.515699 1.326432
H 4.177989 0.097694 -2.690284	C 2.940246 -1.365755 -0.381123	H -0.134009 -0.541201 1.375988
H 4.187243 0.054112 -5.143708	C 3.956982 -1.545621 0.560443	



7D-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.05300781

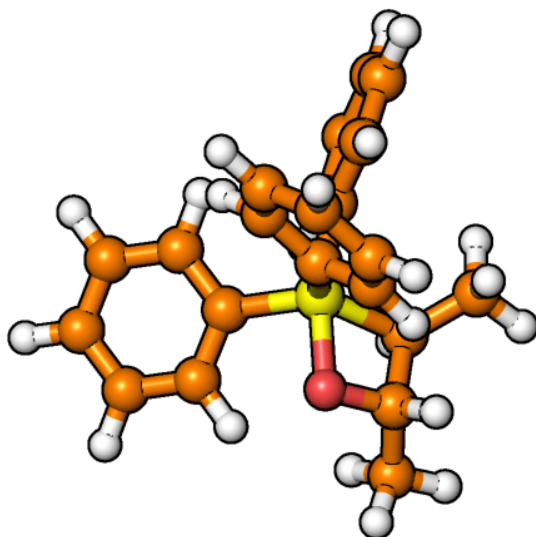
O 0.315073 0.300561 -0.091751	H 3.706742 0.378219 -4.847315	C 4.056978 -1.439979 0.986474
C 0.129244 0.391904 1.344323	C 4.130194 4.187146 -0.157184	C 4.922696 -2.517575 1.104042
C 1.553114 0.079295 1.758761	C 4.880552 3.038251 0.060752	H 5.536183 -4.405688 0.278479
P 1.977145 0.094964 -0.179209	C 4.270758 1.788336 0.047240	H 3.897580 -4.308199 -1.578092
H -0.148019 1.423246 1.582463	C 2.903052 1.674639 -0.192059	H 2.427976 -2.364370 -1.828097
H 1.628556 -0.943441 2.131902	C 2.155986 2.832012 -0.419894	H 4.086609 -0.664769 1.736553
C 1.671890 -0.312959 -4.861535	C 2.764786 4.079786 -0.399016	H 5.627492 -2.552898 1.924636
C 0.566732 -0.617892 -4.077962	H 4.605966 5.158687 -0.143828	C 2.188855 1.043856 2.745075
C 0.625008 -0.475944 -2.694101	H 5.945431 3.111641 0.239447	H 3.238265 0.813731 2.931882
C 1.788979 -0.031173 -2.064020	H 4.870097 0.904469 0.209346	H 2.143645 2.071653 2.384619
C 2.891785 0.267658 -2.868478	H 1.096019 2.749976 -0.623239	H 1.675497 1.006568 3.710865
C 2.838113 0.133989 -4.249267	H 2.173436 4.968410 -0.577096	C -0.953356 -0.562451 1.799422
H 1.626024 -0.419117 -5.937565	C 4.872297 -3.556953 0.180261	H -1.080893 -0.498777 2.881891
H -0.347548 -0.965748 -4.541963	C 3.956662 -3.499848 -0.861056	H -1.908324 -0.328370 1.327354
H -0.243426 -0.711633 -2.098764	C 3.116524 -2.399228 -0.997996	H -0.683619 -1.588682 1.544067
H 3.811788 0.609403 -2.413835	C 3.156722 -1.347225 -0.081295	



7D-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.05163068

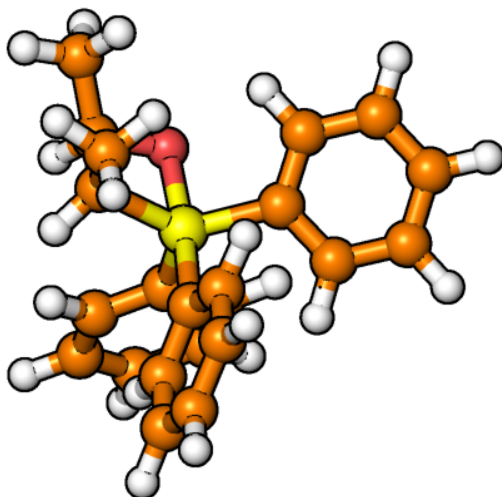
O 0.294879 0.229838 -0.066366	H 3.768267 0.339512 -4.799663	C 4.013401 -1.454609 1.003892
C 0.100760 0.335236 1.370954	C 4.144214 4.195624 -0.224468	C 4.857595 -2.549709 1.117925
C 1.553147 0.134530 1.784158	C 4.865280 3.058151 0.116562	H 5.423689 -4.453516 0.295123
P 1.959179 0.112885 -0.162573	C 4.246489 1.812572 0.132131	H 3.769474 -4.330289 -1.546191
H -0.541022 -0.495681 1.672694	C 2.900553 1.689628 -0.204657	H 2.340240 -2.355468 -1.792601
H 1.691850 -0.872775 2.175554	C 2.185847 2.834678 -0.561477	H 4.062793 -0.680153 1.754077
C 1.698929 -0.239185 -4.856927	C 2.800574 4.079436 -0.564799	H 5.568105 -2.597116 1.932947
C 0.566235 -0.493266 -4.095618	H 4.626341 5.164080 -0.232165	C -0.573189 1.647565 1.715033
C 0.608309 -0.372818 -2.708549	H 5.914471 3.136688 0.370184	H -0.737900 1.719881 2.791562
C 1.782522 0.002755 -2.052976	H 4.825678 0.938820 0.391829	H 0.030340 2.499194 1.404666
C 2.912844 0.252441 -2.837102	H 1.146494 2.745885 -0.849574	H -1.540740 1.713193 1.217057
C 2.877191 0.136572 -4.219462	H 2.232470 4.957752 -0.842070	C 2.176934 1.138012 2.737973
H 1.665877 -0.329952 -5.934875	C 4.776949 -3.591378 0.199202	H 3.228650 0.912125 2.917995
H -0.357426 -0.785774 -4.578883	C 3.852631 -3.519990 -0.833772	H 2.134832 2.157043 2.356910
H -0.280831 -0.571986 -2.131358	C 3.035230 -2.402489 -0.968343	H 1.675089 1.124337 3.709999
H 3.841392 0.541055 -2.362768	C 3.106436 -1.347792 -0.056594	



6D-CHMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.05600242

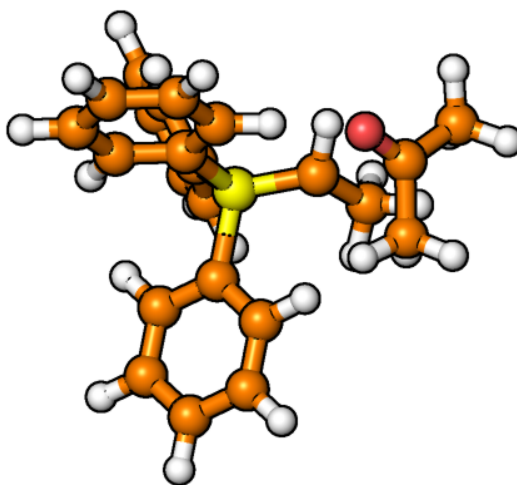
O 1.348473 0.132034 3.643580	C -1.935542 3.971002 -0.359145	C 0.576478 2.958208 6.498066
C 0.451848 -0.859154 3.162667	C -0.650886 3.610643 -0.739438	H 0.470052 4.995859 7.171220
C -0.414034 0.041533 2.283420	C 0.187332 2.945987 0.154136	H 0.445827 5.922202 4.871202
P 0.734115 1.488741 2.638656	C -0.232595 2.632835 1.446271	H 0.484230 4.424876 2.940721
H -1.365704 0.272076 2.769651	C -1.536317 2.997321 1.806175	H 0.733495 1.043206 5.542411
C 4.835954 1.904152 0.529981	C -2.378019 3.658473 0.923509	H 0.591377 2.542166 7.496936
C 4.203696 0.668104 0.597886	H -2.587343 4.487854 -1.051121	H 0.990414 -1.596641 2.550329
C 2.982676 0.543149 1.248677	H -0.294448 3.843033 -1.734972	C -0.664647 -0.370337 0.843191
C 2.360090 1.657472 1.810473	H 1.178401 2.668415 -0.174552	H -1.236998 0.384075 0.306943
C 2.999280 2.894430 1.733611	H -1.899538 2.770913 2.801718	H 0.268104 -0.532135 0.301656
C 4.234925 3.014954 1.109970	H -3.378172 3.932365 1.234601	H -1.231795 -1.303734 0.817767
H 5.793691 1.999308 0.035724	C 0.509441 4.333117 6.316611	C -0.267949 -1.582099 4.287029
H 4.667830 -0.204460 0.157289	C 0.494878 4.852572 5.027211	H -0.955148 -2.331832 3.888049
H 2.524246 -0.430976 1.330003	C 0.530407 4.001199 3.931825	H 0.447946 -2.085871 4.937300
H 2.538321 3.770353 2.165624	C 0.608012 2.613481 4.099098	H -0.841033 -0.874988 4.889919
H 4.724850 3.979082 1.074301	C 0.638887 2.106627 5.400991	



6D-CHMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1267.05297906

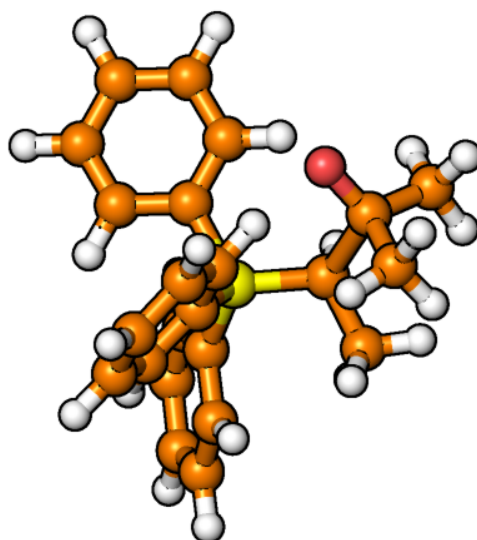
O 0.172788 0.465582 -0.061346	H 3.464705 2.538670 -4.456663	C 1.801918 -2.495953 -0.209983
C 0.190718 0.145184 1.322024	C 6.654238 0.448178 0.155271	C 1.586325 -3.760789 -0.744254
C 1.701570 0.331411 1.555540	C 5.884921 1.606874 0.194747	H 1.144613 -4.894591 -2.514451
P 1.947755 0.304933 -0.305204	C 4.511253 1.536136 0.008790	H 1.021439 -2.888982 -3.964396
H -0.081019 -0.908794 1.471879	C 3.860555 0.315908 -0.214731	H 1.377158 -0.652931 -3.018068
H 2.200212 -0.526040 2.012304	C 4.651224 -0.833317 -0.253525	H 2.025651 -2.403253 0.843705
C 1.819583 3.601202 -3.569787	C 6.031489 -0.770713 -0.073297	H 1.637392 -4.629044 -0.100381
C 0.915043 3.635649 -2.516920	H 7.726269 0.498577 0.293524	C -0.773875 1.010064 2.110216
C 0.937430 2.645055 -1.540611	H 6.356494 2.566793 0.362876	H -0.730492 0.776324 3.176220
C 1.890562 1.627483 -1.586091	H 3.938597 2.454707 0.018033	H -0.555675 2.069576 1.977925
C 2.807444 1.611430 -2.642541	H 4.198872 -1.795467 -0.443175	H -1.791065 0.828561 1.762655
C 2.760004 2.577800 -3.636527	H 6.618093 -1.679567 -0.119362	C 2.141006 1.600259 2.273674
H 1.792978 4.364919 -4.336036	C 1.310092 -3.910143 -2.097564	H 3.226157 1.668341 2.307993
H 0.179538 4.427223 -2.458534	C 1.243189 -2.784528 -2.910380	H 1.761440 2.500704 1.790136
H 0.206255 2.642080 -0.748579	C 1.452186 -1.519038 -2.376873	H 1.773425 1.594885 3.301352
H 3.562982 0.840634 -2.688043	C 1.741275 -1.361211 -1.021394	



5D-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1306.28167734

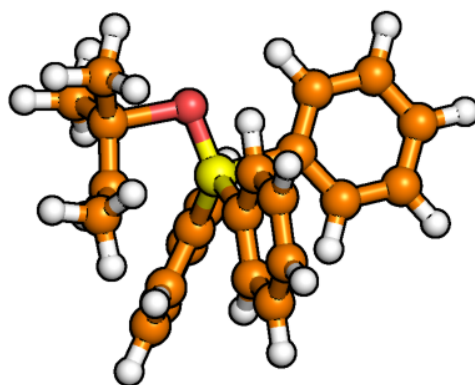
H 4.283481 1.244244 -1.086229	H -3.503160 1.767957 -0.353292	C -2.831299 3.798880 -0.361119
H 3.466094 -0.233396 -0.518362	H -3.834452 4.204178 -0.376695	C -1.731703 4.651726 -0.353557
H 4.972303 0.263125 0.234811	H -1.878998 5.724009 -0.364069	C -0.446515 4.123514 -0.322082
C 4.050175 0.636990 -0.215600	H 0.415995 4.775578 -0.301863	C -0.255129 2.747256 -0.299984
H 3.850742 0.579577 2.656102	H 0.745540 2.350933 -0.239255	C -1.801351 -0.428574 1.384636
H 2.470849 -0.207745 1.890684	H -2.322384 1.082461 -2.748971	C -1.353281 1.888643 -0.323822
H 2.258636 1.378811 2.678067	H -3.597817 -0.039414 -4.523278	C -2.626796 0.053337 -2.616426
C 2.931910 0.759097 2.091148	H -4.284073 -2.405109 -4.261916	C -3.341261 -0.582496 -3.622996
H 0.758970 -2.352261 -1.176837	H -3.677117 -3.636859 -2.199448	C -3.727156 -1.910818 -3.476955
H 0.376356 -2.283776 0.535705	H -2.420498 -2.512885 -0.413323	C -3.387537 -2.601103 -2.318779
H 1.981299 -1.858782 -0.015783	H 1.043852 0.299132 -1.073366	C -2.677260 -1.963956 -1.309697
C 0.917934 -1.766696 -0.260988	C -3.169290 -0.609017 1.594999	C -2.297642 -0.623550 -1.438577
H -3.860397 -0.519448 0.768840	C -3.649846 -0.912447 2.862389	C 0.505375 -0.316358 -0.361568
H -4.712162 -1.049990 3.016258	C -2.768104 -1.042465 3.930024	P -1.117832 0.096092 -0.224661
H -3.143644 -1.282593 4.915975	C -1.404552 -0.860540 3.727852	C 3.265642 1.447148 0.789455
H -0.715622 -0.957096 4.556649	C -0.924495 -0.547717 2.462606	O 2.938105 2.592369 0.566520
H 0.129845 -0.383188 2.289291	C -2.643706 2.424159 -0.345366	



TS_{5→6}D-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1306.26377911

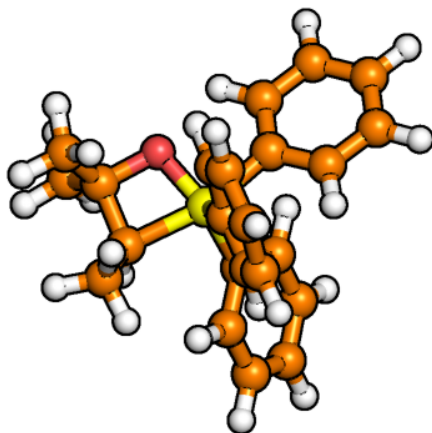
H 3.040554 1.551433 -0.793651	H -3.374710 1.766531 -0.261766	C -2.842074 3.825337 -0.475446
H 3.481699 -0.170781 -0.728955	H -3.869939 4.161627 -0.500811	C -1.800043 4.745004 -0.568430
H 4.137541 0.966674 0.456253	H -2.019869 5.799810 -0.670471	C -0.483343 4.309672 -0.511543
C 3.251005 0.712472 -0.130328	H 0.328059 5.023757 -0.551693	C -0.190828 2.955265 -0.381284
H 3.084470 -0.364663 2.506698	H 0.827904 2.625901 -0.234279	C -1.544392 -0.134332 1.548696
H 2.716272 -1.565666 1.265980	H -2.159144 1.116841 -2.623305	C -1.233176 2.032857 -0.314001
H 1.436734 -0.959434 2.331838	H -3.371345 -0.099988 -4.376712	C -2.382606 0.068931 -2.486160
C 2.333937 -0.684938 1.780428	H -3.886053 -2.506780 -4.097789	C -3.064747 -0.620821 -3.479532
H 0.407011 -2.010204 -1.592731	H -3.151128 -3.688375 -2.047806	C -3.352501 -1.971720 -3.323617
H 0.627705 -2.277777 0.136955	H -1.934629 -2.481179 -0.295964	C -2.942493 -2.634313 -2.172433
H 2.002121 -1.869339 -0.869531	H 1.020541 0.417300 -1.302327	C -2.258055 -1.948805 -1.178371
C 0.944816 -1.662617 -0.706730	C -2.774161 -0.763730 1.757779	C -1.985340 -0.582309 -1.314888
H -3.371101 -1.097864 0.923368	C -3.247231 -0.952572 3.050096	C 0.767153 -0.175913 -0.420163
H -4.197609 -1.445167 3.205320	C -2.504568 -0.504503 4.136121	P -0.924898 0.266806 -0.105393
H -2.874392 -0.654322 5.142115	C -1.294092 0.147442 3.926847	C 2.082584 0.515879 0.851119
H -0.721101 0.512823 4.768564	C -0.810251 0.343965 2.640450	O 1.658132 1.584023 1.417237
H 0.121723 0.881230 2.462131	C -2.561417 2.475352 -0.342812	



TS_{7→8}D-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1306.28455863

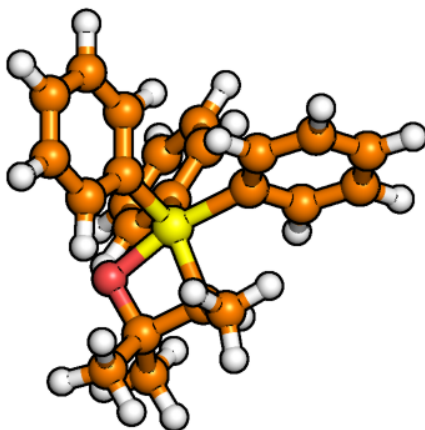
H 0.239575 2.392498 1.493469	C 4.618512 -2.818634 0.238032	H 3.827833 0.262573 -5.357842
H -0.405363 1.482286 2.856224	C 4.028304 -1.564160 0.199130	H 3.990471 0.181095 -2.912103
H -1.233170 1.432514 1.290962	C 2.914029 -1.328912 -0.609425	H -0.261139 0.491161 -2.596403
C -0.257325 1.467119 1.772643	C 2.380454 -2.390030 -1.345212	H -0.433585 0.578709 -5.062986
H -0.358099 -1.243291 2.596676	C 2.947980 -3.656625 -1.273210	H 1.612747 0.462701 -6.452461
H 0.448237 -1.870534 1.157617	C 4.076872 -3.872016 -0.493500	C 2.928108 0.313094 -4.758460
H -1.109423 -1.037391 1.004900	H 2.681026 5.094954 -0.496051	C 3.015970 0.267520 -3.375064
C -0.159991 -1.051534 1.538517	H 1.395958 2.998042 -0.660544	C 1.869825 0.329687 -2.577566
H 2.367326 1.399060 3.506882	H 5.049339 0.759366 -0.518035	C 0.629232 0.442413 -3.204473
H 2.413753 2.359946 2.034566	H 6.321547 2.844270 -0.353845	C 0.537598 0.490603 -4.593094
H 3.730256 1.274234 2.402598	H 5.153753 5.028283 -0.332011	C 1.684215 0.425386 -5.373298
C 2.643587 1.376689 2.444706	C 3.200353 4.145608 -0.490846	H 2.347480 -0.726995 1.969548
H 5.491276 -2.980013 0.856950	C 2.474207 2.966357 -0.578709	P 2.060960 0.277777 -0.726318
H 4.418377 -0.773996 0.821759	C 3.126385 1.729292 -0.571109	C 1.977116 0.252663 1.690074
H 1.520938 -2.224056 -1.979534	C 4.519196 1.699123 -0.496111	C 0.570484 0.261597 1.415388
H 2.512691 -4.470690 -1.837528	C 5.241489 2.882818 -0.409882	O 0.547420 0.418883 -0.386118
H 4.528480 -4.854038 -0.448126	C 4.587457 4.109368 -0.401487	



7D-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1306.31700664

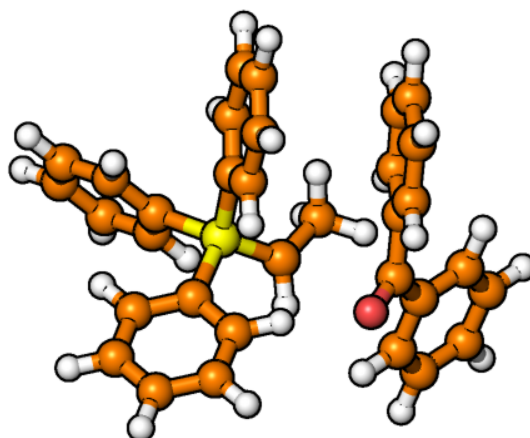
H -0.889497 -0.747336 2.949778	C 4.859282 -2.544464 1.134362	H 3.740356 0.310983 -4.792845
H -0.349999 -1.708424 1.565518	C 4.031264 -1.437088 1.020444	H 3.844507 0.537066 -2.359341
H -1.760991 -0.650795 1.412137	C 3.110698 -1.326387 -0.027965	H -0.286155 -0.528343 -2.067603
C -0.772855 -0.748855 1.864536	C 3.009430 -2.389579 -0.927083	H -0.394185 -0.767615 -4.512203
H 0.157575 2.557369 1.405420	C 3.810155 -3.519003 -0.791874	H 1.618093 -0.347934 -5.896385
H -0.620263 1.854017 2.826291	C 4.748112 -3.594563 0.228486	C 2.854042 0.123640 -4.200199
H -1.445587 1.831596 1.262613	H 2.313010 4.982296 -0.878610	C 2.907216 0.253658 -2.819565
C -0.474584 1.742145 1.751006	H 1.198731 2.784311 -0.850875	C 1.783682 0.024549 -2.019781
H 1.751626 1.198725 3.728074	H 4.860748 0.946933 0.395244	C 0.598029 -0.345187 -2.657745
H 2.219399 2.212411 2.362796	H 5.978619 3.130310 0.336456	C 0.538196 -0.480068 -4.042837
H 3.297465 0.956373 2.930488	H 4.712576 5.165749 -0.285407	C 1.664519 -0.246151 -4.819954
C 2.248430 1.196519 2.752991	C 2.871205 4.100438 -0.592506	H 1.743576 -0.811529 2.218121
H 5.580897 -2.594563 1.939338	C 2.240440 2.863861 -0.568699	P 1.982369 0.150962 -0.130580
H 4.103430 -0.655503 1.761330	C 2.942318 1.714778 -0.199727	C 1.605556 0.191392 1.814410
H 2.303611 -2.339433 -1.741872	C 4.291873 1.824930 0.127234	C 0.138343 0.388209 1.429286
H 3.703606 -4.335360 -1.494132	C 4.926873 3.061824 0.090610	O 0.326798 0.297938 -0.019355
H 5.382091 -4.466079 0.324568	C 4.218230 4.203748 -0.261636	



6D-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1692.48758376

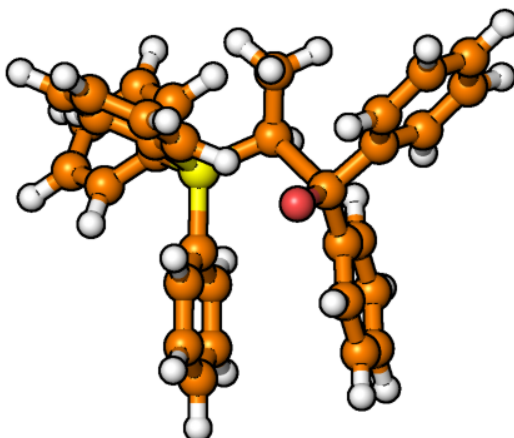
H -0.879324 -0.334006 4.827874	C 0.884759 2.723402 6.451981	H 4.598870 4.208085 1.141136
H 0.178430 -1.718037 5.127345	C 0.896204 1.925349 5.314173	H 2.399508 3.808059 2.149987
H -1.289646 -1.918312 4.159901	C 0.649998 2.470954 4.050543	H 2.735541 -0.358834 1.242607
C -0.464815 -1.240199 4.386565	C 0.422101 3.849674 3.964826	H 4.892259 0.054604 0.136489
H 1.459603 -1.999246 1.609207	C 0.426964 4.649651 5.099341	H 5.850317 2.339312 0.100607
H 0.094359 -2.898745 2.273939	C 0.649558 4.087986 6.350853	C 4.183243 3.208881 1.140076
H 1.561208 -2.668090 3.235421	H -3.376574 3.854746 1.168329	C 2.942012 2.979818 1.718570
C 0.891533 -2.193804 2.517022	H -1.899660 2.665509 2.712502	C 2.397355 1.695197 1.750796
H -1.178594 -1.317224 0.639346	H 1.212439 2.704598 -0.229097	C 3.120876 0.646591 1.186803
H 0.336038 -0.525855 0.202841	H -0.263243 3.895658 -1.770667	C 4.348970 0.879304 0.578512
H -1.167688 0.381459 0.168528	H -2.572719 4.487094 -1.093680	C 4.886578 2.160131 0.558057
C -0.617259 -0.383520 0.711664	C -2.369637 3.605389 0.859280	H -1.424471 0.283557 2.575252
H 1.071637 2.274338 7.418722	C -1.527513 2.928977 1.729672	P 0.758906 1.413535 2.535242
H 1.120958 0.875419 5.392437	C -0.212648 2.596719 1.376200	C -0.448358 0.012016 2.171008
H 0.233595 4.309156 3.008017	C 0.214108 2.955506 0.098152	C 0.332346 -0.912950 3.124304
H 0.252078 5.713208 5.002441	C -0.625757 3.631486 -0.785532	O 1.398442 0.000177 3.415404
H 0.645424 4.709415 7.236819	C -1.919448 3.962048 -0.409198	



5D-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1689.20366900

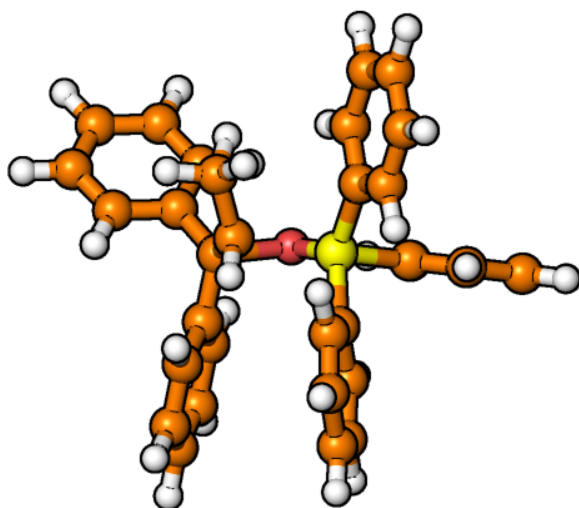
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H 2.586795 -3.861686 -0.203503	C 5.833355 -0.832639 1.409213	C -1.358479 0.206339 3.376397
H 3.414512 -2.349148 0.130013	C 3.435015 -0.422400 2.751359	C -0.644430 -0.373158 2.336304
C 2.455370 -2.771566 -0.180794	C 4.887188 0.041849 0.887459	C -0.632658 0.296767 -1.109305
H 2.465241 2.672428 -4.100121	C 3.675842 0.248935 1.549514	C -0.701470 1.112714 -2.228811
H 2.010316 4.317109 -2.309009	H -2.937083 -2.665749 1.337838	C -0.520737 0.574659 -3.498120
H 2.969535 0.321301 -3.517571	H -4.194283 -1.635479 3.178429	C -0.268061 -0.783268 -3.643719
H 2.073889 3.599596 0.068353	H -3.193919 0.208481 4.493387	C -0.218313 -1.606363 -2.524623
H 3.079184 -0.366690 -1.153817	H -0.911524 1.015184 3.938923	C -1.204661 -1.413097 1.588454
C 2.508506 2.368279 -3.062441	H 0.341999 -0.009645 2.098945	C -0.406519 -1.074509 -1.247219
C 2.249037 3.292577 -2.055646	H -0.753140 0.728832 -0.126249	C -2.350813 -3.575116 -1.072246
C 2.804303 1.050108 -2.736176	H -0.879409 2.172331 -2.108118	C -3.031909 -4.741508 -1.394043
C 2.290501 2.899157 -0.726175	H -0.565357 1.214466 -4.369349	C -2.568910 -5.969444 -0.929103
C 2.870825 0.660513 -1.406344	H -0.116479 -1.205846 -4.628541	C -1.424877 -6.026225 -0.142000
C 2.622669 1.585281 -0.391027	H -0.049584 -2.667557 -2.648790	C -0.744798 -4.856610 0.179440
H 1.490579 -2.349651 1.790086	H -2.711682 -2.624352 -1.441363	C -1.202283 -3.623098 -0.278186
H 6.303189 -2.206363 2.988806	H -3.921789 -4.694927 -2.008318	C 1.348417 -2.295323 0.720159
H 4.164616 -1.836652 4.181855	H -3.097457 -6.878474 -1.184165	P -0.238599 -2.131059 0.231605
H 6.771194 -0.981221 0.891002	H -1.060840 -6.979723 0.217287	C 2.646692 1.207894 1.053257
H 2.501898 -0.245493 3.265475	H 0.152081 -4.884815 0.786492	O 1.843591 1.709140 1.824869
H 5.098912 0.573917 -0.027996	C -2.491314 -1.858512 1.899246	
C 5.572083 -1.515856 2.589153	C -3.201189 -1.277046 2.942610	



TS_{5→6}D-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1689.18840828

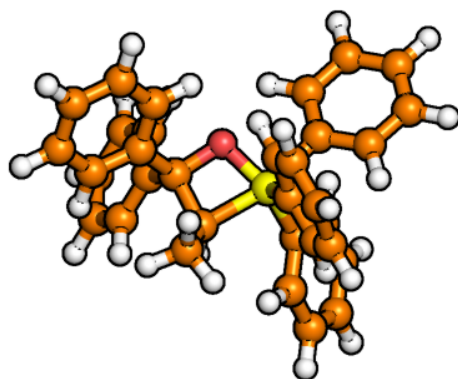
H 1.161636 -0.133875 -2.683143	C 2.630050 0.249916 3.809627	C -0.871298 -0.645091 4.114971
H 0.943744 -1.850222 -2.993130	C 3.549532 -1.796624 2.968983	C -0.181911 -1.790538 3.733064
H 2.556450 -1.193717 -2.711461	C 2.263893 0.612461 2.520718	C -0.003809 -2.074560 2.388766
C 1.514631 -1.125594 -2.403276	C 3.182743 -1.427332 1.680206	C -1.230771 0.681292 -1.532474
H 6.080360 1.595160 -3.415332	C 2.536452 -0.214381 1.429778	C -2.140357 1.392362 -2.303720
H 3.947951 2.861183 -3.369277	H -1.554132 0.633559 1.057790	C -3.230887 0.751086 -2.881620
H 6.430064 -0.257214 -1.805632	H -1.898648 1.116945 3.444531	C -3.415299 -0.612699 -2.688466
H 2.182924 2.244916 -1.725777	H -1.007093 -0.421835 5.164833	C -2.514913 -1.335023 -1.915438
H 4.684846 -0.847984 -0.202520	H 0.230216 -2.454565 4.479694	C -0.506012 -1.206752 1.416095
C 5.302932 1.331565 -2.709993	H 0.536105 -2.964422 2.098990	C -1.422926 -0.690156 -1.330575
C 4.106272 2.038516 -2.683138	H -0.366883 1.162170 -1.079151	C -1.786377 -3.855263 0.276713
C 5.495945 0.290331 -1.808942	H -1.990566 2.452925 -2.456791	C -2.158402 -5.186338 0.154441
C 3.113070 1.697432 -1.774226	H -3.932842 1.311267 -3.485390	C -1.446123 -6.035123 -0.687459
C 4.499011 -0.047477 -0.901063	H -4.257748 -1.118434 -3.140960	C -0.361228 -5.548716 -1.406334
C 3.285806 0.642375 -0.877839	H -2.664971 -2.395284 -1.777848	C 0.012672 -4.215234 -1.286789
H 2.026266 -2.168532 -0.556787	H -2.335384 -3.201476 0.939944	C -0.696800 -3.359137 -0.445055
H 3.561885 -1.244162 5.046751	H -3.000287 -5.562836 0.719841	C 1.423822 -1.329741 -0.895422
H 2.402147 0.910317 4.636805	H -1.734507 -7.073835 -0.778487	P -0.228076 -1.603481 -0.325037
H 4.045144 -2.745337 3.132913	H 0.197340 -6.205969 -2.059018	C 2.113624 0.330914 0.057596
H 1.743322 1.538436 2.325942	H 0.859061 -3.841759 -1.844488	O 1.180230 1.198524 0.078854
H 3.394271 -2.112765 0.873340	C -1.186767 -0.054872 1.801597	
C 3.277753 -0.957438 4.042535	C -1.372444 0.219024 3.150234	



TS_{7→8}D-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1689.19827913

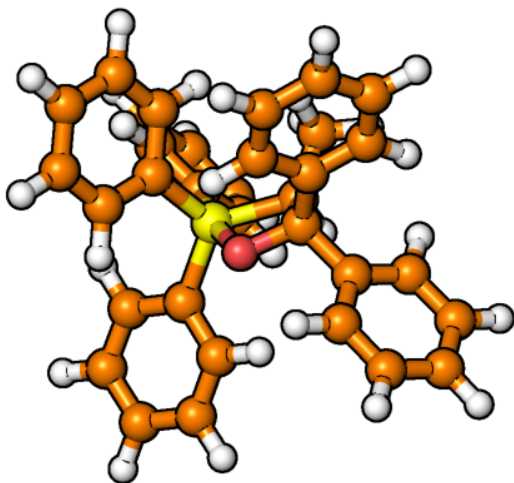
H 3.050682 2.540825 1.748568	C -0.649811 3.546735 1.955773	C 3.930612 1.554847 -0.928861
H 4.530716 1.612292 1.896114	C 0.312694 1.356430 3.348025	C 5.290154 1.267703 -1.061342
H 3.353935 1.622551 3.210363	C 0.058489 2.554096 1.284887	C 6.220815 2.297910 -1.111084
C 3.462237 1.602989 2.119367	C 0.549662 1.449590 1.973897	C 5.809426 3.623734 -1.036004
H -1.102582 -4.444140 1.552555	H 5.508793 -3.524485 0.450923	H 3.745182 -0.119134 -5.695970
H -2.165185 -2.520706 0.401497	H 4.974445 -1.133614 0.322758	H 4.208438 -0.142644 -3.288408
H 1.100157 -4.144897 2.646863	H 1.366172 -2.051911 -1.796581	H 0.130146 0.849749 -2.473352
H -1.014637 -0.343246 0.322433	H 1.840267 -4.451590 -1.558779	H -0.340843 0.888816 -4.899601
H 2.227268 -1.969127 2.578986	H 3.929967 -5.203496 -0.458293	H 1.466197 0.400778 -6.520757
C -0.604819 -3.483791 1.524267	C 4.599990 -3.204628 -0.041652	C 2.949665 0.096979 -4.994797
C -1.200499 -2.403244 0.877675	C 4.311529 -1.850841 -0.136592	C 3.207809 0.084539 -3.632139
C 0.628122 -3.315874 2.136457	C 3.151729 -1.419311 -0.781629	C 2.197946 0.356392 -2.705125
C -0.559636 -1.176067 0.838143	C 2.273673 -2.371650 -1.304563	C 0.918710 0.644289 -3.180763
C 1.269836 -2.082007 2.094004	C 2.545003 -3.726680 -1.174408	C 0.657532 0.662176 -4.548136
C 0.693468 -1.000951 1.432779	C 3.713538 -4.147757 -0.552922	C 1.669826 0.388271 -5.458038
H -1.430577 4.221173 3.840412	H 4.122960 4.942931 -0.862768	H 3.271125 -0.535312 1.753597
H -0.567665 2.253455 5.080624	H 2.469277 3.122809 -0.772145	P 2.617757 0.315079 -0.894090
H -1.026474 4.397710 1.402957	H 5.630531 0.246545 -1.141320	C 2.799464 0.400473 1.497605
H 0.687171 0.499786 3.892982	H 7.271618 2.061240 -1.215508	C 1.370840 0.344635 1.359363
H 0.224530 2.625636 0.222262	H 6.537447 4.422767 -1.073403	O 1.186650 0.683770 -0.383217
C -0.878477 3.448902 3.321453	C 4.455175 3.914631 -0.916994	
C -0.394201 2.344985 4.016372	C 3.521407 2.889747 -0.865459	



7D-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1689.22830685

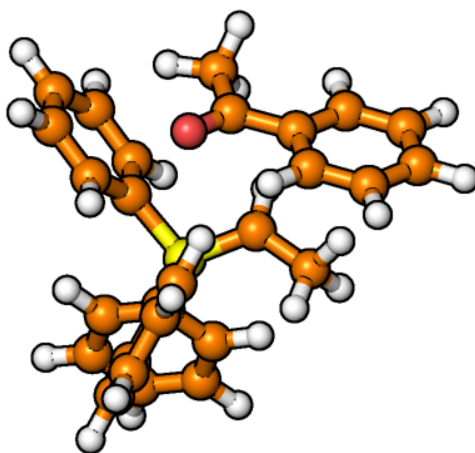
H -2.685392 -4.370453 2.848467	H 1.671742 1.207350 3.786782	C 2.766463 1.710069 -0.128822
H -0.914563 -3.511810 4.352396	H 1.731680 2.261898 2.381898	C 4.131620 1.826038 0.123627
H -3.195173 -3.162942 0.745086	H 3.120327 1.269356 2.786425	C 4.750288 3.071185 0.093558
H 0.338977 -1.487139 3.755566	C 2.029905 1.285023 2.757678	C 4.010388 4.215533 -0.177162
H -1.944859 -1.118742 0.160488	H 5.546343 -2.539838 1.901090	H 3.456981 0.426843 -4.759646
C -2.139059 -3.473331 2.589840	H 4.030204 -0.624262 1.767256	H 3.616558 0.630230 -2.329188
C -1.146212 -2.991597 3.432295	H 2.145974 -2.347361 -1.672302	H -0.452355 -0.628414 -1.943461
C -2.423454 -2.795260 1.408879	H 3.590622 -4.319378 -1.468701	H -0.618961 -0.831821 -4.385035
C -0.438710 -1.843182 3.093205	H 5.326766 -4.417261 0.296335	H 1.335079 -0.306255 -5.816871
C -1.720738 -1.645749 1.076974	C 4.798616 -2.503041 1.119294	C 2.595114 0.195511 -4.146915
C -0.716252 -1.159380 1.913019	C 3.947995 -1.410829 1.031521	C 2.680102 0.311882 -2.766676
H -2.943541 4.361251 3.138533	C 2.991045 -1.321705 0.014288	C 1.589433 0.025122 -1.939940
H -2.095086 2.725598 4.796895	C 2.880243 -2.385196 -0.882090	C 0.404583 -0.389516 -2.552697
H -2.449323 4.026029 0.732961	C 3.705152 -3.499315 -0.771833	C 0.312194 -0.508259 -3.937262
H -0.774705 0.792354 4.061752	C 4.675710 -3.556369 0.218687	C 1.405909 -0.215883 -4.740594
H -1.108658 2.086068 0.005183	H 2.062737 4.990445 -0.648685	H 1.802757 -0.798721 2.324845
C -2.352319 3.514814 2.814985	H 0.976005 2.785892 -0.626854	P 1.836244 0.126872 -0.054830
C -1.874669 2.596681 3.745232	H 4.724793 0.946966 0.328458	C 1.503842 0.153422 1.896501
C -2.072359 3.327302 1.468447	H 5.813702 3.144252 0.281272	C 0.008261 0.125880 1.540492
C -1.121308 1.508464 3.329467	H 4.492004 5.184212 -0.194872	O 0.174544 0.156081 0.097000
C -1.311611 2.238037 1.054061	C 2.647743 4.106577 -0.431509	
C -0.820230 1.322308 1.979619	C 2.033028 2.862234 -0.414407	



6D-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1689.23521271

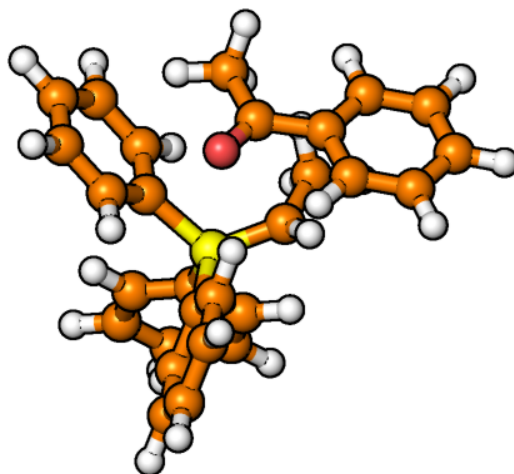
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H 0.978751 -4.954955 0.687999	H 0.163630 -0.768442 0.176625	C 0.229231 3.335587 0.278084
H 4.488110 -2.586974 1.338183	H -1.187420 0.376503 0.168486	C -0.564234 4.186308 -0.490202
H -0.356483 -3.310067 1.927491	C -0.732229 -0.452914 0.707382	C -1.911484 4.341704 -0.199075
H 3.126237 -0.928562 2.567237	H -0.397309 2.492828 7.222032	H 5.478843 2.422588 2.460663
C 2.823688 -3.876985 0.919438	H -0.080392 0.974193 5.309265	H 3.226011 2.361153 3.451452
C 1.456184 -4.070961 1.090433	H 1.014719 4.306239 2.852516	H 1.674400 0.737288 -0.197117
C 3.423663 -2.745286 1.455668	H 0.828598 5.801384 4.790888	H 3.929133 0.746940 -1.163749
C 0.701297 -3.136163 1.784881	H 0.087902 4.909998 6.982140	H 5.845922 1.599170 0.153364
C 2.663639 -1.806948 2.146412	C -0.073173 2.890775 6.269443	C 4.646115 2.052379 1.877519
C 1.293719 -1.986032 2.308925	C 0.087469 2.032624 5.186908	C 3.374080 2.029486 2.433553
H -2.117689 -3.367323 7.135296	C 0.480665 2.530807 3.944837	C 2.289631 1.558640 1.692654
H 0.215003 -2.576660 7.405688	C 0.729317 3.899742 3.812077	C 2.501387 1.104699 0.391826
H -3.279885 -3.031126 4.973538	C 0.611129 4.747483 4.903939	C 3.777201 1.114113 -0.157720
H 1.367199 -1.455297 5.523795	C 0.197732 4.246227 6.134516	C 4.852515 1.589903 0.582001
H -2.128697 -1.917892 3.112140	H -3.506379 3.766110 1.123170	H -1.361873 0.157940 2.660353
C -1.609608 -2.880319 6.313567	H -2.106668 2.295481 2.482176	P 0.656958 1.423617 2.489342
C -0.299507 -2.435250 6.463964	H 1.276928 3.245405 0.034196	C -0.426623 -0.055418 2.139646
C -2.260419 -2.692048 5.101667	H -0.121259 4.729011 -1.315637	C 0.465743 -0.940071 3.055188
C 0.352708 -1.810157 5.410297	H -2.528450 5.001052 -0.795380	O 1.280439 0.102734 3.563203
C -1.605191 -2.060290 4.048836	C -2.459471 3.646191 0.875319	
C -0.294583 -1.612665 4.191031	C -1.661830 2.804287 1.635480	



5D-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.74550309

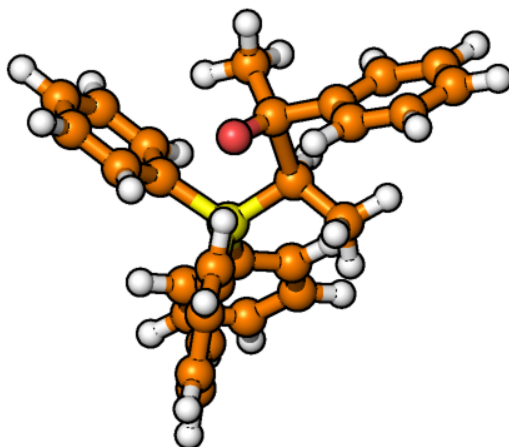
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C 2.258805 0.900046 1.863829	C -3.340248 -0.822411 1.255430	H 0.618310 -3.352864 -0.421921
P -0.991633 -0.359400 -0.264756	H 1.246069 -0.777576 -0.789083	C 2.698961 1.672380 0.643477
C 0.461876 -1.174683 -0.157434	H -1.398389 -2.694491 -1.872683	H 3.761016 1.917233 0.718215
C -2.218156 -0.736366 -1.595473	H -3.000681 -3.320551 -3.655887	H 2.554294 1.086037 -0.261841
C -2.158676 -1.994176 -2.193559	H -4.698021 -1.687601 -4.416846	H 2.119700 2.587295 0.574062
C -3.052708 -2.340282 -3.200341	H -4.800457 0.558318 -3.382631	C 2.876804 -0.434415 2.130725
C -4.006522 -1.423095 -3.627683	H -3.224544 1.164210 -1.584906	C 2.508698 -1.124373 3.288116
C -4.064809 -0.160418 -3.045412	H -0.068987 1.099288 -2.576668	C 3.816751 -1.007773 1.272791
C -3.176437 0.180261 -2.032951	H 0.533934 3.459164 -2.954369	C 3.063626 -2.360275 3.579629
C -0.670298 1.405324 -0.533082	H 0.229481 5.121491 -1.143818	C 4.375534 -2.245026 1.564669
C -1.966127 -0.578572 1.256670	H -0.648486 4.398597 1.056185	C 4.001365 -2.923577 2.718837
C -0.182413 1.818640 -1.776454	H -1.197667 2.036281 1.452441	H 1.785531 -0.668775 3.949195
C 0.149913 3.149206 -1.991408	H -0.224960 -0.300524 2.475567	H 4.109157 -0.495986 0.367592
C -0.022210 4.082918 -0.974064	H -1.441567 -0.559743 4.609168	H 2.767341 -2.887292 4.476914
C -0.519270 3.678821 0.259206	H -3.881390 -0.996276 4.597156	H 5.099326 -2.681739 0.889532
C -0.837601 2.344588 0.482663	H -5.089697 -1.168592 2.444270	H 4.434372 -3.889131 2.944423
C -1.287091 -0.491545 2.475574	H -3.875667 -0.904402 0.321340	
C -1.975882 -0.637338 3.671548	C 0.602008 -2.583329 0.361000	
C -3.345697 -0.879442 3.664085	H 1.525501 -2.699759 0.932542	



5D-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.74378442

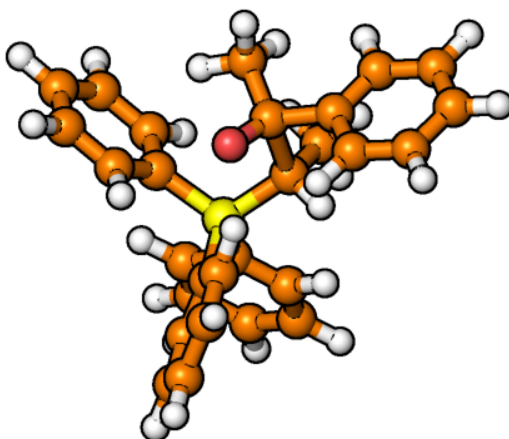
O 1.451050 1.352821 2.711212	C -4.046780 -0.948596 2.448052	H 2.029665 2.670569 0.682303
C 2.254945 0.937970 1.894911	C -3.323852 -0.778504 1.273331	C 2.896366 -0.399292 2.071998
P -0.992579 -0.293528 -0.193998	H -1.405176 -2.717792 -1.621802	C 2.513364 -1.189875 3.159230
C 0.358953 -1.271322 -0.118817	H -2.919347 -3.400806 -3.479397	C 3.856347 -0.888111 1.184610
C -2.092542 -0.698633 -1.599808	H -4.467517 -1.743944 -4.471902	C 3.062550 -2.447497 3.343501
C -2.085850 -2.008859 -2.076141	H -4.499728 0.579680 -3.622176	C 4.411906 -2.146990 1.371636
C -2.935780 -2.384266 -3.108989	H -2.975229 1.250202 -1.801922	C 4.013308 -2.930638 2.447463
C -3.805740 -1.453412 -3.666261	H 0.059997 1.218483 -2.418595	H 1.776649 -0.799194 3.846523
C -3.823430 -0.146071 -3.189884	H 0.664820 3.579793 -2.743094	H 4.165884 -0.295248 0.336974
C -2.967183 0.231457 -2.163465	H 0.202818 5.238192 -0.960984	H 2.751467 -3.055656 4.182551
C -0.747516 1.511776 -0.442610	H -0.864643 4.505998 1.150742	H 5.151427 -2.517785 0.674310
C -1.960669 -0.481869 1.322607	H -1.458641 2.147164 1.484094	H 4.441746 -3.913832 2.589351
C -0.141373 1.934993 -1.632117	H -0.288699 -0.077922 2.622480	H 0.620619 -1.634033 0.861904
C 0.198429 3.266583 -1.818105	H -1.567438 -0.398280 4.690184	C 1.346112 -1.402264 -1.245468
C -0.062016 4.199040 -0.817044	H -3.981166 -0.951007 4.594334	H 2.125971 -0.624959 -1.270255
C -0.661994 3.788217 0.366859	H -5.101379 -1.184810 2.398120	H 1.871085 -2.358152 -1.186811
C -1.001312 2.452805 0.555036	H -3.819997 -0.885775 0.319954	H 0.857749 -1.372388 -2.224849
C -1.333461 -0.343317 2.564615	C 2.633706 1.769607 0.696420	
C -2.061542 -0.513749 3.734383	H 3.691587 2.037950 0.739541	
C -3.417501 -0.818962 3.680180	H 2.471235 1.211377 -0.224828	



TS_{5→6}D-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.72742839

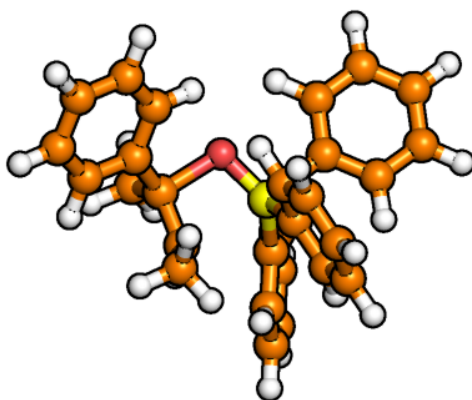
O 1.149444 0.893450 2.350447	C -4.181321 -0.968410 2.428738	H 2.830321 0.623397 -0.498143
C 1.810486 0.271945 1.444441	C -3.349002 -0.783195 1.332537	H 1.742123 1.913609 0.032614
P -0.926415 -0.074514 0.114877	H 1.112865 -0.989208 -0.571310	C 2.780984 -0.802633 1.940126
C 0.623012 -0.889238 0.397631	H -0.502896 -2.430964 -1.560023	C 2.760642 -1.132214 3.293064
C -1.786996 -0.723207 -1.352999	H -1.687125 -3.325917 -3.525784	C 3.681935 -1.471710 1.109155
C -1.359970 -1.906250 -1.954156	H -3.643335 -2.124146 -4.448973	C 3.601058 -2.114835 3.803125
C -2.027961 -2.408686 -3.065493	H -4.405575 -0.016804 -3.395275	C 4.526847 -2.452858 1.613581
C -3.125736 -1.733635 -3.583182	H -3.219323 0.881879 -1.435682	C 4.486569 -2.782572 2.964951
C -3.555412 -0.549465 -2.991035	H -0.414382 1.394517 -2.329329	H 2.072405 -0.588798 3.925438
C -2.889896 -0.045421 -1.883556	H -0.032774 3.776401 -2.799946	H 3.721395 -1.238554 0.053523
C -0.770288 1.694542 -0.224822	H -0.170992 5.439118 -0.970576	H 3.567369 -2.359456 4.857700
C -2.043770 -0.320144 1.516951	H -0.683950 4.697056 1.334674	H 5.217835 -2.961203 0.952603
C -0.480950 2.114570 -1.525780	H -1.023033 2.311255 1.817809	H 5.142371 -3.548202 3.359318
C -0.265190 3.458824 -1.792492	H -0.539393 0.274483 2.933740	C 0.421455 -2.238532 1.091443
C -0.342659 4.390990 -0.763575	H -2.047533 -0.039864 4.891124	H -0.413016 -2.829497 0.700825
C -0.634747 3.976033 0.530294	H -4.367421 -0.842043 4.563017	H 1.325650 -2.834804 0.988929
C -0.843022 2.631384 0.805361	H -5.189023 -1.331826 2.279097	H 0.247223 -2.098828 2.157909
C -1.570346 -0.058806 2.807855	H -3.718221 -1.011623 0.344570	
C -2.415515 -0.243786 3.894208	C 2.451060 1.164443 0.368224	
C -3.717734 -0.695096 3.710123	H 3.288189 1.685788 0.837403	



TS_{5→6}D-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.72808904

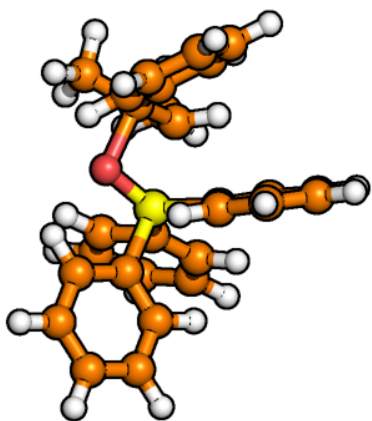
O 1.091768 0.872813 2.288996	C -4.158540 -0.739064 2.369262	H 1.794008 2.105454 0.141581
C 1.830922 0.344113 1.381867	C -3.321558 -0.520293 1.284808	C 2.771994 -0.770140 1.854809
P -0.876481 -0.022383 0.058781	H -1.182483 -2.730190 -0.804104	C 2.470920 -1.425570 3.050017
C 0.735317 -0.760011 0.215279	H -2.504363 -3.825195 -2.569810	C 3.920826 -1.161994 1.165001
C -1.810425 -0.741720 -1.328930	H -3.899962 -2.465160 -4.098706	C 3.267193 -2.457617 3.524618
C -1.784133 -2.131696 -1.475118	H -3.974587 -0.004717 -3.836114	C 4.726746 -2.192968 1.639503
C -2.533580 -2.748660 -2.465744	H -2.657606 1.090303 -2.070479	C 4.399640 -2.851478 2.817277
C -3.319213 -1.984197 -3.322925	H -0.186372 1.499327 -2.331440	H 1.608709 -1.088053 3.606869
C -3.358469 -0.603065 -3.178226	H 0.157686 3.900907 -2.723756	H 4.207280 -0.654531 0.255398
C -2.609899 0.017203 -2.183980	H -0.206336 5.521785 -0.888461	H 3.012301 -2.950632 4.454345
C -0.760091 1.748095 -0.267626	H -0.906130 4.720189 1.346106	H 5.615214 -2.476026 1.089223
C -1.951950 -0.311303 1.487165	H -1.219738 2.310468 1.751847	H 5.025434 -3.653173 3.187528
C -0.356087 2.200846 -1.526846	H -0.375290 -0.089382 2.917014	H 0.612272 -1.635309 0.851296
C -0.160618 3.556345 -1.749206	H -1.874493 -0.537752 4.863651	C 1.386462 -1.106363 -1.114549
C -0.364523 4.465242 -0.716405	H -4.292708 -0.928180 4.503948	H 2.390335 -1.484203 -0.921538
C -0.762712 4.016815 0.537387	H -5.215172 -0.902801 2.204338	H 0.859142 -1.871695 -1.689333
C -0.956165 2.661406 0.767088	H -3.737632 -0.520349 0.288259	H 1.486301 -0.228947 -1.754713
C -1.430874 -0.318197 2.783219	C 2.511537 1.349165 0.443350	
C -2.281053 -0.538505 3.860751	H 3.293518 1.846479 1.021157	
C -3.638881 -0.752409 3.659700	H 2.970659 0.920870 -0.445645	



TS_{7→8}D-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.73989260

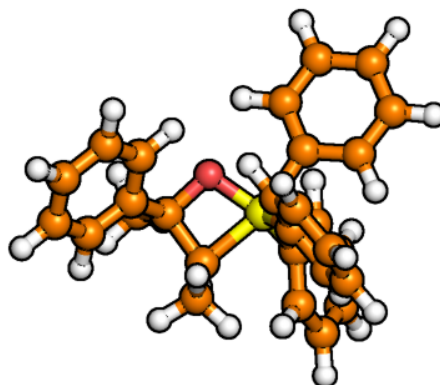
O 0.599112 0.176348 -0.095770	C 2.392319 2.822631 -0.247799	H 2.254753 2.233497 2.345353
C 0.650248 0.034040 1.683473	C 3.070065 4.031393 -0.184958	H 2.571072 1.241263 3.756874
C 2.054084 0.108341 1.964007	H 4.987711 5.002133 -0.172082	C -0.252358 1.155335 2.124140
P 2.107848 0.117690 -0.484888	H 6.247057 2.879009 -0.375340	C -0.981003 1.971160 1.261911
H 2.486533 -0.847661 2.234987	H 5.059813 0.741455 -0.504620	C -0.390504 1.351251 3.501500
C 1.562334 0.167566 -5.112274	H 1.312305 2.807477 -0.206501	C -1.812753 2.967746 1.763113
C 0.441697 0.162564 -4.292673	H 2.509687 4.953109 -0.100833	C -1.226419 2.339146 4.002280
C 0.584671 0.143621 -2.907934	C 4.386108 -3.886731 -0.213021	C -1.939401 3.157561 3.132664
C 1.851517 0.131394 -2.324370	C 3.231292 -3.762384 -0.974106	H -0.893491 1.819043 0.198004
C 2.970943 0.137004 -3.161154	C 2.581016 -2.536993 -1.060946	H 0.170463 0.727518 4.184514
C 2.831538 0.153903 -4.540949	C 3.059262 -1.428327 -0.358208	H -2.366285 3.594512 1.075794
H 1.450945 0.182478 -6.188541	C 4.203312 -1.571381 0.430610	H -1.315652 2.474029 5.072340
H -0.549065 0.172435 -4.728386	C 4.873172 -2.784171 0.484386	H -2.586878 3.932940 3.520183
H -0.285968 0.134624 -2.270407	H 4.901027 -4.836425 -0.155855	C -0.000144 -1.328106 1.807050
H 3.964679 0.126997 -2.733346	H 2.839262 -4.615329 -1.512020	H -0.951578 -1.363099 1.279560
H 3.711224 0.157651 -5.171255	H 1.700062 -2.441299 -1.680265	H 0.658510 -2.101095 1.413282
C 4.459726 4.059587 -0.224993	H 4.554385 -0.741538 1.024463	H -0.181722 -1.536990 2.863258
C 5.165695 2.867502 -0.335579	H 5.766553 -2.875316 1.087950	
C 4.492320 1.654009 -0.402028	C 2.681796 1.284814 2.666716	
C 3.097873 1.620235 -0.350306	H 3.753652 1.335064 2.458747	



TS_{7→8}D-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.74271605

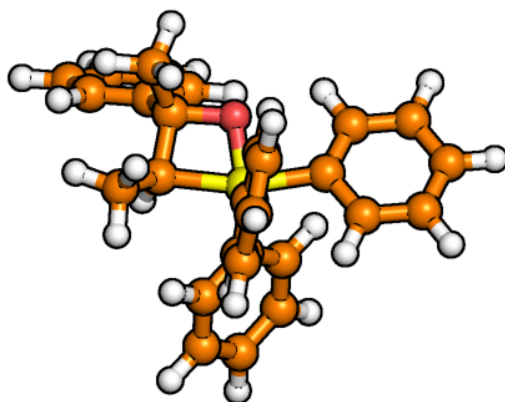
O 0.48140 0.61175 -0.59305	C 2.60654 3.05987 -0.66296	H 1.78556 2.63844 1.80782
C 0.33663 0.26483 1.17081	C 3.40284 4.19067 -0.54768	H 1.68668 1.76889 3.33272
C 1.69823 0.47344 1.57809	H 5.39203 4.94640 -0.24631	C -0.17456 -1.15118 1.13541
P 2.02101 0.40041 -0.76536	H 6.40356 2.69018 -0.10078	C -1.14404 -1.53745 0.20504
H 2.19868 -0.41110 1.94097	H 5.00904 0.69013 -0.31442	C 0.28669 -2.10373 2.04215
C 2.11957 0.41459 -5.43258	H 1.54296 3.16074 -0.83600	C -1.61565 -2.84014 0.16638
C 0.91374 0.62280 -4.77663	H 2.95289 5.17175 -0.62507	C -0.18543 -3.41166 2.00626
C 0.86081 0.61639 -3.38522	C 3.49141 -3.92604 -0.14618	C -1.13321 -3.78708 1.06543
C 2.01419 0.40571 -2.63001	C 2.43269 -3.62686 -0.99403	H -1.49318 -0.81566 -0.51824
C 3.22139 0.20069 -3.30383	C 2.05376 -2.30705 -1.19768	H 1.02227 -1.82644 2.78229
C 3.27734 0.20160 -4.68966	C 2.70335 -1.27029 -0.52402	H -2.35423 -3.12122 -0.57309
H 2.16028 0.41767 -6.51398	C 3.74924 -1.58144 0.34570	H 0.19544 -4.13613 2.71394
H 0.00843 0.78911 -5.34637	C 4.15460 -2.89747 0.51592	H -1.49498 -4.80626 1.03089
H -0.07719 0.77415 -2.87538	H 3.79360 -4.95360 0.00610	C -0.71977 1.28758 1.50920
H 4.13067 0.03352 -2.74090	H 1.89890 -4.41986 -1.50020	H -1.63147 1.12115 0.93967
H 4.22219 0.03717 -5.19123	H 1.23731 -2.08125 -1.86853	H -0.95916 1.19862 2.57210
C 4.77128 4.06528 -0.33700	H 4.22686 -0.80190 0.91933	H -0.36519 2.29780 1.32207
C 5.33730 2.79835 -0.25109	H 4.97559 -3.12212 1.18408	
C 4.54461 1.66306 -0.36507	C 2.09859 1.72654 2.31660	
C 3.16880 1.78386 -0.56365	H 3.18479 1.78259 2.40613	



7D-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.77273913

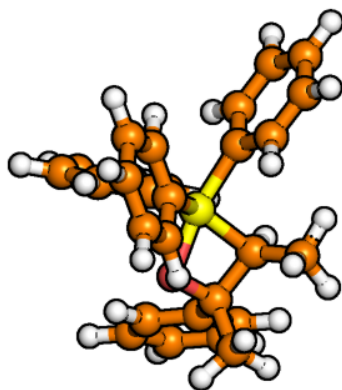
O 0.428581 0.416617 0.035627	C 2.513243 2.932328 -0.637719	H 2.240446 2.526280 2.163262
C 0.290238 0.517034 1.481883	C 3.241297 4.109504 -0.742510	H 2.111285 1.569867 3.633694
C 1.788287 0.425226 1.815880	H 5.187372 5.015255 -0.632373	C -0.511270 -0.693266 1.953897
P 2.075673 0.246838 -0.139714	H 6.330157 2.882985 -0.101448	H -1.510147 -0.681265 1.517564
H 1.993902 -0.523063 2.309885	H 5.042882 0.805251 0.100397	H -0.005357 -1.610773 1.651618
C 1.557226 -0.256560 -4.804807	H 1.445329 2.949108 -0.804292	H -0.609376 -0.694042 3.039076
C 0.438236 -0.344498 -3.988520	H 2.732760 5.034171 -0.981783	C -0.412262 1.808613 1.842435
C 0.557236 -0.183500 -2.609806	C 4.549840 -3.674659 0.308617	C -0.866913 2.688024 0.863415
C 1.795820 0.071214 -2.016529	C 3.560150 -3.583194 -0.660585	C -0.637142 2.130573 3.182553
C 2.910640 0.155027 -2.856889	C 2.845874 -2.400916 -0.823730	C -1.514088 3.868830 1.213146
C 2.799508 -0.005743 -4.230510	C 3.087755 -1.299850 -0.001067	C -1.280616 3.308656 3.534451
H 1.465224 -0.379876 -5.876023	C 4.059959 -1.420718 0.998285	C -1.719833 4.186809 2.548939
H -0.534943 -0.539280 -4.421262	C 4.801646 -2.584994 1.136503	H -0.721753 2.435376 -0.175933
H -0.322380 -0.258620 -1.990596	H 5.116699 -4.588838 0.425279	H -0.300446 1.458833 3.960789
H 3.887802 0.347699 -2.434896	H 3.346597 -4.428729 -1.301141	H -1.860645 4.538521 0.436687
H 3.681867 0.066229 -4.853470	H 2.098300 -2.337295 -1.599916	H -1.438913 3.542177 4.579230
C 4.617946 4.099473 -0.546164	H 4.239957 -0.602382 1.679905	H -2.221267 5.105858 2.821694
C 5.257569 2.903693 -0.244631	H 5.565913 -2.647372 1.900106	
C 4.526500 1.726341 -0.126724	C 2.446847 1.548350 2.594254	
C 3.146971 1.729831 -0.321703	H 3.530478 1.422898 2.604095	



7D-CPhMe-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.77229701

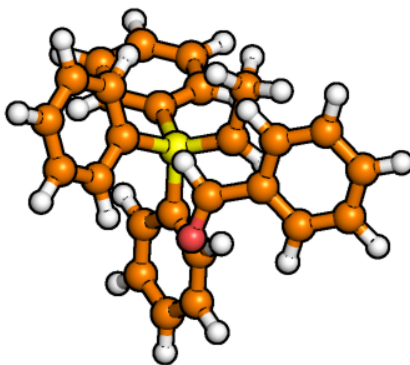
O 0.527915 0.343247 -0.537438	C 2.573944 2.888754 -0.651097	H 2.343370 1.879033 2.127796
C 0.289305 0.211379 0.891813	C 3.257717 4.084129 -0.475126	H 1.861425 0.683749 3.332211
C 1.747903 -0.051191 1.297236	H 5.133319 5.004457 0.028799	C -0.616525 -0.974248 1.156432
P 2.182010 0.159194 -0.621822	H 6.292882 2.842141 0.365244	C -1.100093 -1.771090 0.122777
H 1.863914 -1.096646 1.575155	H 5.081206 0.728958 0.072397	C -0.952188 -1.306225 2.470888
C 2.049025 0.541812 -5.321773	H 1.538412 2.901434 -0.965201	C -1.904253 -2.873875 0.395139
C 0.859544 0.362660 -4.629865	H 2.746577 5.024012 -0.637514	C -1.753410 -2.405979 2.744148
C 0.861499 0.258335 -3.240221	C 4.637298 -3.798844 -0.710814	C -2.234818 -3.195749 1.704545
C 2.051324 0.329695 -2.513873	C 3.706536 -3.532460 -1.705860	H -0.841169 -1.526850 -0.896142
C 3.239094 0.510402 -3.230021	C 3.007182 -2.330140 -1.707765	H -0.577760 -0.706085 3.290335
C 3.244524 0.615912 -4.612894	C 3.204194 -1.386530 -0.698812	H -2.270798 -3.482236 -0.421357
H 2.047684 0.625688 -6.400899	C 4.114051 -1.686970 0.320602	H -2.000710 -2.648979 3.769325
H -0.077932 0.305037 -5.168571	C 4.843121 -2.867435 0.302270	H -2.858935 -4.053789 1.916299
H -0.073123 0.125508 -2.718391	H 5.191501 -4.728032 -0.716244	C -0.332199 1.511781 1.385771
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H 4.180227 0.757600 -5.138373	H 2.305048 -2.127698 -2.502450	H -0.506490 1.481002 2.460317
C 4.598094 4.073671 -0.103311	H 4.253024 -1.000873 1.143027	H 0.320139 2.354584 1.166061
C 5.246897 2.860256 0.088703	H 5.559050 -3.068706 1.088633	
C 4.558634 1.662709 -0.074439	C 2.369788 0.818903 2.372858	
C 3.215312 1.666043 -0.442786	H 3.416670 0.553654 2.527071	



6D-CPhMe-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1497.77561168

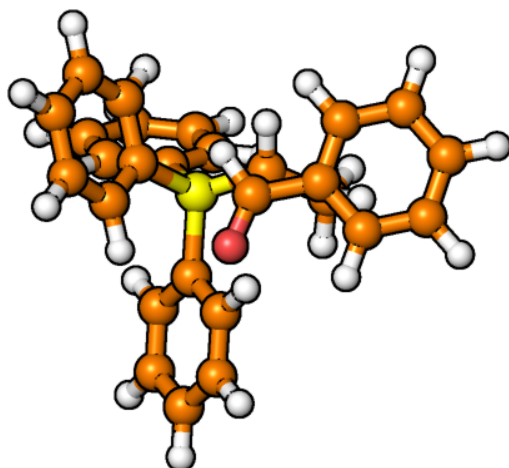
O 1.583068 -0.176469 3.025150	C -1.243794 3.374232 1.829558	H 0.383710 -0.738050 0.005209
C 0.497885 -1.085534 2.893664	C -2.013105 4.196274 1.008286	H -1.084305 -1.584650 0.483869
C -0.387495 -0.198169 1.977369	H -2.434309 4.812791 -1.006680	C 0.996269 -2.395221 2.284682
P 0.740471 1.257404 2.323497	H -0.724605 3.304432 -1.987801	H 1.711027 -2.849895 2.969986
H -1.370423 0.014167 2.399685	H 0.640531 1.885157 -0.541148	H 0.178655 -3.099944 2.129261
C 4.745491 2.696833 0.476054	H -1.392086 3.430573 2.897315	H 1.496095 -2.218412 1.333388
C 4.496111 1.336972 0.603818	H -2.744190 4.860147 1.452086	C -0.160440 -1.376926 4.236918
C 3.306033 0.892876 1.171284	C 0.145487 2.932903 6.587303	C -1.445384 -1.913226 4.303640
C 2.334277 1.805196 1.581027	C 1.364589 3.081790 5.935998	C 0.523107 -1.121664 5.421554
C 2.588316 3.172544 1.432640	C 1.531024 2.606100 4.641422	C -2.044551 -2.172404 5.530582
C 3.791835 3.615409 0.904368	C 0.474972 1.983303 3.976263	C -0.071099 -1.382249 6.649948
H 5.677469 3.041708 0.047679	C -0.745238 1.837393 4.637183	C -1.358174 -1.904027 6.710142
H 5.233267 0.616318 0.274909	C -0.908071 2.306441 5.933831	H -1.990645 -2.122572 3.390953
H 3.132246 -0.160785 1.317309	H 0.020221 3.296079 7.598672	H 1.509438 -0.685251 5.364595
H 1.841670 3.893990 1.731807	H 2.193758 3.562292 6.438668	H -3.046472 -2.580409 5.565786
H 3.980385 4.677157 0.815884	H 2.491559 2.705426 4.156707	H 0.467906 -1.164216 7.562758
C -1.839076 4.173514 -0.368014	H -1.572304 1.335570 4.156462	H -1.824111 -2.099406 7.667020
C -0.881093 3.326556 -0.916796	H -1.856620 2.168860 6.435220	
C -0.116085 2.515072 -0.091101	C -0.565615 -0.625239 0.528110	
C -0.282240 2.512886 1.300180	H -1.163407 0.103195 -0.014909	



5D-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.47469083

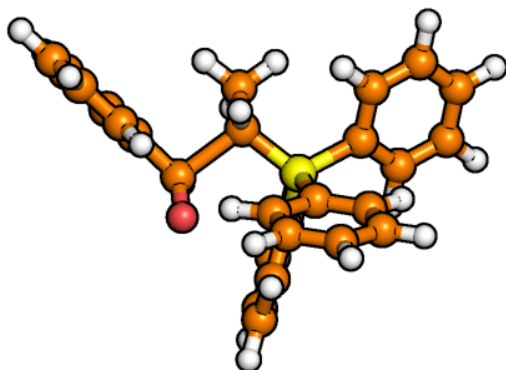
O 1.033291 0.918527 2.885377	C -3.811200 -0.622254 3.577642	C 2.836344 -1.305607 3.235553
C 1.785867 0.588004 1.990392	C -4.376931 -0.384099 2.329785	C 3.797330 -0.592701 1.141212
P -1.114947 -0.348596 -0.137001	C -3.570356 -0.310334 1.202096	C 3.819449 -2.273614 3.354953
C 0.257401 -1.293286 0.079154	H -1.622487 -2.770543 -1.522510	C 4.790444 -1.555409 1.265763
C -2.212637 -0.715589 -1.571314	H -3.072245 -3.425997 -3.428289	C 4.799003 -2.399482 2.370299
C -2.244949 -2.035733 -2.018889	H -4.465805 -1.720510 -4.557572	H 2.073951 -1.182520 3.992751
C -3.055933 -2.399361 -3.086639	H -4.414556 0.627823 -3.779713	H 3.776213 0.063410 0.280263
C -3.838949 -1.441146 -3.720890	H -2.970786 1.272060 -1.887983	H 3.831784 -2.931169 4.214470
C -3.808943 -0.120132 -3.284818	H -0.098954 1.088849 -2.466286	H 5.552632 -1.650793 0.503492
C -2.997026 0.242115 -2.217008	H 0.726723 3.385895 -2.780561	H 5.568726 -3.154167 2.467685
C -0.688235 1.398139 -0.417661	H 0.577870 5.022966 -0.928577	C 1.313622 -1.393865 -0.991199
C -2.186938 -0.472556 1.313778	H -0.382524 4.334959 1.248879	H 2.189187 -1.915976 -0.604448
C -0.151243 1.793226 -1.646942	H -1.154950 2.026998 1.585102	H 0.998003 -1.930664 -1.896566
C 0.307187 3.091628 -1.827611	H -0.553433 -0.800272 2.667438	H 1.658586 -0.408488 -1.320503
C 0.222954 4.010745 -0.787197	H -1.988146 -0.960477 4.662962	H 0.130396 -2.129971 0.753271
C -0.317816 3.625593 0.434651	H -4.440372 -0.679113 4.456221	H 1.785706 1.120534 1.024890
C -0.768339 2.325154 0.622231	H -5.447370 -0.259064 2.232606	
C -1.623149 -0.706210 2.570457	H -4.019620 -0.136023 0.235450	
C -2.435462 -0.783923 3.693919	C 2.814532 -0.463789 2.121416	



5D-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.47616486

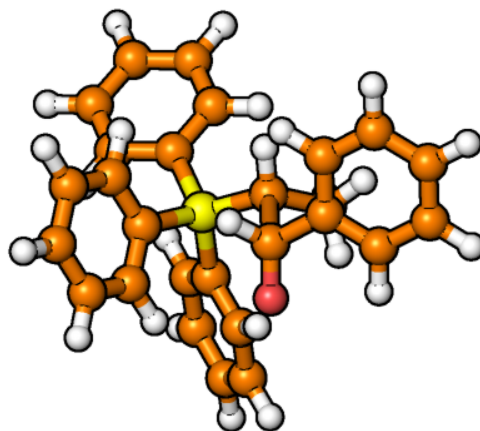
O 1.199736 1.068732 2.849766	C -3.775311 -0.670414 3.594834	C 0.421711 -2.631965 0.681229
C 1.886806 0.648229 1.939758	C -4.360485 -0.651423 2.333856	H 1.313673 -2.749412 1.303553
P -1.079658 -0.385391 -0.129003	C -3.565024 -0.576863 1.197315	H -0.436119 -2.854163 1.319273
C 0.343557 -1.237079 0.117120	H 1.151422 -0.906002 -0.523314	H 0.465627 -3.421639 -0.079727
C -2.195426 -0.778201 -1.545024	H -1.516994 -2.810380 -1.580984	C 2.802458 -0.505143 2.057579
C -2.178153 -2.083892 -2.035569	H -2.966537 -3.462142 -3.478473	C 2.845480 -1.260872 3.230113
C -2.986448 -2.446403 -3.105912	H -4.432605 -1.777762 -4.546351	C 3.637421 -0.839112 0.991747
C -3.811063 -1.500246 -3.705186	H -4.462817 0.546773 -3.698571	C 3.710101 -2.340433 3.330047
C -3.828012 -0.193214 -3.228725	H -3.039369 1.184578 -1.788559	C 4.502487 -1.919058 1.090149
C -3.025629 0.165847 -2.152373	H 0.005809 0.985806 -2.434340	C 4.538877 -2.671665 2.260871
C -0.657951 1.353581 -0.419233	H 0.804191 3.288938 -2.794947	H 2.194693 -0.984162 4.047943
C -2.174675 -0.520657 1.313850	H 0.568044 4.978495 -1.000184	H 3.592901 -0.254397 0.081042
C -0.087699 1.717577 -1.642835	H -0.457128 4.343439 1.162868	H 3.740097 -2.927962 4.238263
C 0.356952 3.016655 -1.848139	H -1.214188 2.036307 1.541915	H 5.144626 -2.178345 0.258860
C 0.222730 3.965795 -0.839716	H -0.517730 -0.489131 2.678867	H 5.210005 -3.516966 2.339036
C -0.355270 3.610863 0.373543	H -1.929823 -0.627744 4.695465	H 1.906725 1.161099 0.963858
C -0.792966 2.309440 0.586325	H -4.395949 -0.728723 4.479393	
C -1.591680 -0.543525 2.584179	H -5.436967 -0.698843 2.232918	
C -2.391180 -0.616618 3.716870	H -4.028560 -0.573007 0.221860	



TS_{5→6}D-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.46786881

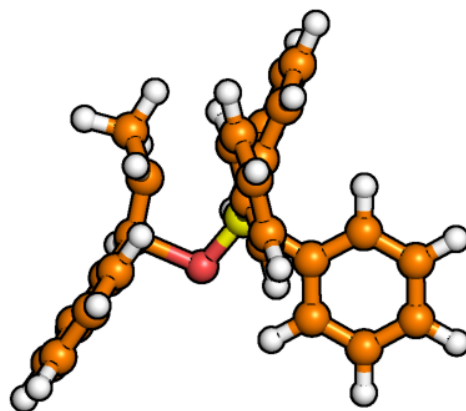
O 0.694005 1.149796 2.669356	C -4.021660 -0.790556 3.687387	C 1.454661 -1.019354 -0.521499
C 1.457359 0.681526 1.766941	C -4.438531 -0.851123 2.361563	H 2.381487 -1.472987 -0.175057
P -1.012518 -0.053605 0.301757	C -3.530617 -0.625918 1.336883	H 1.000966 -1.700012 -1.246536
C 0.582585 -0.701750 0.680626	H 0.471804 -1.532314 1.374436	H 1.729495 -0.107604 -1.057591
C -1.773817 -0.817715 -1.163689	H -1.071843 -2.768534 -0.599461	H 1.690096 1.322585 0.891036
C -1.647266 -2.200403 -1.318570	H -2.152480 -3.916716 -2.496375	C 2.687185 -0.085482 2.198652
C -2.258765 -2.846011 -2.383610	H -3.475848 -2.618806 -4.138635	C 2.643449 -0.880156 3.343809
C -3.003125 -2.116335 -3.305318	H -3.720430 -0.171248 -3.866042	C 3.885426 0.009231 1.495115
C -3.138362 -0.741488 -3.154299	H -2.640641 0.975573 -1.972838	C 3.764653 -1.582241 3.762025
C -2.527196 -0.092786 -2.087457	H 0.015207 1.395697 -1.995301	C 5.015789 -0.686033 1.914416
C -0.895545 1.711161 -0.066925	H 0.332232 3.793027 -2.448855	C 4.957085 -1.489131 3.046661
C -2.194510 -0.338726 1.636751	H -0.398160 5.475352 -0.786284	H 1.720693 -0.919077 3.907764
C -0.303550 2.125340 -1.263977	H -1.425470 4.743259 1.342370	H 3.936268 0.644724 0.619029
C -0.127586 3.477265 -1.522145	H -1.712243 2.342563 1.815403	H 3.716751 -2.196431 4.652497
C -0.537935 4.421098 -0.586221	H -0.748798 0.012868 3.185194	H 5.942475 -0.594981 1.361883
C -1.119560 4.011446 0.607425	H -2.371064 -0.438920 5.015268	H 5.834477 -2.029681 3.377076
C -1.294092 2.659465 0.873348	H -4.730285 -0.970343 4.485306	
C -1.774820 -0.273621 2.968529	H -5.469190 -1.077267 2.123245	
C -2.695997 -0.498123 3.984833	H -3.862941 -0.682464 0.310652	



TS_{5→6}D-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.46821848

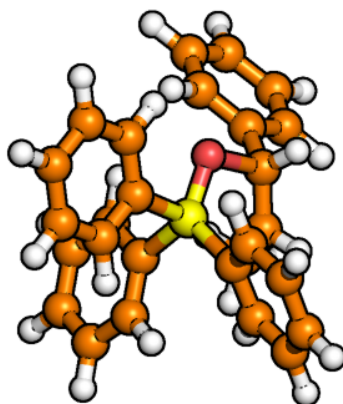
O 1.075995 0.767945 2.521525	C -3.878939 -0.857948 3.576976	C 0.574743 -2.106534 1.157194
C 1.615047 0.517968 1.399654	C -4.322659 -1.060436 2.275226	H 1.525936 -2.610790 0.990384
P -1.017731 -0.087370 0.073466	C -3.468180 -0.831237 1.204937	H 0.505810 -1.895542 2.225803
C 0.556308 -0.804622 0.370735	H 1.078537 -0.854569 -0.583584	H -0.225274 -2.808399 0.905860
C -1.827037 -0.703110 -1.434666	H -0.598587 -2.460126 -1.531362	H 1.585239 1.293711 0.611147
C -1.414579 -1.915988 -1.985153	H -1.715995 -3.359688 -3.540531	C 2.945094 -0.201259 1.369489
C -2.043015 -2.419389 -3.118406	H -3.570558 -2.104079 -4.592274	C 3.431093 -0.799981 2.528243
C -3.084699 -1.713943 -3.708161	H -4.306154 0.052785 -3.625831	C 3.706845 -0.271652 0.203555
C -3.499247 -0.501223 -3.165261	H -3.192857 0.950001 -1.619904	C 4.646772 -1.474753 2.517401
C -2.874385 0.003182 -2.033762	H -0.369169 1.488635 -2.276261	C 4.921679 -0.943698 0.187346
C -0.860179 1.697284 -0.187895	H 0.036161 3.890327 -2.617016	C 5.394113 -1.553721 1.347006
C -2.160868 -0.396435 1.437274	H -0.220531 5.471275 -0.728514	H 2.840126 -0.708690 3.429351
C -0.484336 2.173486 -1.447291	H -0.869309 4.628264 1.506220	H 3.342724 0.210448 -0.697145
C -0.257235 3.528361 -1.640865	H -1.245963 2.225414 1.860246	H 5.015297 -1.936498 3.424820
C -0.400831 4.414946 -0.578717	H -0.682699 0.125005 2.913972	H 5.504819 -0.987982 -0.724054
C -0.769123 3.943370 0.675339	H -2.225406 -0.277960 4.819897	H 6.341952 -2.075852 1.338868
C -0.996823 2.588146 0.876002	H -4.545860 -1.039785 4.409547	
C -1.708673 -0.202351 2.747198	H -5.332242 -1.401568 2.089954	
C -2.576050 -0.430563 3.807743	H -3.820859 -1.001282 0.198831	



TS_{7→8}D-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.47783232

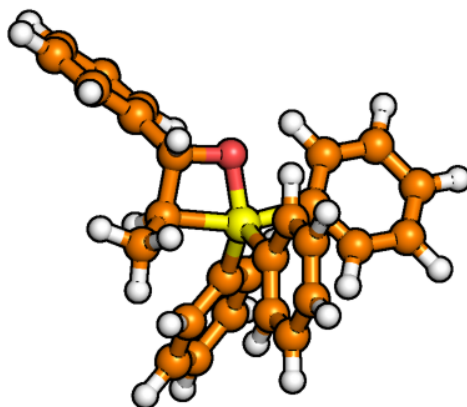
O 0.173977 0.510261 0.090619	C 2.579054 2.125723 -0.053808	C 1.881127 1.815698 2.941877
C 0.146698 0.336833 1.833582	C 1.783057 3.275145 -0.049579	H 2.945852 2.041106 2.839176
C 1.508154 0.546570 2.216730	C 2.363539 4.531588 0.044818	H 1.341458 2.678215 2.548086
P 1.704490 0.558067 -0.234299	H 4.197598 5.640036 0.210312	H 1.667757 1.762991 4.016589
H 2.021670 -0.332419 2.583392	H 5.618429 3.611728 0.179311	H -0.532198 1.166276 2.005911
C 1.357899 0.537148 -4.877216	H 4.603807 1.389904 -0.004020	C -0.527258 -0.976768 1.995661
C 0.211670 0.392966 -4.106871	H 0.707714 3.177805 -0.122376	C -1.911913 -1.013590 2.169213
C 0.293616 0.401158 -2.717193	H 1.734796 5.412216 0.047637	C 0.174105 -2.185775 1.981618
C 1.525188 0.555405 -2.080707	C 4.213075 -3.290838 0.197932	C -2.581294 -2.219672 2.334279
C 2.671068 0.701156 -2.867238	C 3.122793 -3.231508 -0.659602	C -0.493564 -3.391876 2.132875
C 2.591794 0.691564 -4.251972	C 2.408564 -2.047571 -0.800499	C -1.873611 -3.415236 2.312921
H 1.293248 0.531079 -5.957403	C 2.756363 -0.916225 -0.058103	H -2.468156 -0.084596 2.171186
H -0.751778 0.272870 -4.585233	C 3.837909 -0.993722 0.822972	H 1.244957 -2.187851 1.846439
H -0.595884 0.287402 -2.116819	C 4.573000 -2.163960 0.933449	H -3.654387 -2.225562 2.474020
H 3.637214 0.823963 -2.395812	H 4.776110 -4.208871 0.300713	H 0.065929 -4.318048 2.113417
H 3.490517 0.805833 -4.843897	H 2.827590 -4.104238 -1.226680	H -2.391055 -4.357453 2.436229
C 3.745340 4.660466 0.134114	H 1.572817 -2.005605 -1.484200	
C 4.541677 3.521322 0.120225	H 4.084127 -0.148446 1.446844	
C 3.966033 2.260427 0.023484	H 5.415912 -2.204234 1.610591	



TS_{7→8}D-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.47397951

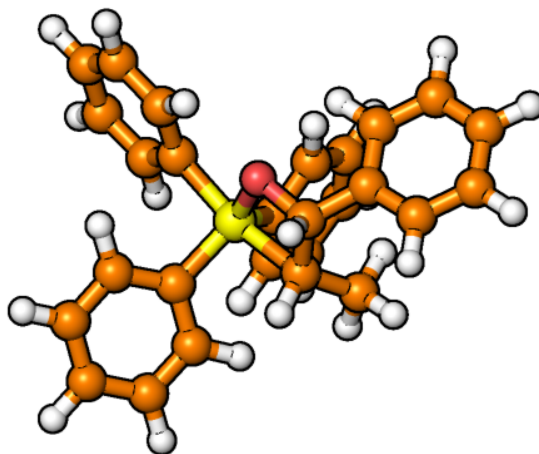
O 0.60730 0.05653 0.02584	C 4.44576 1.64425 -0.35713	H 5.87208 -2.81215 1.09866
C 0.69578 -0.03187 1.76242	C 3.05302 1.57701 -0.28056	C 2.70720 1.20926 2.77941
C 2.08644 0.03037 2.07744	C 2.32253 2.76104 -0.13974	H 3.77765 1.27384 2.56513
P 2.10150 0.05420 -0.43280	C 2.97395 3.98320 -0.06418	H 2.26639 2.15367 2.46259
H 0.25070 -1.02083 1.82033	H 4.86910 4.99737 -0.06462	H 2.60477 1.16437 3.87067
H 2.52939 -0.92744 2.31917	H 6.17225 2.90829 -0.33497	C -0.25373 1.03186 2.22981
C 1.38156 0.12971 -5.02593	H 5.03122 0.74705 -0.48953	C -1.00193 1.84886 1.38528
C 0.29559 0.03084 -4.16642	H 1.24432 2.72136 -0.07752	C -0.40666 1.18249 3.61116
C 0.49095 0.00663 -2.78840	H 2.39440 4.88968 0.04989	C -1.86819 2.80393 1.90813
C 1.77695 0.08290 -2.25325	C 4.55066 -3.85057 -0.24199	C -1.27943 2.12675 4.13315
C 2.86156 0.18298 -3.12891	C 3.39680 -3.75963 -1.00888	C -2.01124 2.94802 3.28179
C 2.66889 0.20553 -4.50217	C 2.68952 -2.56451 -1.06714	H -0.90599 1.72770 0.31775
H 1.22896 0.14923 -6.09702	C 3.11030 -1.45412 -0.33065	H 0.17084 0.55600 4.27798
H -0.70869 -0.02820 -4.56550	C 4.25496 -1.56509 0.46335	H -2.43706 3.43269 1.23526
H -0.35196 -0.07364 -2.11935	C 4.98017 -2.74618 0.48973	H -1.38232 2.22656 5.20586
H 3.86797 0.24559 -2.73712	H 5.10935 -4.77628 -0.20648	H -2.68669 3.69005 3.68654
H 3.52121 0.28413 -5.16423	H 3.04943 -4.61457 -1.57359	
C 4.36173 4.04427 -0.12850	H 1.80935 -2.49488 -1.69078	
C 5.09233 2.87121 -0.27648	H 4.56279 -0.73554 1.08079	



7D-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.50952659

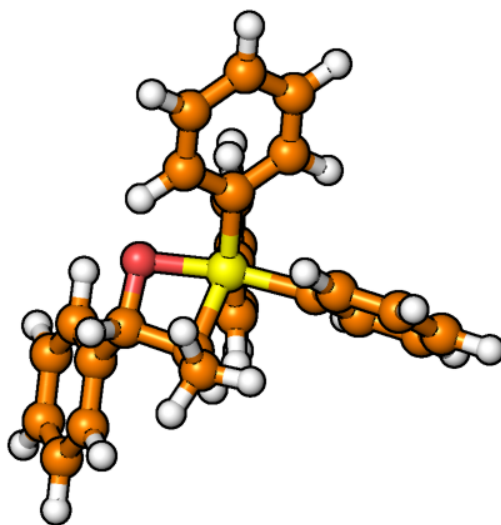
O 0.295339 0.332903 -0.018471	C 2.907963 1.658165 -0.143553	C 2.251916 0.935982 2.793894
C 0.146165 0.380901 1.416738	C 2.178256 2.836729 -0.311336	H 3.300721 0.680189 2.947117
C 1.579943 0.022125 1.785834	C 2.812149 4.071105 -0.261069	H 2.215737 1.978185 2.476076
P 1.952823 0.097664 -0.160154	H 4.679972 5.104869 -0.013887	H 1.758221 0.864379 3.767657
H 1.637264 -1.013478 2.119961	H 5.987783 3.020359 0.261988	H -0.102223 1.405157 1.707036
C 1.501949 -0.145743 -4.839367	H 4.868315 0.836342 0.180976	C -0.919389 -0.556119 1.905097
C 0.409242 -0.441330 -4.035163	H 1.112254 2.782703 -0.491197	C -1.136443 -1.786500 1.285649
C 0.509675 -0.347408 -2.649558	H 2.234337 4.976567 -0.392458	C -1.667649 -0.228533 3.033688
C 1.704877 0.038600 -2.039547	C 4.751676 -3.638392 0.008989	C -2.079670 -2.671851 1.790000
C 2.794510 0.329600 -2.864478	C 3.809158 -3.524944 -1.003223	C -2.607947 -1.116229 3.544139
C 2.698551 0.243859 -4.246629	C 2.998929 -2.396769 -1.084950	C -2.816777 -2.341799 2.923099
H 1.423069 -0.214359 -5.916489	C 3.096930 -1.373497 -0.140558	H -0.570684 -2.043505 0.400637
H -0.528555 -0.743434 -4.483856	C 4.024294 -1.522381 0.897331	H -1.514611 0.730606 3.513597
H -0.351009 -0.572078 -2.038912	C 4.860036 -2.627643 0.959243	H -2.242098 -3.621466 1.296857
H 3.736992 0.627221 -2.424922	H 5.391799 -4.508914 0.064449	H -3.182209 -0.847152 4.421046
H 3.557665 0.480735 -4.861075	H 3.705398 -4.310413 -1.740255	H -3.552330 -3.032121 3.314135
C 4.184908 4.143639 -0.050057	H 2.288913 -2.317719 -1.893723	
C 4.917637 2.973662 0.107667	H 4.098055 -0.770539 1.667859	
C 4.283150 1.736839 0.065098	H 5.586278 -2.707558 1.757607	



7D-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.50718383

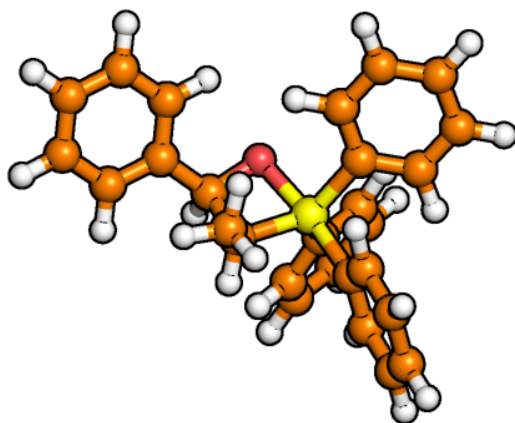
O 0.375669 0.203153 0.159983	C 4.397141 1.785775 -0.036200	H 5.713828 -2.591514 1.805044
C 0.287594 0.306842 1.597833	C 3.021830 1.711694 -0.246924	C 2.379621 1.450585 2.687485
C 1.788880 0.297491 1.899635	C 2.325616 2.878412 -0.564709	H 3.468548 1.388704 2.702914
P 2.031151 0.168792 -0.073304	C 2.985920 4.096191 -0.652734	H 2.117053 2.417215 2.260659
H -0.203507 -0.597125 1.966297	H 4.875867 5.110344 -0.513996	H 2.034674 1.445927 3.724281
H 2.069456 -0.645942 2.364152	H 6.132089 3.042103 0.014512	C -0.516051 1.503284 2.028791
C 1.414431 -0.193845 -4.736515	H 4.963565 0.894754 0.190661	C -0.973129 2.453599 1.121330
C 0.318115 -0.346563 -3.899613	H 1.261603 2.834906 -0.750506	C -0.814893 1.667930 3.382257
C 0.463872 -0.233114 -2.518522	H 2.428444 4.991781 -0.893575	C -1.695026 3.559368 1.559171
C 1.707565 0.038983 -1.944402	C 4.721298 -3.620998 0.200285	C -1.533779 2.770393 3.821643
C 2.799641 0.189440 -2.805649	C 3.706259 -3.553726 -0.744506	C -1.973071 3.725472 2.909654
C 2.661788 0.074734 -4.181141	C 2.924024 -2.408980 -0.852578	H -0.776424 2.312773 0.069158
H 1.301281 -0.280686 -5.809282	C 3.124006 -1.323064 0.001136	H -0.479565 0.926194 4.096994
H -0.658509 -0.555537 -4.317600	C 4.123398 -1.421711 0.975648	H -2.044919 4.288987 0.840381
H -0.398242 -0.358709 -1.883388	C 4.930905 -2.546840 1.059352	H -1.753704 2.884593 4.875076
H 3.779601 0.398968 -2.398188	H 5.340223 -4.505369 0.274209	H -2.534355 4.585508 3.249880
H 3.526767 0.196897 -4.820385	H 3.525159 -4.388703 -1.408429	
C 4.358484 4.163165 -0.440090	H 2.156032 -2.362381 -1.609791	
C 5.061511 3.003305 -0.139545	H 4.272898 -0.617565 1.681083	



6D-CPhH-trans

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.51218510

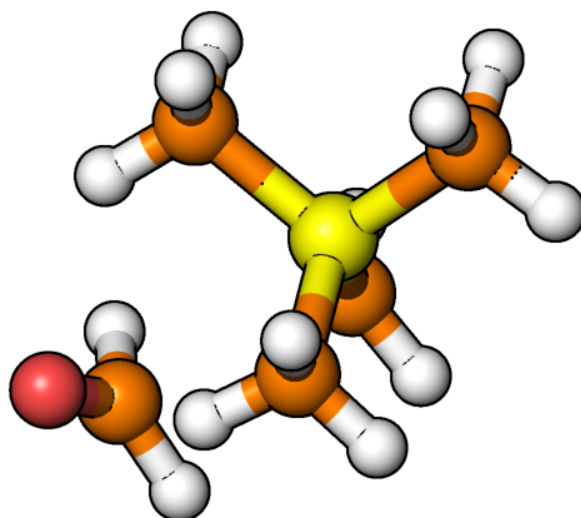
O 0.181167 0.351503 -0.118954	C 3.889410 0.287902 -0.238885	C 2.148018 1.446893 2.290901
C 0.192379 0.101198 1.271032	C 4.719333 -0.830147 -0.328199	H 3.231678 1.533121 2.329919
C 1.709970 0.219120 1.506326	C 6.097277 -0.726587 -0.148374	H 1.744656 2.363780 1.857724
P 1.980949 0.231731 -0.348282	H 7.748323 0.584525 0.266446	H 1.779608 1.374833 3.316263
H 2.173227 -0.671583 1.933901	H 6.307948 2.599646 0.422372	H -0.343574 0.899813 1.800643
C 1.807837 3.622990 -3.506300	H 3.894707 2.417363 0.078522	C -0.420257 -1.226918 1.660079
C 0.907538 3.618907 -2.449201	H 4.301211 -1.798402 -0.558750	C -1.106205 -1.994528 0.725121
C 0.940239 2.598293 -1.504566	H 6.714745 -1.611801 -0.233444	C -0.301824 -1.699075 2.967232
C 1.901177 1.590767 -1.585549	C 1.388432 -3.928652 -2.264736	C -1.654363 -3.219955 1.086360
C 2.813922 1.612775 -2.645266	C 1.227668 -2.775807 -3.024671	C -0.846900 -2.923922 3.330576
C 2.754898 2.608559 -3.608918	C 1.433554 -1.525419 -2.454982	C -1.524552 -3.690811 2.387468
H 1.772369 4.409593 -4.248589	C 1.811507 -1.413036 -1.117219	H -1.183069 -1.627785 -0.287857
H 0.166650 4.402851 -2.363585	C 1.968506 -2.574495 -0.359876	H 0.225095 -1.107636 3.707206
H 0.210326 2.565224 -0.711842	C 1.757002 -3.823057 -0.929413	H -2.177549 -3.811566 0.346297
H 3.573873 0.848207 -2.717150	H 1.221606 -4.901199 -2.708281	H -0.742448 -3.280908 4.347024
H 3.455627 2.599269 -4.433254	H 0.933729 -2.846877 -4.063688	H -1.948015 -4.646574 2.666965
C 6.678178 0.502550 0.128899	H 1.282840 -0.637052 -3.051137	
C 5.869393 1.631367 0.217234	H 2.237903 -2.515144 0.684809	
C 4.498600 1.520250 0.032078	H 1.870783 -4.711729 -0.323180	



6D-CPhH-cis

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1458.51084887

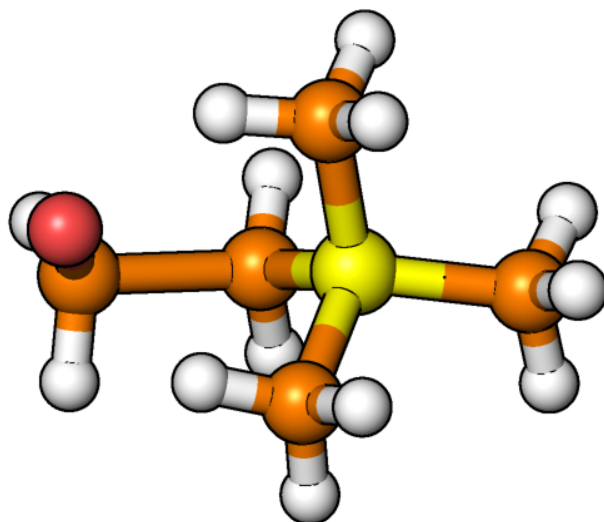
O 0.181798 0.418285 0.022021	C 4.502663 1.589173 -0.063419	H 1.823956 -4.640756 0.057823
C 0.253447 0.081399 1.391173	C 3.878284 0.347664 -0.240951	C 2.120251 1.685351 2.244008
C 1.763805 0.357277 1.590755	C 4.698478 -0.780051 -0.296507	H 3.193898 1.857362 2.211157
P 1.967753 0.291620 -0.268382	C 6.082472 -0.676453 -0.173773	H 1.618145 2.522269 1.758102
H 0.054274 -0.989371 1.540494	H 7.754012 0.644396 0.106528	H 1.807608 1.681983 3.288348
H 2.323854 -0.448249 2.069597	H 6.330826 2.675150 0.200379	C -0.703957 0.855692 2.257387
C 1.686921 3.545700 -3.556698	H 3.905881 2.491980 -0.046981	C -1.518877 1.850912 1.728553
C 0.862361 3.618911 -2.441818	H 4.266787 -1.756933 -0.455678	C -0.781009 0.575669 3.622261
C 0.925961 2.637496 -1.458352	H 6.692113 -1.569294 -0.231295	C -2.385084 2.564875 2.550961
C 1.841841 1.591614 -1.561521	C 1.326817 -3.975190 -1.922662	C -1.641154 1.288641 4.445826
C 2.684066 1.539210 -2.676611	C 1.165377 -2.870310 -2.750923	C -2.446060 2.290666 3.911449
C 2.592240 2.495760 -3.676921	C 1.375684 -1.588082 -2.260405	H -1.478920 2.044077 0.666754
H 1.627299 4.301897 -4.328423	C 1.763815 -1.393242 -0.934841	H -0.161091 -0.207996 4.042489
H 0.158755 4.434490 -2.338904	C 1.919705 -2.506855 -0.107308	H -3.016938 3.333894 2.125466
H 0.262086 2.673490 -0.610451	C 1.699996 -3.788819 -0.597707	H -1.687153 1.062164 5.503161
H 3.416500 0.749300 -2.761727	H 1.158453 -4.972759 -2.305759	H -3.119453 2.846159 4.550674
H 3.236560 2.429317 -4.543574	H 0.866771 -3.004620 -3.782272	
C 6.679164 0.562444 0.012540	H 1.223180 -0.738185 -2.909655	
C 5.880037 1.700123 0.066012	H 2.220711 -2.383299 0.923761	



5A-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-614.13048550

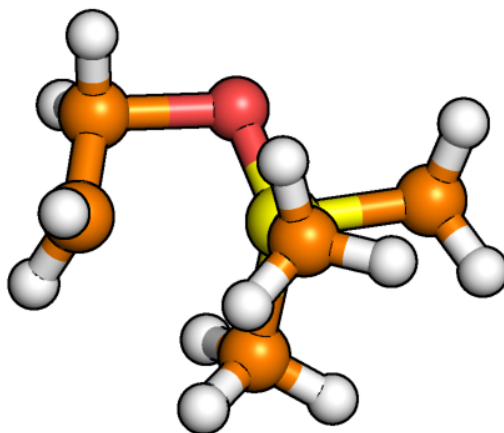
H 2.254533 0.166848 -0.940358	H 2.780567 2.491593 0.655335	C 2.629388 1.918186 1.570067
H 5.349744 -0.733558 1.108475	H 1.573945 1.933441 1.838106	H -0.183277 -1.208714 0.773604
H 5.272620 0.876871 0.385627	H 3.224589 2.361387 2.367753	C 2.256176 -0.428796 -0.034802
H 5.365946 0.705702 2.153986	H 2.335684 -1.498514 -0.190479	P 3.121260 0.202570 1.273894
H 1.699708 -0.643695 2.998223	H -0.272075 0.478493 0.005433	O -0.169881 0.385356 2.031255
H 2.991312 -1.796707 2.587300	C 4.957134 0.275001 1.237845	C -0.153418 -0.119357 0.920679
H 3.358600 -0.394311 3.609431	C 2.759627 -0.747366 2.770604	



TS_{5→6}A-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-614.12823645

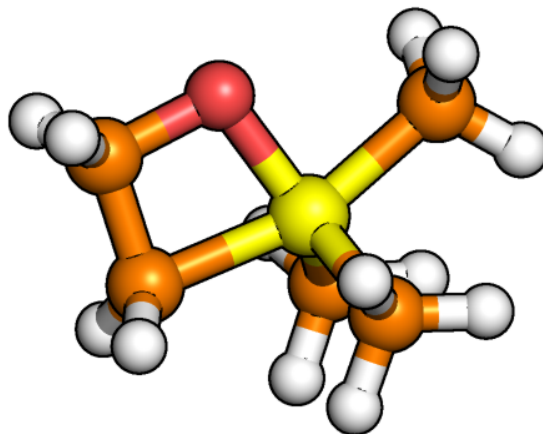
H 1.814881 0.447675 -0.674934	H 2.574198 2.586492 1.026265	C 2.280566 1.948270 1.859417
H 4.844326 -0.854299 1.150585	H 1.191477 1.946923 1.969203	H -0.063390 -1.418408 1.021329
H 4.848895 0.790148 0.495903	H 2.768441 2.291388 2.770990	C 1.778064 -0.277807 0.134626
H 5.013539 0.533753 2.247675	H 2.027596 -1.279870 -0.207781	P 2.720502 0.243520 1.495772
H 1.247144 -0.593319 3.129282	H -0.530344 -0.116209 -0.157198	O -0.296317 0.462144 1.796728
H 2.491962 -1.810784 2.718977	C 4.532996 0.173339 1.336242	C -0.077159 -0.326410 0.828552
H 2.908047 -0.460602 3.797089	C 2.309199 -0.758962 2.937410	



TS_{7→8}A-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-614.13828761

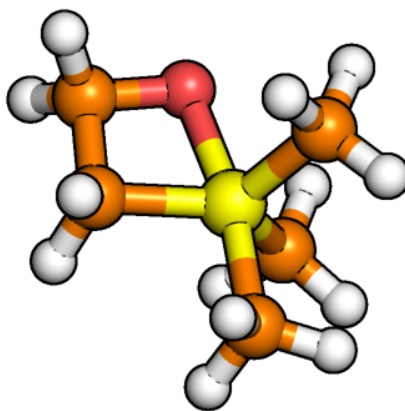
H 2.153934 -0.683766 2.383196	H 3.424403 -1.025710 0.246806	C 2.601211 -1.365721 -0.373588
H 1.369923 2.302726 -0.163500	H 2.152712 -2.236991 0.101807	H -0.555096 0.664879 1.982198
H 2.969970 1.610031 0.092221	H 2.961409 -1.651408 -1.364102	P 1.325705 -0.069657 -0.500647
H 2.355734 1.858714 -1.569662	H 1.842737 1.110709 2.276866	C 1.535628 0.112988 1.988662
H 0.404736 -1.238236 -2.424466	H -0.247550 -1.105863 2.085526	C 0.154782 -0.136834 1.812435
H 0.105149 0.498011 -2.526291	C 2.092579 1.583325 -0.546243	O -0.103517 -0.281330 0.100017
H 1.715855 -0.143745 -2.912861	C 0.845839 -0.255703 -2.263064	



7A-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-614.16901266

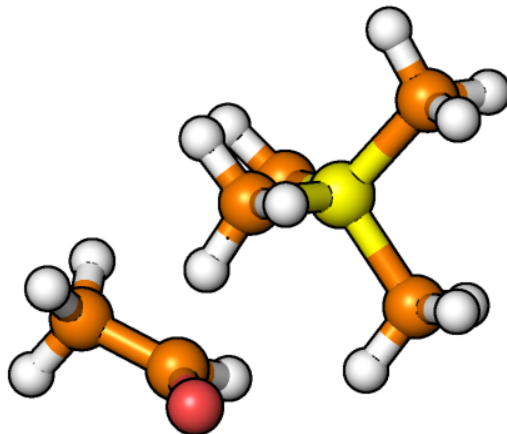
H 0.357101 1.892180 -2.757497	C 2.834757 2.118313 -1.136156	H -0.037512 -0.617479 1.182085
H 0.288780 0.160223 -3.072823	H 2.113187 -1.706312 -1.509758	H 0.020141 1.128286 1.502297
H 1.721092 1.087902 -3.556228	H 3.617108 -0.902681 -1.057374	P 1.733719 0.642997 -1.114745
C 0.951263 0.978876 -2.791485	H 2.981459 -0.753787 -2.720490	C 1.943347 0.287179 0.815595
H 3.728105 1.923358 -0.544765	C 2.718548 -0.811056 -1.665589	C 0.435853 0.322709 0.895323
H 2.296679 2.946709 -0.670806	H 2.393784 -0.672762 1.063828	O 0.165829 0.588508 -0.504696
H 3.108922 2.412611 -2.147838	H 2.450441 1.070097 1.377652	



6A-CHH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-614.17305458

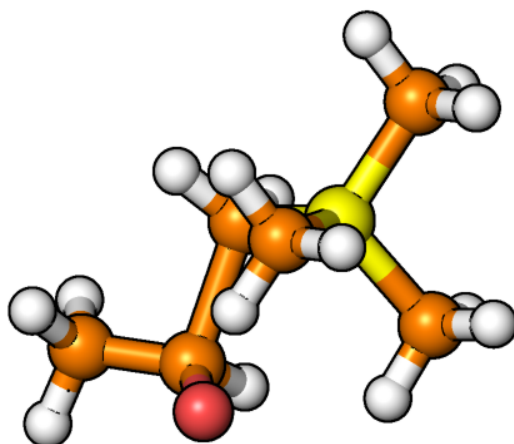
H 2.496295 -0.189828 1.105901	H 2.108933 -1.674254 -2.712666	C 1.498076 -1.612970 -1.813525
H 3.467728 1.546498 -1.412406	H 1.925173 -2.274900 -1.058319	H -0.272920 1.006165 1.347879
H 3.953906 -0.129415 -1.149550	H 0.480439 -1.940528 -2.006679	P 1.470461 0.081831 -1.129671
H 3.375983 0.382229 -2.740201	H 2.068161 1.501454 0.826602	C 1.748759 0.471497 0.666704
H -0.352161 0.934889 -2.462967	H 0.185693 -0.661926 1.732250	C 0.295663 0.138615 0.992883
H 0.565100 2.230596 -1.704296	C 3.233876 0.509927 -1.665748	O -0.116101 -0.275609 -0.295962
H 1.223617 1.448584 -3.149195	C 0.652250 1.282513 -2.237532	



5A-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.40096878

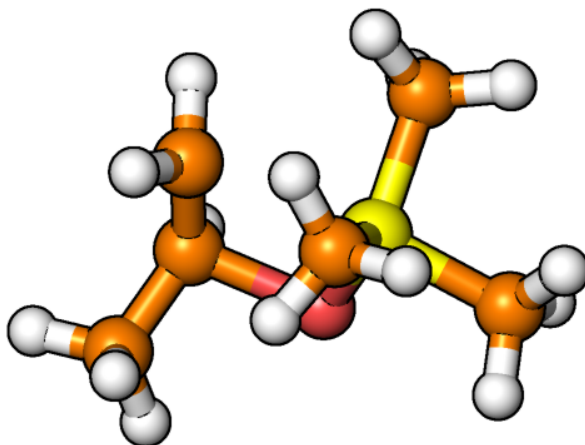
H 1.640735 0.048446 -0.783974	H 1.227408 -0.858442 3.170756	C 2.283960 -0.868326 2.910074
H -1.368018 1.250567 0.139298	H 2.598066 -1.891941 2.704526	C 1.880493 1.788902 1.742075
H -2.592403 -0.027013 0.079495	H 2.875490 -0.479218 3.738180	H -0.711258 -1.569903 1.194791
H -1.081140 -0.231075 -0.820648	H 1.956752 2.379646 0.828897	C 1.729699 -0.562455 0.106457
C -1.514631 0.172524 0.091225	H 0.835203 1.708459 2.033632	P 2.527953 0.128272 1.416488
H 4.845584 -0.569250 1.249196	H 2.449137 2.282153 2.529822	O -0.829181 0.049236 2.385139
H 4.604543 1.035348 0.550818	H 1.898236 -1.618353 -0.069204	C -0.934509 -0.496370 1.305084
H 4.717093 0.847490 2.316236	C 4.351674 0.391680 1.393601	



TS_{5→6}A-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.39449856

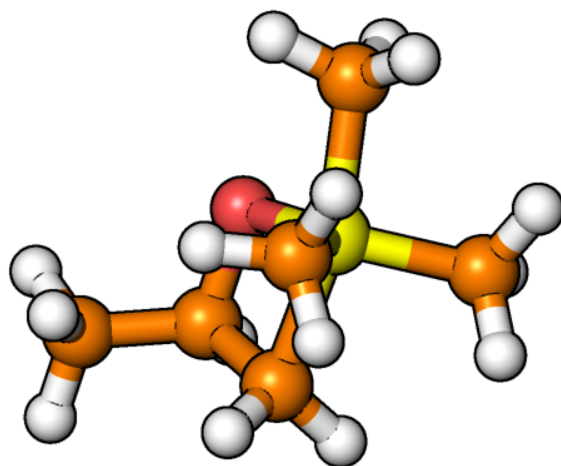
H 2.153704 -1.179650 -0.275016	H 5.015302 0.541201 2.328415	C 2.302848 -0.800251 2.946876
H -0.663736 0.908648 -0.952674	H 1.229443 -0.688770 3.129208	C 2.274296 1.972692 1.968219
H -1.823152 -0.343153 -0.480229	H 2.534466 -1.840579 2.700296	H 0.037441 -1.458330 0.911354
H -0.389162 -0.791524 -1.433829	H 2.874203 -0.508094 3.832529	C 1.820598 -0.214729 0.117538
C -0.756829 -0.135665 -0.634842	H 2.605240 2.646814 1.172510	P 2.715845 0.271241 1.542430
H 1.881586 0.558487 -0.653638	H 1.180601 1.992524 2.044625	O -0.296280 0.415117 1.674889
H 4.860667 -0.807268 1.173790	H 2.739961 2.271832 2.911658	C -0.023488 -0.361178 0.695907
H 4.864806 0.865738 0.582006	C 4.539385 0.214093 1.397328	



TS_{7→8}A-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.40126740

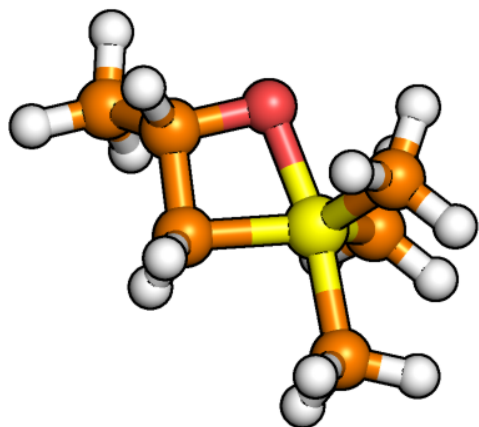
H 1.769522 1.076703 2.166234	H 2.339075 1.841975 -1.651429	C 0.868257 -0.293498 -2.365042
H -0.594044 -1.495933 3.297446	H 0.440861 -1.283417 -2.547460	C 2.620042 -1.399870 -0.462304
H 0.207586 -2.357696 1.977065	H 0.122122 0.454647 -2.646719	H -0.597306 0.620183 1.872184
H -1.447859 -1.747624 1.760647	H 1.751403 -0.168175 -3.002162	P 1.316523 -0.109169 -0.574401
C -0.473875 -1.532128 2.207287	H 3.434165 -1.063815 0.179557	C 1.484896 0.067920 1.875759
H 2.109146 -0.709989 2.313472	H 2.183419 -2.297700 -0.016507	C 0.093806 -0.212628 1.739636
H 1.350999 2.285101 -0.241414	H 3.003465 -1.656606 -1.456453	O -0.135539 -0.336116 -0.019316
H 2.960818 1.598776 0.011280	C 2.076483 1.562434 -0.624866	



7A-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.43398055

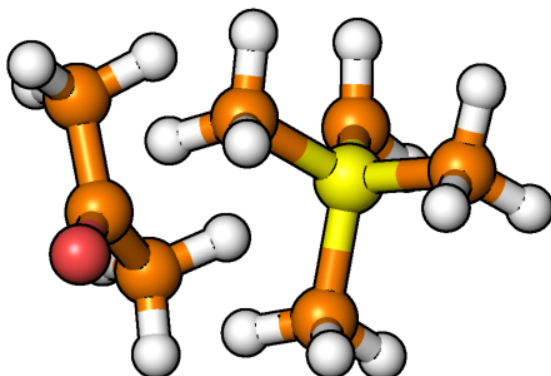
H 2.389419 -0.655522 1.070683	C 0.968429 0.998059 -2.784241	C 2.713511 -0.812813 -1.647633
H 0.279618 2.419219 1.488154	H 3.744417 1.921787 -0.529779	H 2.451229 1.085565 1.390644
H 0.011688 1.272666 2.810184	H 2.325202 2.957281 -0.680497	H -0.014314 -0.609512 1.173484
H -1.244972 1.528138 1.588111	H 3.145827 2.399986 -2.144092	P 1.743021 0.652694 -1.103989
C -0.168515 1.458114 1.749171	C 2.859174 2.118894 -1.132455	C 1.945513 0.306817 0.820148
H 0.386853 1.919614 -2.749602	H 2.098744 -1.700491 -1.485561	C 0.434892 0.351090 0.910231
H 0.295725 0.188712 -3.068239	H 3.611888 -0.908677 -1.040494	O 0.174897 0.589798 -0.504054
H 1.741646 1.099739 -3.546868	H 2.975775 -0.764501 -2.703009	



6A-CHMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-653.43771380

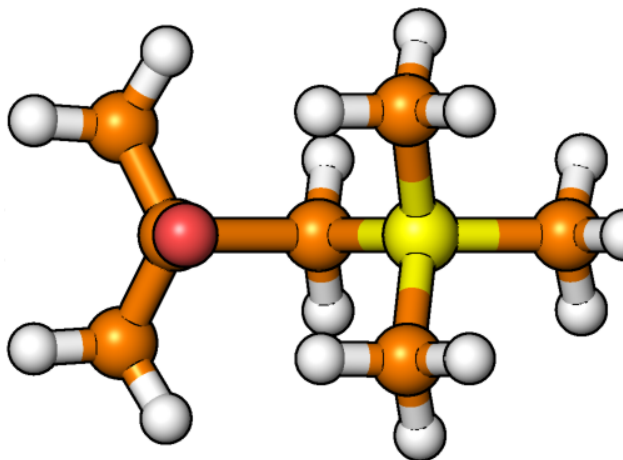
H 2.506033 -0.103690 1.131220	H -0.343026 0.908047 -2.480498	C 0.657739 1.266152 -2.257018
H 0.456400 -0.690630 3.006664	H 0.563700 2.225394 -1.745449	C 1.544819 -1.609721 -1.776964
H 0.745676 -1.865306 1.708998	H 1.233918 1.414520 -3.168213	H -0.291120 0.988310 1.343257
H -0.899108 -1.327602 2.061793	H 2.154655 -1.668347 -2.677045	P 1.479520 0.095155 -1.120167
C 0.141291 -1.006199 2.009047	H 1.990847 -2.248492 -1.013178	C 1.733080 0.511106 0.668338
H 3.456321 1.586620 -1.410045	H 0.535365 -1.965248 -1.961753	C 0.291873 0.122499 1.003376
H 3.966839 -0.076081 -1.112193	H 1.999596 1.558509 0.811532	O -0.110493 -0.266317 -0.301835
H 3.397808 0.397428 -2.717765	C 3.242573 0.542004 -1.647271	



5A-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.67114446

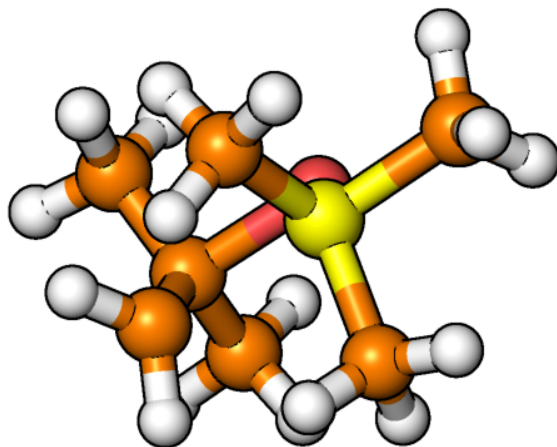
H 1.953214 -0.124638 -1.085241	H 4.833195 -0.565526 1.381139	H 2.131762 -1.749705 -0.264544
H -1.200278 -2.411263 1.949401	H 4.650708 1.006760 0.598939	C 4.302838 0.385789 1.425057
H -0.510076 -2.213811 0.316966	H 4.534311 0.882303 2.369654	C 2.085530 -0.873314 2.705941
H -2.262892 -2.291516 0.520072	H 1.007913 -0.856419 2.854475	C 1.782172 1.725574 1.390132
C -1.335573 -1.941504 0.978251	H 2.417804 -1.903378 2.574785	C 1.905995 -0.694128 -0.163738
H -1.731325 1.400981 0.090592	H 2.583540 -0.452620 3.578941	P 2.497143 0.068384 1.211632
H -2.495954 -0.031094 -0.656678	H 1.924398 2.272026 0.457274	O -1.099257 0.106545 2.172319
H -0.752046 0.209081 -0.803551	H 0.718041 1.634831 1.596755	C -1.337178 -0.440860 1.114732
C -1.610524 0.345548 -0.141299	H 2.267505 2.274226 2.196896	



TS_{5→6}A-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.65910266

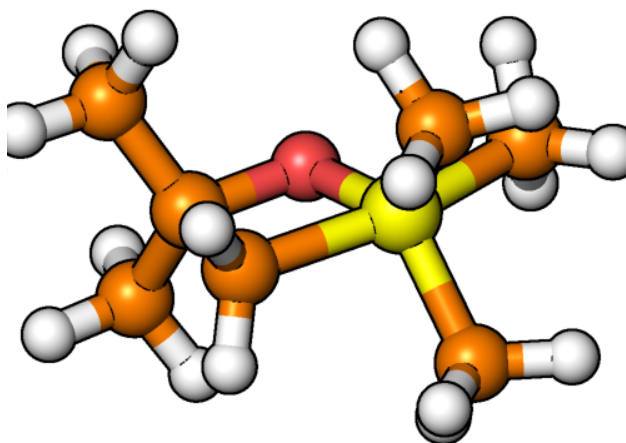
H 1.989968 0.030134 -0.664185	H 4.958809 -0.592190 1.186327	H 2.230883 -1.549968 0.133016
H 0.261772 -2.603059 1.494220	H 4.717782 0.979688 0.398924	C 4.522760 0.403216 1.307373
H -0.038370 -2.525672 -0.262367	H 5.004368 0.902034 2.155625	C 2.513614 -0.659969 3.122039
H -1.356995 -2.225161 0.893864	H 1.435806 -0.714926 3.308744	C 2.112365 1.952488 1.807630
C -0.286183 -2.075301 0.706549	H 2.927157 -1.666215 3.003996	C 1.854898 -0.530817 0.265719
H -0.318707 1.237686 -0.431537	H 3.030536 -0.154214 3.942808	P 2.718879 0.262342 1.577750
H -1.718443 0.165954 -0.305397	H 2.284204 2.529565 0.893899	O -0.176745 -0.006502 1.924707
H -0.380389 -0.260042 -1.398249	H 1.038307 1.870878 2.005975	C 0.005213 -0.557393 0.771122
C -0.628159 0.187234 -0.427912	H 2.631207 2.436692 2.640110	



TS_{7→8}A-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.66590315

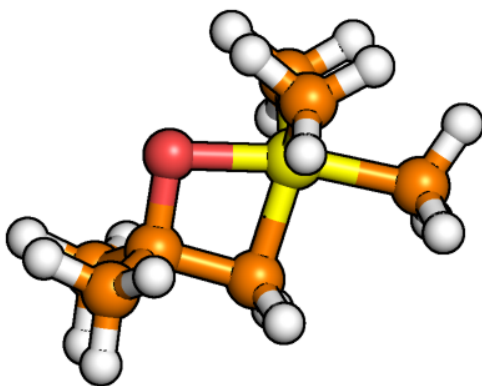
H 2.043721 -0.708859 2.351932	H 1.403778 2.338251 -0.144561	H 1.739473 1.082829 2.251427
H -0.597494 -1.552462 3.300097	H 2.992008 1.624361 0.161604	C 2.127679 1.601113 -0.502446
H 0.187233 -2.315657 1.911157	H 2.428093 1.875025 -1.519691	C 0.966962 -0.223252 -2.289816
H -1.480154 -1.720436 1.767790	H 0.534387 -1.205224 -2.501297	C 2.621297 -1.374189 -0.338144
C -0.499660 -1.518224 2.207261	H 0.244207 0.537733 -2.597449	P 1.338052 -0.061269 -0.472314
H -0.536941 1.931151 1.686524	H 1.878766 -0.104470 -2.886909	C 1.437528 0.088762 1.925537
H -1.049692 1.098025 3.159689	H 3.435296 -1.047148 0.309160	C 0.032331 -0.156269 1.810841
H -1.911191 0.806945 1.633800	H 2.167026 -2.262572 0.108998	O -0.142603 -0.281614 -0.002410
C -0.926823 0.986302 2.074574	H 3.012009 -1.643991 -1.325369	



7A-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.69882545

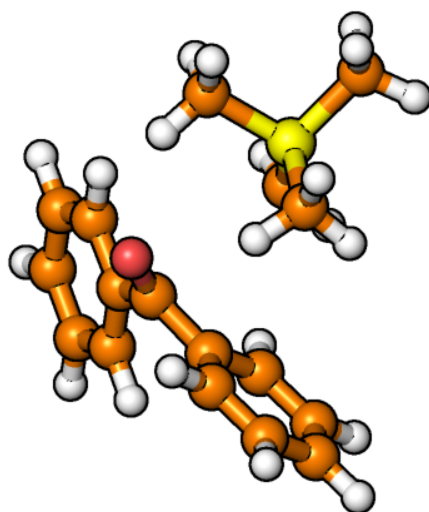
H 2.355207 -0.677655 1.090284	H 0.388998 1.843555 -2.777969	H 3.652632 -0.884804 -0.975602
H 0.297463 2.427367 1.381852	H 0.364276 0.108640 -3.086287	H 3.072753 -0.734443 -2.658538
H 0.003839 1.361576 2.762921	H 1.789832 1.064127 -3.536175	C 2.774563 -0.802730 -1.613786
H -1.246438 1.579677 1.526819	C 1.002252 0.942235 -2.791358	H 2.418865 1.062163 1.410196
C -0.171476 1.493332 1.693509	H 3.699530 1.958009 -0.482208	P 1.745882 0.632286 -1.088390
H -0.084226 -1.215210 2.345934	H 2.250615 2.950233 -0.640934	C 1.918513 0.286398 0.832082
H 0.148742 -1.810496 0.696839	H 3.104018 2.428810 -2.099138	C 0.401399 0.323447 0.909061
H -1.334752 -0.947321 1.120772	C 2.814973 2.132070 -1.092782	O 0.171267 0.563450 -0.520427
C -0.257960 -0.992078 1.291826	H 2.177702 -1.707795 -1.485222	



6A-CMeMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-692.70260180

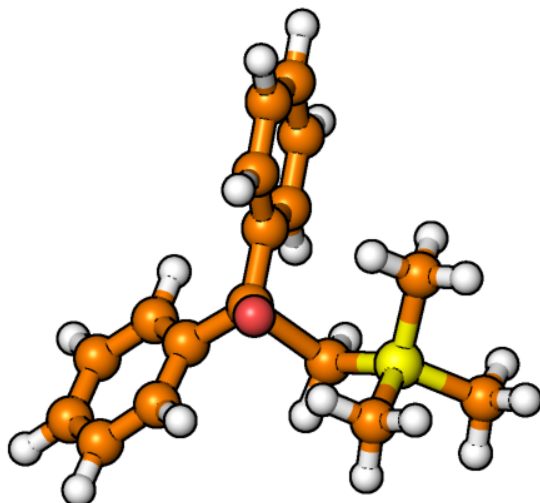
H 2.535730 -0.070143 1.099742	H 3.423448 1.570525 -1.505337	H 2.033329 1.591373 0.774256
H -0.143240 1.712752 2.526673	H 3.930465 -0.085071 -1.165157	C 3.196734 0.520068 -1.702162
H -1.546901 1.102882 1.634537	H 3.324995 0.339788 -2.770898	C 0.610654 1.238015 -2.282052
H -0.419295 2.210514 0.848745	H -0.408994 0.902896 -2.448202	C 1.484957 -1.625890 -1.711167
C -0.494713 1.376864 1.548660	H 0.568669 2.225751 -1.820326	P 1.443223 0.102177 -1.116315
H 0.596964 -0.722522 3.003668	H 1.156121 1.318801 -3.220412	C 1.753945 0.544367 0.652947
H 0.801756 -1.835706 1.640196	H 2.077744 -1.721578 -2.619381	C 0.313722 0.184952 1.044381
H -0.815418 -1.310687 2.111425	H 1.941987 -2.239643 -0.933692	O -0.129064 -0.205186 -0.256428
C 0.222172 -0.990133 2.013353	H 0.470301 -1.981238 -1.864817	



5A-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1075.58406208

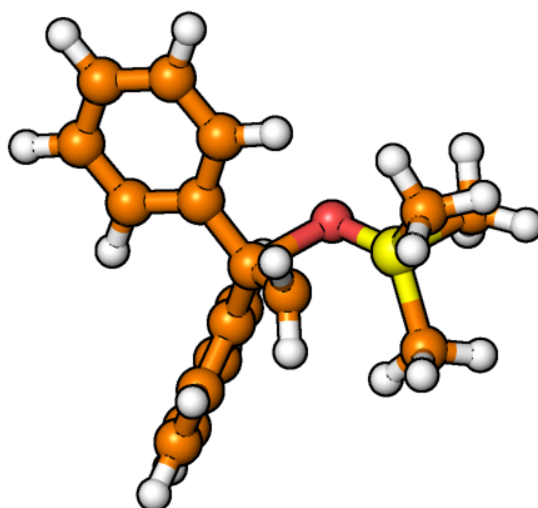
H 3.140391 1.106224 -0.491086	H -0.535749 -3.929130 3.281938	H 3.861202 -0.978820 3.684999
H -1.538177 3.473872 -2.561260	H 0.583611 -1.255581 -0.722447	H 3.668080 2.771725 1.771830
H -2.517367 1.212488 -2.345036	H -0.556061 -1.448495 3.385930	H 2.341927 1.989792 2.663901
H 0.158148 4.245191 -0.930307	C 0.043571 -3.983465 1.213681	H 3.969327 2.095326 3.381764
H -1.784486 -0.280578 -0.525129	C 0.351596 -3.229618 0.085017	H 3.077333 -0.720384 -0.297796
H 0.863031 2.745743 0.915303	C -0.293196 -3.345827 2.403536	C 5.650693 0.303325 1.851848
C -1.221676 2.820351 -1.758864	C 0.315286 -1.843427 0.141801	C 3.254077 -0.940268 2.781678
C -1.767489 1.548882 -1.641186	C -0.313943 -1.959619 2.464563	C 3.409636 1.963607 2.456598
C -0.269337 3.255600 -0.839092	C -0.015262 -1.197764 1.334106	C 3.076344 0.254077 0.173279
C -1.351914 0.705340 -0.616885	H 6.002883 -0.649900 1.456145	P 3.814054 0.379335 1.671204
C 0.129516 2.422597 0.192247	H 6.096411 1.100806 1.256592	O 0.304256 0.803507 2.533864
C -0.399273 1.135501 0.306841	H 5.976136 0.403199 2.889421	C 0.009001 0.290232 1.465342
H 0.067860 -5.064565 1.166023	H 2.213905 -0.762418 3.042693	
H 0.626940 -3.722950 -0.837788	H 3.326552 -1.895379 2.261523	



TS_{5→6}A-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1075.57448054

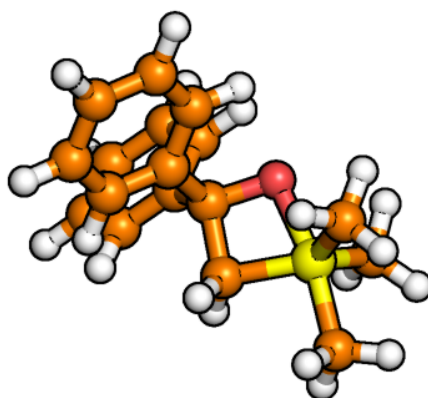
H 3.163427 -1.437840 0.836421	H 0.171508 0.685266 -3.668852	H 3.513475 -0.425237 3.428024
H 1.615110 -6.499310 -0.088892	H -1.662328 -0.104796 0.840106	H 2.679754 1.075984 3.900201
H 1.043218 -5.084369 -2.040308	H 1.451084 -0.597180 -2.026367	H 1.382434 2.271012 0.201424
H 1.703016 -5.478837 2.171623	C -1.494962 1.027235 -2.358003	H 0.476852 1.487971 1.512172
H 0.600323 -2.694345 -1.749872	C -2.013175 0.796206 -1.089057	H 1.581449 2.850774 1.873153
H 1.230886 -3.056344 2.449959	C -0.243223 0.516684 -2.683119	C 4.284590 1.699618 1.306337
C 1.424998 -5.441819 0.041068	C -1.281730 0.071790 -0.155829	C 2.663547 0.224667 3.220663
C 1.109404 -4.646299 -1.052253	C 0.481982 -0.210829 -1.746392	C 1.413890 1.974068 1.248513
C 1.476635 -4.866340 1.307864	C -0.021056 -0.440256 -0.464188	C 2.574394 -0.608688 0.453563
C 0.865551 -3.285503 -0.887257	H 2.851127 -0.378031 -0.570436	P 2.731969 0.773389 1.509336
C 1.227070 -3.511607 1.469406	H 5.130117 1.035726 1.480675	O 0.301039 -0.928590 1.841462
C 0.934241 -2.696657 0.373870	H 4.347379 2.084149 0.288943	C 0.691088 -1.210952 0.658816
H -2.058663 1.595446 -3.086417	H 4.331157 2.535050 2.006886	
H -2.989456 1.181417 -0.824114	H 1.732352 -0.338051 3.311304	



TS_{7→8}A-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1075.57548416

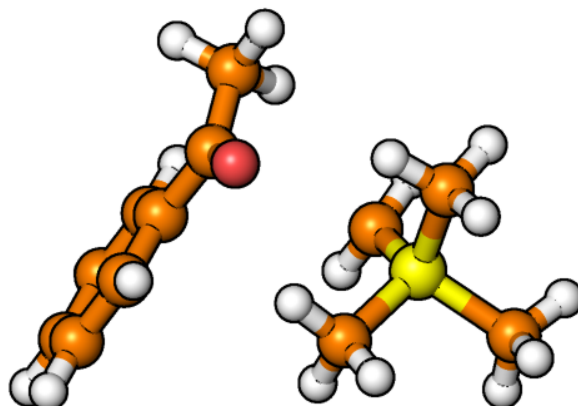
H 2.783522 -0.428258 1.798428	H -0.782806 4.497851 1.304709	H 2.205705 -0.314513 -3.348728
H -0.906176 -4.843709 3.030275	H -1.336342 -0.010416 3.265189	H 3.833624 -1.263240 -0.234878
H 0.996165 -3.712732 4.162494	H 0.649217 2.656310 0.546411	H 2.356984 -2.231374 -0.113393
H -2.064567 -3.702285 1.149924	C -1.873205 3.292640 2.720439	H 3.100343 -1.964825 -1.706032
H 1.730059 -1.479510 3.416783	C -2.018279 2.020231 3.260955	H 2.433716 1.345470 1.657340
H -1.316241 -1.469579 0.402672	C -0.902267 3.510524 1.741818	C 2.926455 1.479707 -1.167394
C -0.580170 -3.860733 2.703261	C -1.205282 0.972597 2.828141	C 1.331425 -0.224706 -2.693496
C 0.486930 -3.229018 3.333970	C -0.088798 2.468621 1.316716	C 2.894279 -1.508419 -0.732682
C -1.229221 -3.218993 1.648485	C -0.224066 1.179440 1.852435	P 1.855900 -0.001147 -0.917950
C 0.907590 -1.969667 2.907096	H 2.339933 2.378604 -0.958145	C 2.120536 0.335787 1.404459
C -0.813416 -1.960274 1.227206	H 3.774914 1.460087 -0.483423	C 0.708636 0.068735 1.443357
C 0.269070 -1.320726 1.845193	H 3.278409 1.534727 -2.203215	O 0.382917 0.032503 -0.361838
H -2.509724 4.107387 3.052446	H 0.719808 -1.125115 -2.795103	
H -2.769780 1.833107 4.022586	H 0.733381 0.629959 -3.022663	



6A-CPhPh

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-1075.61583900

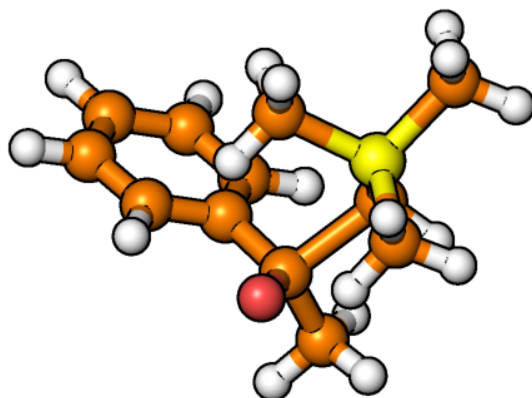
H 2.421962 1.638855 0.606688	H -0.082742 4.132784 3.409923	H 0.558903 2.154708 -1.739254
H 0.434402 -3.489795 4.861164	H -1.736648 0.914329 0.050814	H 1.280941 1.514881 -3.229655
H -1.014435 -3.666869 2.859279	H 1.301774 2.215975 2.749231	H 2.419861 -1.638058 -2.805827
H 2.035039 -1.607112 5.049343	C -1.712557 3.613920 2.110176	H 2.360472 -2.177953 -1.119197
H -0.851248 -1.969001 1.059038	C -2.176686 2.705466 1.166593	H 0.851927 -1.973577 -1.999816
H 2.177129 0.075802 3.266985	C -0.454983 3.430414 2.675154	C 3.441524 0.667725 -1.941154
C 0.496687 -2.747611 4.075905	C -1.390504 1.622083 0.789877	C 0.764842 1.248602 -2.309612
C -0.315548 -2.845205 2.951803	C 0.327197 2.346476 2.297562	C 1.855652 -1.577378 -1.876971
C 1.393701 -1.690894 4.181343	C -0.131490 1.431208 1.351284	P 1.762351 0.137915 -1.260259
C -0.233707 -1.893554 1.942108	H 2.912732 -0.037390 0.896181	C 2.127734 0.597847 0.487077
C 1.472306 -0.740409 3.170779	H 3.613557 1.728230 -1.745560	C 0.705244 0.219356 0.937298
C 0.659338 -0.830242 2.042074	H 4.243828 0.103175 -1.461329	O 0.259089 -0.316656 -0.294965
H -2.323209 4.457775 2.403009	H 3.508894 0.505009 -3.018271	
H -3.153619 2.839656 0.720634	H -0.188965 0.773556 -2.522321	



5A-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.12899261

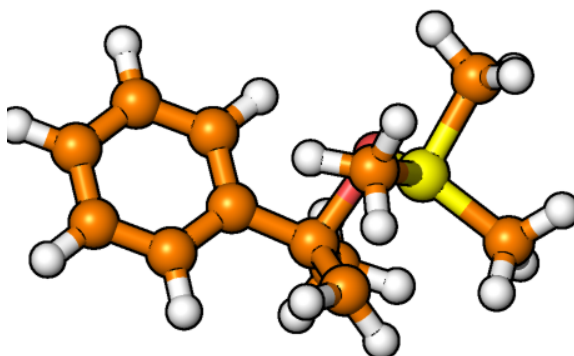
H 2.138715 -1.533193 -0.187387	C -0.602997 -4.160398 0.374459	H 0.812283 1.836585 1.660688
H -1.731648 1.141377 0.026244	C -0.890757 -2.551737 2.620503	H 2.353630 2.486288 2.278356
H -2.415271 -0.422906 -0.490122	C -0.804876 -2.795140 0.227368	C 4.412769 0.640294 1.412671
H -0.709424 -0.053960 -0.799400	C -0.943243 -1.976864 1.349292	C 2.245544 -0.655741 2.752103
C -1.531040 0.080211 -0.095248	H 2.003357 0.091080 -1.035045	C 1.876565 1.944827 1.461641
H -0.392379 -5.788725 1.759254	H 4.954064 -0.304338 1.359631	C 1.983996 -0.464864 -0.105135
H -0.662047 -4.353330 3.758409	H 4.728127 1.260058 0.572600	P 2.605919 0.296434 1.252569
H -0.481864 -4.784170 -0.501066	H 4.664361 1.147130 2.346777	O -0.985846 0.215499 2.214333
H -1.005138 -1.909194 3.482140	H 1.180210 -0.597842 2.961929	C -1.129394 -0.498825 1.237376
H -0.823454 -2.362178 -0.761543	H 2.519491 -1.697402 2.586274	
C -0.548657 -4.723874 1.645054	H 2.809752 -0.270235 3.600562	
C -0.697313 -3.916643 2.768927	H 2.014163 2.508607 0.538300	



TS_{5→6}A-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.11835127

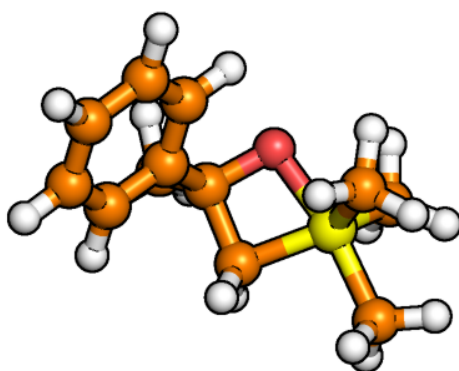
H 2.429410 -1.924920 0.722893	C -0.655198 0.207998 -2.879844	H 0.557321 1.603077 1.634618
H 0.359820 -3.203417 1.276112	C -1.397087 0.701008 -0.248999	H 2.012251 2.601766 1.977037
H 0.331519 -3.010500 -0.496462	C -0.118928 -0.552798 -1.844308	C 4.287768 0.761193 1.309824
H -1.170518 -2.884960 0.441901	C -0.470501 -0.311369 -0.510057	C 2.373764 -0.288307 3.247092
C -0.097901 -2.656325 0.446518	H 2.259949 -0.725757 -0.598656	C 1.588514 1.815237 1.345833
H -1.984873 1.822598 -3.408791	H 4.929601 -0.114725 1.436536	C 1.988674 -0.966877 0.431487
H -2.657152 2.249016 -1.053532	H 4.433610 1.155145 0.300016	P 2.536810 0.283972 1.538397
H -0.364870 0.003024 -3.906962	H 4.580333 1.527296 2.036186	O -0.266338 -0.718836 1.851789
H -1.691855 0.864729 0.782615	H 1.331458 -0.601444 3.370671	C 0.064609 -1.136795 0.684633
H 0.584847 -1.344315 -2.086956	H 3.040293 -1.140245 3.411989	
C -1.565347 1.228154 -2.602169	H 2.630976 0.510706 3.948517	
C -1.937128 1.467222 -1.281559	H 1.609102 2.137483 0.301333	



TS_{7→8}A-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.12197360

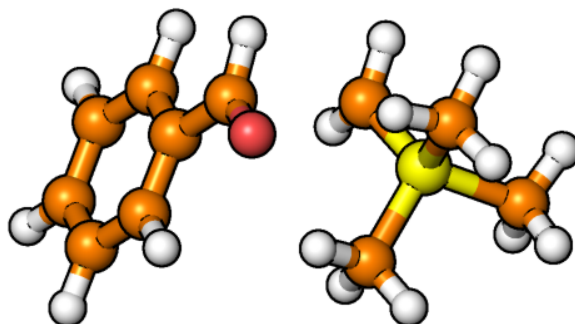
H 2.425581 -0.623611 2.221473	C -0.748259 3.314793 3.573910	H 3.533758 -1.102135 -1.499314
H -0.310844 -1.162376 3.134392	C -1.457562 1.801344 1.350822	H 2.370198 1.193332 2.285421
H 0.394422 -1.932626 1.700511	C 0.030141 2.222503 3.192359	C 2.671029 2.054336 -0.326841
H -1.188263 -1.128036 1.593921	C -0.309116 1.452676 2.074154	C 1.527584 0.447267 -2.329675
C -0.195160 -1.079278 2.046597	H 1.973772 2.728258 0.177955	C 3.123830 -0.941170 -0.496331
H -2.484487 4.511501 3.132469	H 3.571393 1.976169 0.283919	P 1.869691 0.407469 -0.498961
H -3.110608 3.155116 1.145793	H 2.921249 2.476076 -1.305843	C 1.933749 0.285416 1.879854
H -0.466099 3.896499 4.446830	H 1.086309 -0.499185 -2.655121	C 0.511047 0.229206 1.737235
H -1.727086 1.225329 0.473343	H 0.822287 1.249101 -2.564671	O 0.370291 0.189525 -0.084130
H 0.904320 1.957032 3.777318	H 2.452963 0.614800 -2.893262	
C -1.879799 3.657816 2.840738	H 3.927508 -0.712088 0.204057	
C -2.230638 2.894852 1.727244	H 2.638757 -1.864258 -0.166801	



6A-CPhMe

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-884.16050491

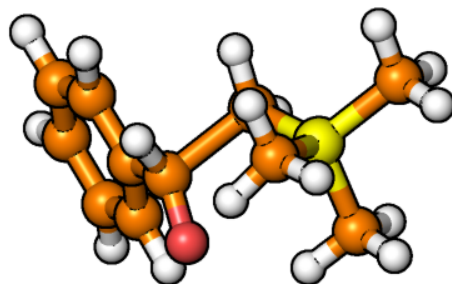
H 2.427111 -0.412403 1.137101	H 0.350269 -0.750306 3.058895	H 0.474443 -1.846582 -2.094689
H -2.464411 4.489037 2.552785	H 0.580279 -1.937264 1.757819	H 2.145901 1.328362 0.998267
H -0.417759 3.816026 3.776567	H -1.030828 -1.287734 2.094289	C 3.252381 0.550351 -1.567204
H -3.244424 3.130789 0.634392	C 0.030640 -1.043854 2.057870	C 0.665118 1.400973 -2.042237
H 0.831593 1.813317 3.086681	H 3.490276 1.560789 -1.228631	C 1.495929 -1.528913 -1.907433
H -1.966451 1.116442 -0.057441	H 3.967177 -0.134066 -1.104839	P 1.487156 0.094246 -1.068265
C -1.915478 3.607150 2.250268	H 3.393661 0.509600 -2.648510	C 1.751032 0.346667 0.741556
C -0.766243 3.228980 2.936643	H -0.306016 1.040752 -2.370484	C 0.267253 0.074615 1.042719
C -2.350521 2.844473 1.173440	H 0.495370 2.256800 -1.388629	O -0.097909 -0.359375 -0.259667
C -0.062112 2.097828 2.544208	H 1.268198 1.715870 -2.891582	
C -1.641704 1.713374 0.782627	H 2.072952 -1.493690 -2.829949	
C -0.489407 1.328952 1.461503	H 1.958215 -2.255804 -1.237921	



5A-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-844.86077946

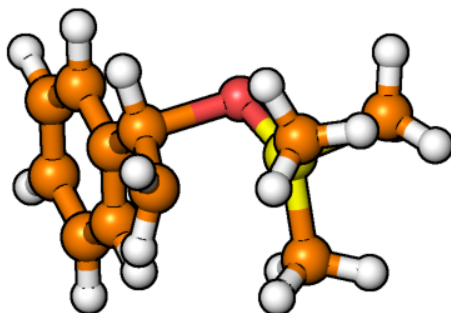
H 1.799677 -1.764754 0.082211	C -1.111289 -1.867201 1.205975	H -0.967298 0.014501 0.104720
H -1.560107 -5.703501 1.391660	H 1.758709 -0.170650 -0.833341	C 4.339430 0.215364 1.506399
H -1.388683 -4.583881 -0.808979	H 4.769065 -0.786339 1.493962	C 2.073122 -0.743958 2.969462
H -1.462267 -4.367955 3.470932	H 4.698385 0.749844 0.626394	C 1.961673 1.803801 1.532634
H -1.084709 -2.126563 -0.920057	H 4.672946 0.738505 2.405266	C 1.754987 -0.684411 0.119910
H -1.188809 -1.898060 3.341121	H 1.012905 -0.591864 3.161361	P 2.504980 0.079869 1.415494
C -1.435965 -4.629628 1.339215	H 2.268775 -1.811626 2.870948	O -0.928919 0.335237 2.099151
C -1.340412 -4.000276 0.100783	H 2.660470 -0.349056 3.797515	C -0.959117 -0.396376 1.125303
C -1.378019 -3.877736 2.509777	H 2.159713 2.300957 0.582355	
C -1.179000 -2.624359 0.036927	H 0.891145 1.818272 1.730647	
C -1.221221 -2.501046 2.443984	H 2.495790 2.330077 2.323061	



TS_{5→6}A-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-844.85460761

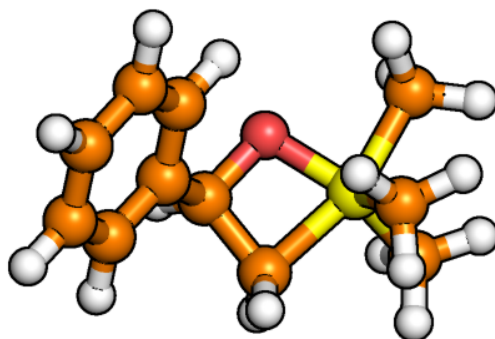
H 2.311552 -0.891936 -0.157976	C -0.319546 -3.001927 2.308863	H 2.571525 -1.854753 1.337648
H 0.071875 -0.132621 0.513300	C -0.092697 -2.176844 1.205817	C 4.746827 0.733967 1.168063
H -1.224835 -5.867517 0.711260	H 5.348843 -0.155351 1.372623	C 3.056233 0.179554 3.489662
H -0.855004 -4.402133 -1.261213	H 4.773455 0.930780 0.092515	C 2.137768 1.994269 1.365477
H -0.897010 -4.956876 2.998162	H 5.180357 1.589465 1.697639	C 2.210917 -0.907404 0.930343
H -0.141937 -2.052010 -0.942287	H 2.018125 0.003281 3.793447	P 3.020859 0.445250 1.701240
H -0.193996 -2.579932 3.301321	H 3.664724 -0.700841 3.716634	O 0.197592 -0.192727 2.562239
C -0.907136 -4.837823 0.848615	H 3.473717 1.049887 4.004151	C 0.350379 -0.733653 1.413807
C -0.697320 -4.014893 -0.258055	H 2.076038 2.159818 0.285927	
C -0.720361 -4.324646 2.131792	H 1.132646 1.892942 1.785230	
C -0.294225 -2.694336 -0.076371	H 2.659536 2.838216 1.825545	



TS_{7→8}A-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-844.85676628

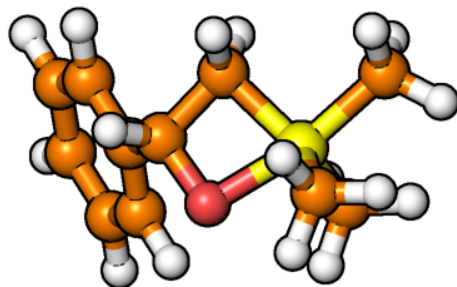
H 1.032033 1.434178 2.062022	C -0.637557 -1.573913 2.024707	C 1.983406 1.674667 -0.591452
H -1.917658 -5.015629 3.334056	H 1.694201 -0.169830 2.585626	C 1.578651 -0.566083 -2.242632
H -3.517809 -3.364872 2.388664	H 1.069419 2.270105 -0.513272	C 2.984552 -1.077154 0.129972
H 0.500005 -4.455580 3.443501	H 2.650979 1.968341 0.218880	H -1.033376 0.432356 1.366128
H -2.699062 -1.192289 1.544606	H 2.452931 1.881700 -1.559463	P 1.535353 -0.102009 -0.443368
H 1.307917 -2.279284 2.636503	H 1.398633 -1.638288 -2.359381	C 1.051732 0.360703 1.888003
C -1.562321 -4.057084 2.967679	H 0.798534 -0.030452 -2.790440	C -0.191983 -0.242062 1.518888
C -2.458201 -3.131351 2.438185	H 2.551613 -0.320833 -2.683870	O 0.051621 -0.578456 -0.213454
C -0.205282 -3.741632 3.027653	H 3.513090 -0.552892 0.925590	
C -1.996458 -1.905178 1.967957	H 2.623278 -2.031830 0.522647	
C 0.250812 -2.511628 2.564873	H 3.665656 -1.283801 -0.702877	



7A-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-844.89029182

H 2.041066 -1.013728 0.910840	C -0.181501 1.455568 1.658209	H 3.321187 -0.438245 -2.640417
H -1.301355 4.471509 3.829681	H 0.318893 1.751696 -2.784708	C 2.926785 -0.666196 -1.651344
H -0.192887 2.521237 4.884145	H 0.487585 0.040431 -3.171698	H 2.367564 0.638190 1.472047
H -1.696905 4.479880 1.385594	H 1.831984 1.148941 -3.492542	H -0.306185 -0.610490 1.127442
H 0.521281 0.609562 3.502608	C 1.020053 0.917862 -2.802632	P 1.697961 0.591164 -1.081123
H -0.986792 2.547327 0.008673	H 3.466419 2.036618 -0.247407	C 1.769413 0.034502 0.792421
C -0.989948 3.630324 3.224675	H 1.921176 2.878426 -0.367472	C 0.269677 0.271940 0.837574
C -0.368216 2.534166 3.816140	H 2.880826 2.607096 -1.832418	O 0.081588 0.488733 -0.579544
C -1.209566 3.634013 1.853459	C 2.588501 2.180261 -0.874835	
C 0.032097 1.457071 3.037536	H 2.423498 -1.634219 -1.699325	
C -0.809459 2.551923 1.074500	H 3.738228 -0.746527 -0.928974	



6A-CPhH

E(DLPNO-CCSD(T)/CBS(def2-TZVPP,def2-QZVPP))=-844.89531731

H 2.105388 1.425771 0.889195	C -0.514397 1.347274 1.457601	H 0.153895 -0.652262 1.763129
H -2.503068 4.464910 2.634119	H 2.448585 -0.289917 1.150040	C 3.267154 0.462751 -1.605528
H -0.599275 3.623606 3.978642	H 3.492315 1.501134 -1.353858	C 0.685921 1.237897 -2.195059
H -3.138000 3.296420 0.546078	H 3.981786 -0.171678 -1.076803	C 1.529561 -1.660594 -1.777905
H 0.659825 1.642379 3.233185	H 3.422686 0.329709 -2.677306	P 1.501077 0.032017 -1.093105
H -1.858482 1.297894 -0.193082	H -0.300930 0.869850 -2.460538	C 1.747670 0.414132 0.701078
C -1.949803 3.594490 2.307253	H 0.556216 2.169291 -1.642972	C 0.269940 0.133048 1.004892
C -0.879932 3.121873 3.061742	H 1.279518 1.435995 -3.085302	O -0.102607 -0.349103 -0.268325
C -2.302882 2.938753 1.134750	H 2.151857 -1.720171 -2.669075	
C -0.170828 2.005845 2.639024	H 1.942234 -2.326344 -1.018650	
C -1.589714 1.820635 0.713379	H 0.513290 -1.982511 -1.986335	