

An Actinide Metallacyclopentene Complex: Synthesis, Structure, Reactivity and Computational Studies

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Walter*

Complete reference 32

(32) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A.02, Gaussian, Inc.: Wallingford CT, 2009.

Magnetic Susceptibility Study.

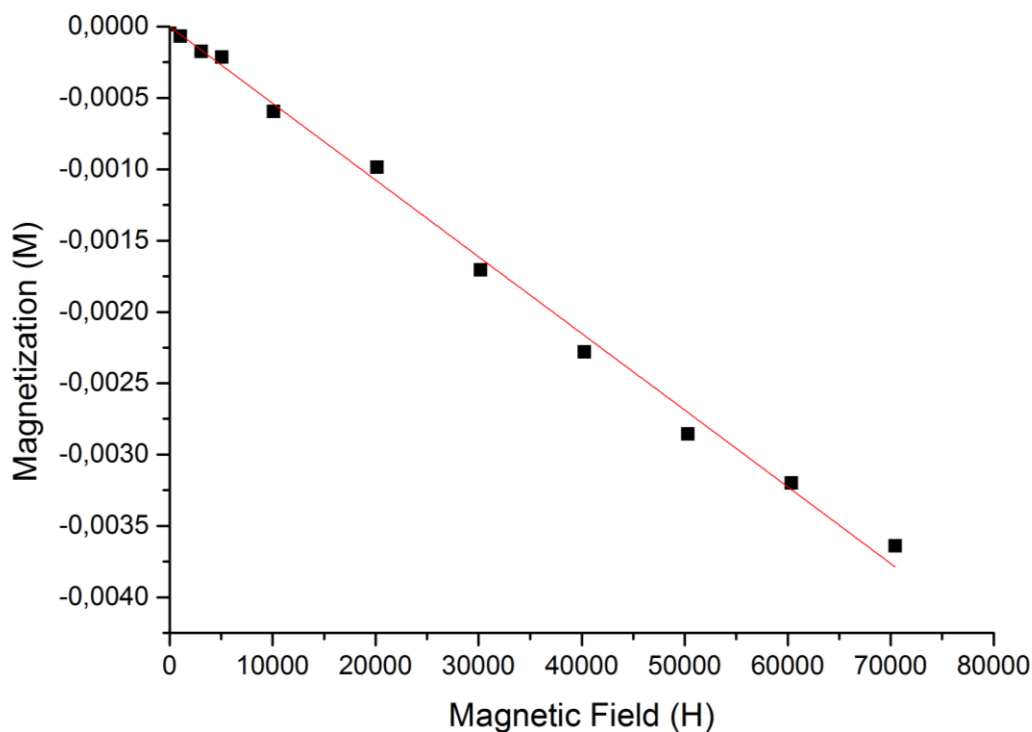
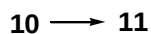


Figure S1. M vs. H plot for **2** recorded at 300 K and at variable magnetic field (H) 0-70 kG. Linear fit results: $\chi_{\text{raw}} = -5.38 \times 10^{-8}$, $R^2 = 0.9978$.

Table S1. Corrected magnetic susceptibility data for **2**

T (K)	χ_{raw}	MW (g mol ⁻¹)	mass (g)	χ_{mol} (cm ³ mol ⁻¹)	Pascal's constants	χ (cm ³ mol ⁻¹)
200	-5.60×10^{-8}	877	0.079	-6.21×10^{-4}	-5.18×10^{-4}	-1.03×10^{-4}
250	-4.50×10^{-8}	877	0.079	-4.99×10^{-4}	-5.18×10^{-4}	1.89×10^{-5}
300	-5.38×10^{-8}	877	0.079	-5.97×10^{-4}	-5.18×10^{-4}	-7.88×10^{-5}
Average						-5.44×10^{-5}
σ_{mean}						3.73×10^{-5}

Kinetic Study. In an attempt to evaluate the reaction



the conversion of **10** to **11** was monitored by ^1H NMR spectroscopy in C_6D_6 solution at 323 K (Figure S2). The reaction was complete after 4 h at 50 °C.

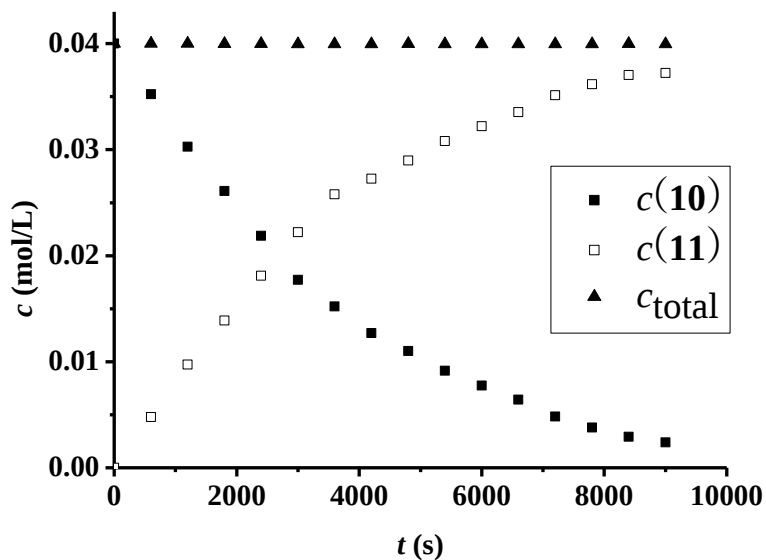


Figure S2. c vs. t plot for the thermal conversion of **10** to **11** at 323 K recorded in C_6D_6 solution. $c_0 = 0.04$ mol/L.

The kinetics for the reaction $\mathbf{10} \xrightarrow{k} \mathbf{11}$ can be described by the following equation:

$$\ln(c_0/c) = kt$$

Figure S3 shows the $\ln(c_0/c)$ vs. t plot of the data presented in Figure S2. The linear fit is of reasonable quality and a value of $k = 3.11(7) \times 10^{-4} \text{ s}^{-1}$ can be derived from this analysis, which corresponds to a barrier $\Delta G^\ddagger(\mathbf{10} \rightarrow \mathbf{11}) = 24.2$ kcal/mol.

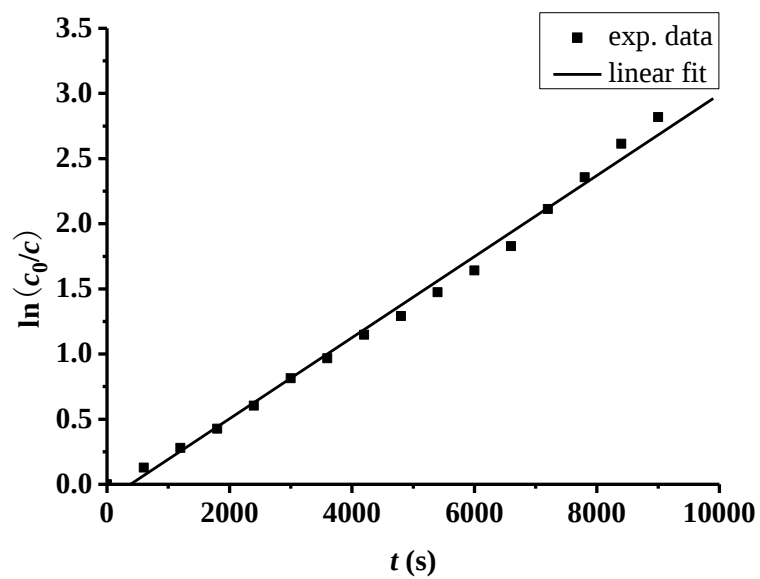


Figure S3. $\ln(c_0/c)$ vs. t plot ($R^2 = 0.976$) for the thermal conversion of **10** to **11** at 323 K recorded in C_6D_6 solution. $c_0 = 0.04$ mol/L. $k = 3.11(7) \times 10^{-4} \text{ s}^{-1}$.

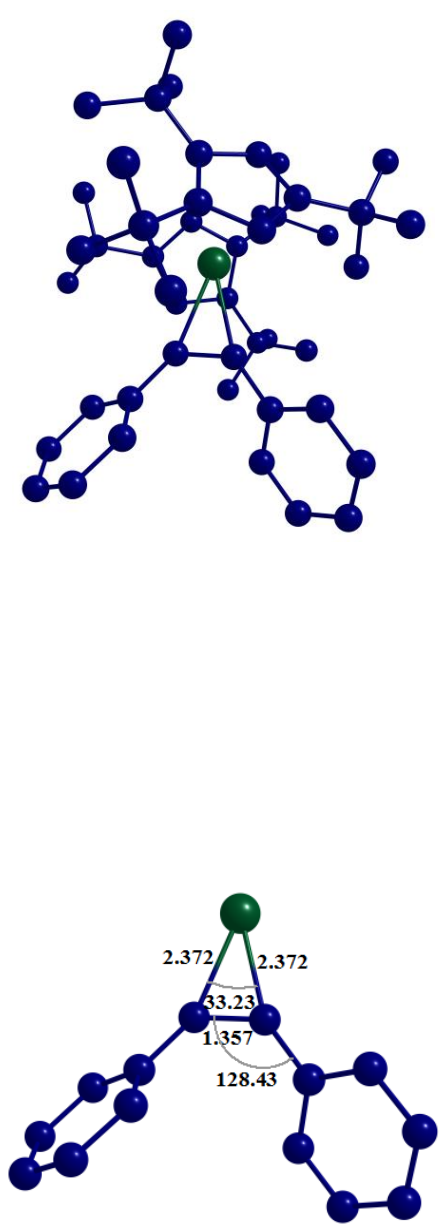
Table S2. Crystal Data and Experimental Parameters for Compounds 2-5

Compound	2	3·C ₆ H ₁₂	2(4)·C ₆ H ₆	5
Formula	C ₄₈ H ₆₈ Th	C ₆₁ H ₈₅ ClOTh	C ₁₀₄ H ₁₄₂ S ₄ Th ₂	C ₅₅ H ₇₃ NSTh
Fw	877.06	1101.78	1984.54	1012.24
crystal system	Monoclinic	triclinic	monoclinic	monoclinic
space group	<i>C2/c</i>	<i>P</i> (-1)	<i>P2</i> ₁ / <i>c</i>	<i>P2</i> ₁ / <i>n</i>
<i>a</i> (Å)	15.809(1)	10.627(1)	30.937(4)	11.734(1)
<i>b</i> (Å)	13.073(1)	12.635(1)	10.764(2)	23.948(1)
<i>c</i> (Å)	21.035(2)	21.431(2)	37.102(4)	18.452(1)
α (deg)	90	92.17(1)	90	90
β (deg)	105.23(1)	103.97(1)	125.21(1)	90.80(1)
γ (deg)	90	104.89(1)	90	90
<i>V</i> (Å ³)	4194.6(5)	2683.4(4)	10096(2)	5184.5(5)
<i>Z</i>	4	2	4	4
<i>D</i> _{calc} (g/cm ³)	1.389	1.364	1.306	1.297
μ (Mo/K α) _{calc} (cm ⁻¹)	3.585	2.867	3.067	2.950
size (mm)	0.45 × 0.38 × 0.25	0.30 × 0.20 × 0.20	0.30 × 0.21 × 0.15	0.15 × 0.12 × 0.09
<i>F</i> (000)	1784	1132	4040	2064
2 θ range (deg)	4.02 to 55.16	3.94 to 55.12	3.82 to 54.92	3.86 to 50.50
no. of reflns, collected	12141	17834	22998	25833
no of obsd reflns	4503	11203	16483	7640
no of variables	231	589	1027	541
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	0.47, 0.30	0.60, 0.48	0.66, 0.46	0.75, 0.62
<i>R</i>	0.019	0.028	0.044	0.029
<i>R</i> _w	0.042	0.065	0.083	0.062
<i>R</i> _{all}	0.043	0.067	0.090	0.067
Gof	1.03	1.05	0.94	1.00

Table S3. Crystal Data and Experimental Parameters for Compounds 6, 7, 11 and 14

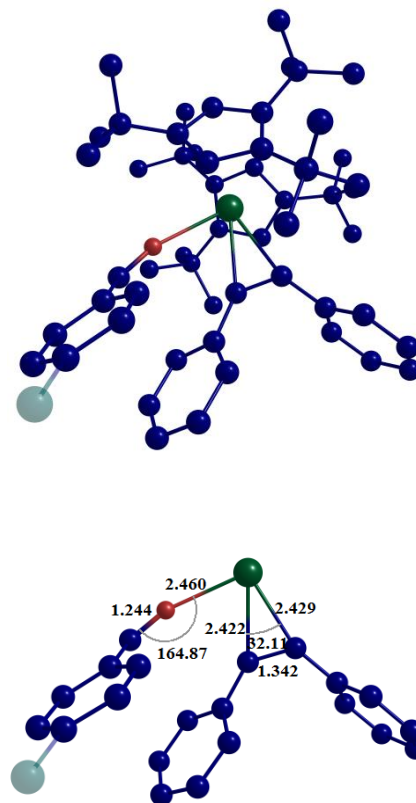
Compound	6	7·4C₆H₁₂	11	14
Formula	C ₆₁ H ₉₀ N ₂ Th	C ₈₄ H ₁₂₆ O ₂ Th	C ₅₁ H ₇₇ NSiTh	C ₆₁ H ₇₆ N ₂ Th
Fw	1083.38	1399.88	964.27	1794.19
crystal system	triclinic	monoclinic	triclinic	monoclinic
space group	<i>P</i> (-1)	<i>C</i> 2/ <i>c</i>	<i>P</i> (-1)	<i>P</i> 2 ₁
<i>a</i> (Å)	13.057(1)	23.875(2)	11.332(1)	10.420(2)
<i>b</i> (Å)	17.487(2)	18.274(2)	12.923(1)	18.183(4)
<i>c</i> (Å)	27.078(3)	19.869(2)	18.201(2)	13.287(3)
α (deg)	80.95(1)	90	76.81(1)	90
β (deg)	81.74(1)	123.61(1)	75.33(1)	93.11(1)
γ (deg)	88.59(1)	90	67.65(1)	90
<i>V</i> (Å ³)	6042.0(11)	7219.3(12)	2358.9(3)	2513.6(9)
<i>Z</i>	4	4	2	2
<i>D</i> _{calc} (g/cm ³)	1.191	1.288	1.358	1.413
μ (Mo/K α) _{calc} (cm ⁻¹)	2.502	2.112	3.219	3.007
size (mm)	0.38 × 0.25 × 0.20	0.40 × 0.33 × 0.25	0.30 × 0.20 × 0.16	0.15 × 0.12 × 0.10
<i>F</i> (000)	2242	2944	988	1092
2 θ range (deg)	3.08 to 50.50	4.10 to 55.27	3.42 to 55.02	3.07 to 56.66
no. of reflns, collected	34882	24056	15932	18269
no of obsd reflns	13888	7515	9629	9828
no of variables	1189	402	507	594
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	0.75, 0.59	0.75, 0.63	0.63, 0.45	0.75, 0.63
<i>R</i>	0.057	0.030	0.028	0.062
<i>R</i> _w	0.119	0.072	0.059	0.109
<i>R</i> _{all}	0.140	0.075	0.062	0.118
Gof	0.97	1.03	1.01	1.06

Table S4. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for 2+*p*-ClPhCHO, obtained with B3PW91-PCM+D3 method.

Species	Cartesian coordinates				
2	C	-0.53212	2.71815	-0.92729	
	C	-1.90839	2.38559	-0.62165	
	C	-2.29546	1.38139	-1.56277	
	H	-3.28872	0.95948	-1.63411	
	C	-1.23991	1.09915	-2.45075	
	C	-0.15960	1.90595	-2.03722	
	H	0.81069	1.91970	-2.50878	
	C	0.43027	3.79898	-0.40412	
	C	-0.13267	5.19692	-0.71985	
	H	-1.05428	5.41313	-0.17594	
	H	-0.34782	5.28910	-1.79077	
	H	0.59877	5.96923	-0.45034	
	C	0.74806	3.66566	1.09549	
	H	1.40706	4.48342	1.41307	
	H	1.27657	2.72599	1.29177	
	H	-0.13938	3.69607	1.72551	
	C	1.78692	3.69204	-1.12812	
	H	2.48285	4.42591	-0.70591	
	H	1.69816	3.89911	-2.20055	
	H	2.22787	2.69848	-0.99659	
	C	-3.03395	3.07202	0.17685	
	C	-3.69324	4.09956	-0.76955	
	H	-4.54878	4.58218	-0.27930	
	H	-4.05053	3.60872	-1.68140	
	H	-2.98532	4.87907	-1.06657	
	C	-2.63930	3.79360	1.47109	
	H	-1.90599	4.58344	1.31090	
	H	-2.24523	3.10306	2.22144	
	H	-3.53007	4.26462	1.90398	
	C	-4.10635	2.03578	0.57398	
	H	-3.65698	1.19652	1.11556	
	H	-4.64117	1.62627	-0.28796	
	H	-4.85543	2.50006	1.22569	
	C	-1.22949	0.09539	-3.59282	
	C	-0.50754	0.68816	-4.81141	
	H	-1.00960	1.59979	-5.15411	
	H	-0.49833	-0.03348	-5.63747	
	H	0.53245	0.94103	-4.58210	
	C	-2.65856	-0.28562	-3.99779	
	H	-3.18846	-0.79455	-3.18556	
	H	-2.63880	-0.97014	-4.85401	
	H	-3.23848	0.60028	-4.27990	
	C	-0.48658	-1.16505	-3.12705	
	H	0.56465	-0.96422	-2.89627	
	H	-0.51733	-1.96657	-3.87570	
	H	-0.96964	-1.58996	-2.23034	
	C	1.91367	0.21176	0.64311	
	C	3.05846	0.55972	1.48650	
	C	4.08939	1.39841	1.02024	
	H	4.04953	1.75736	-0.00399	
	C	5.15079	1.75869	1.84448	
	H	5.93088	2.41297	1.46072	

C	5.22734	1.27448	3.15243
H	6.06068	1.55210	3.79329
C	4.22363	0.42980	3.62712
H	4.27237	0.04083	4.64210
C	3.14823	0.09058	2.80910
H	2.36643	-0.56209	3.18774
Th	-0.35949	0.00016	-0.00110
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C	3.05889	-0.55773	-1.48934
C	4.09812	-1.38354	-1.01848
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C	5.22802	-1.27070	-3.15557
H	6.06152	-1.54766	-3.79651
C	4.21589	-0.43887	-3.63506
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C	-2.29165	-1.38236	1.56435
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C	-1.23503	-1.09834	2.45051
C	-0.15446	-1.90408	2.03555
H	0.81651	-1.91646	2.50568
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C	-0.12472	-5.19516	0.72569
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H	-0.33345	-5.28443	1.79814
H	0.60593	-5.96752	0.45413
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H	1.27565	-2.72924	-1.29832
H	-0.14340	-3.69807	-1.72464
C	1.79432	-3.68591	1.12098
H	2.48986	-4.41958	0.69775
H	1.71066	-3.89035	2.19431
H	2.23273	-2.69186	0.98475
C	-3.03140	-3.07497	-0.17257
C	-3.69186	-4.09665	0.77940
H	-4.54785	-4.58117	0.29182
H	-4.04863	-3.60078	1.68871
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H	-1.90643	-4.59438	-1.29932
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H	-3.53128	-4.27755	-1.89130
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H	-4.63373	-1.62113	0.28452
H	-4.85319	-2.50547	-1.22231
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C	-0.51094	-0.69790	4.81486
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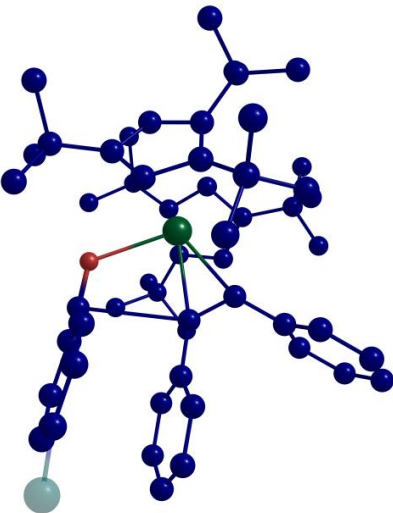
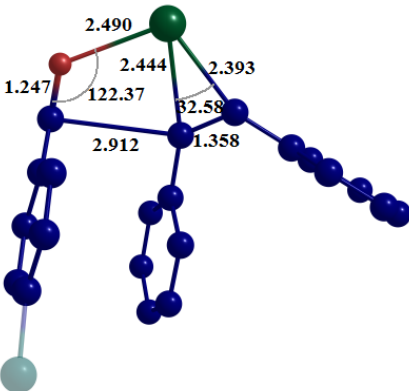
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<i>p</i> -ClPhCHO	C 0.72788 0.86602 -1.31881 O 0.72788 0.78740 -2.53277 H 0.72788 -0.05164 -0.68964 C 0.72788 2.13405 -0.56364 C 0.72788 2.11582 0.83528 C 0.72788 3.35933 -1.24402 C 0.72788 3.30466 1.55718 C 0.72788 4.55384 -0.53812 C 0.72788 4.51270 0.85938 H 0.72788 1.16505 1.36520 H 0.72788 3.35500 -2.33050 H 0.72788 3.30208 2.64243 H 0.72788 5.50926 -1.05324 Cl 0.72788 6.00878 1.75206	
COM3	C 0.29958 1.86312 2.17528 C 1.61083 2.30572 1.75906 C 1.42976 2.91804 0.48066 H 2.21631 3.42581 -0.06187 C 0.06730 2.97836 0.13128 C -0.60802 2.27786 1.15308 H -1.67990 2.16812 1.20510 C -0.25232 1.31138 3.49720 C -0.34999 2.46716 4.51183 H -0.78243 2.11478 5.45726 H -0.98787 3.26753 4.11881 H 0.62819 2.90270 4.73208 C 0.56794 0.15286 4.07474 H 0.64469 -0.65137 3.34096 H 0.07799 -0.24696 4.97152 H 1.57551 0.44006 4.35717 C -1.67909 0.75810 3.29410 H -1.69415 -0.01561 2.51682 H -2.39872 1.53981 3.02659 H -2.03242 0.30485 4.22780 C 2.91610 2.69655 2.49601 C 2.79184 4.21557 2.77423 H 1.90683 4.42573 3.38511 H 2.69613 4.78650 1.84537 H 3.67547 4.58224 3.31282 C 3.24201 2.03557 3.84093 H 3.39453 0.95814 3.75548 H 2.47838 2.22546 4.59711 H 4.17875 2.46270 4.21971 C 4.14450 2.46228 1.59919 H 5.04250 2.87205 2.07754 H 4.05405 2.93107 0.61576 H 4.30507 1.39220 1.44832 C -0.54278 3.91909 -0.90337 C -0.06059 5.34484 -0.56311	



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H	-0.52238	6.07708	-1.23821
H	1.02691	5.43338	-0.66221
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H	0.97715	3.62554	-2.44325
H	-0.53720	4.31338	-3.04719
H	-0.45130	2.59078	-2.62873
C	-2.07250	3.90351	-0.82384
H	-2.47533	2.91346	-1.04129
H	-2.49536	4.60625	-1.55187
H	-2.42357	4.19992	0.17114
C	2.81557	-0.10070	-2.17700
C	2.05794	-1.33009	-2.29005
C	2.29315	-2.05337	-1.08587
H	1.88830	-3.02690	-0.86099
C	3.17048	-1.35373	-0.23723
C	3.44455	-0.13513	-0.89832
H	4.13029	0.61870	-0.54147
C	3.29201	0.95122	-3.19514
C	3.67558	2.26380	-2.48258
H	3.96029	3.02077	-3.22254
H	4.52516	2.14202	-1.80429
H	2.83445	2.65170	-1.90189
C	4.57357	0.40763	-3.86341
H	4.38799	-0.52648	-4.39931
H	5.34117	0.20951	-3.10698
H	4.97456	1.13851	-4.57812
C	2.28035	1.33311	-4.28262
H	1.33583	1.67075	-3.84555
H	2.07109	0.51014	-4.96700
H	2.68083	2.15618	-4.88679
C	1.30611	-1.99597	-3.45579
C	2.26467	-2.27397	-4.62774
H	2.60898	-1.35811	-5.11191
H	1.76078	-2.87950	-5.39205
H	3.14647	-2.82512	-4.28174
C	0.09588	-1.18452	-3.94409
H	-0.61916	-1.07714	-3.12821
H	-0.40311	-1.70355	-4.77275
H	0.35491	-0.18344	-4.28162
C	0.75150	-3.36344	-3.00764
H	1.55443	-4.07160	-2.77482
H	0.15199	-3.79929	-3.81568
H	0.10780	-3.26877	-2.12632
C	3.84585	-1.88522	1.02148
C	5.31423	-1.42693	1.03646
H	5.83222	-1.74243	0.12347
H	5.83652	-1.86177	1.89762
H	5.40544	-0.33879	1.11476
C	3.81951	-3.42055	1.03019
H	2.79601	-3.80293	1.08948
H	4.35971	-3.79789	1.90729
H	4.29505	-3.83072	0.13152
C	3.13841	-1.38203	2.28544
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H	3.72198	-1.60487	3.18845
H	2.15859	-1.85328	2.39056

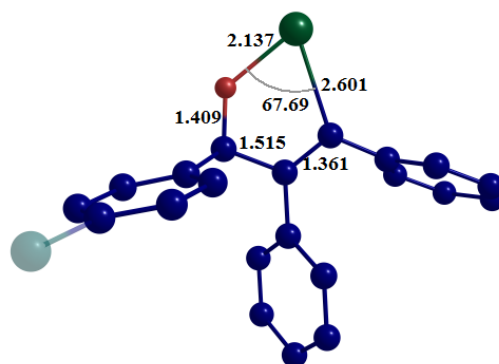
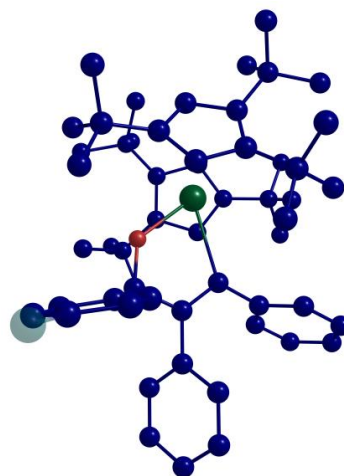
	C -0.57909 -3.02746 3.19288 H -0.91652 -2.10039 3.64301 C -0.58138 -4.19834 3.94914 H -0.90776 -4.16218 4.98664 C -0.17352 -5.40797 3.38806 H -0.16715 -6.31792 3.98287 C 0.21205 -5.43590 2.04688 H 0.51431 -6.37369 1.58533 C 0.20270 -4.26975 1.28711 H 0.47811 -4.30537 0.23615 C -0.17483 -3.03416 1.84725 C -0.15102 -1.82817 1.00889 C -1.01899 -1.58646 0.01474 C -2.30791 -2.13344 -0.34349 C -3.31699 -2.24294 0.63977 H -3.05469 -2.04361 1.67553 C -4.62222 -2.56155 0.29758 H -5.38289 -2.62126 1.07284 C -4.96856 -2.80345 -1.03864 H -5.99527 -3.04245 -1.30327 C -3.98141 -2.74891 -2.01661 H -4.22997 -2.95419 -3.05574 C -2.67156 -2.40363 -1.67795 H -1.91149 -2.36824 -2.44936 C -2.45064 0.42437 -2.05863 H -2.48088 0.15508 -3.12464 C -3.72339 0.66674 -1.40068 C -3.79259 0.83665 -0.00929 H -2.88218 0.74651 0.57023 C -5.00589 1.06850 0.61562 H -5.06324 1.18903 1.69264 C -6.16582 1.12422 -0.16137 C -6.12878 0.93260 -1.54280 H -7.04607 0.96360 -2.12177 C -4.90465 0.69571 -2.15555 H -4.86393 0.53466 -3.23047 Cl -7.69753 1.41561 0.61705 O -1.34438 0.52065 -1.49885 Th 0.68779 0.12265 -0.17031	
TS3	C 0.90158 2.44167 1.46495 C 2.29327 2.24454 1.13645 C 2.39171 2.42887 -0.27946 H 3.32811 2.43751 -0.82083 C 1.16609 2.85096 -0.82541 C 0.24926 2.79180 0.24426 H -0.77543 3.12218 0.18738 C 0.13721 2.58792 2.78763 C 0.44212 3.97530 3.38613 H -0.13788 4.13338 4.30464 H 0.17966 4.76583 2.67319 H 1.49999 4.09234 3.63428 C 0.44346 1.48318 3.80365 H 0.22069 0.50686 3.37182 H -0.17769 1.60962 4.69931 H 1.48042 1.47431 4.12476 C -1.38544 2.52874 2.53495 H -1.66488 1.61540 1.99590	

H	-1.74988	3.39296	1.96800
H	-1.91606	2.53309	3.49440
C	3.62128	2.42432	1.91488
C	4.01340	3.90958	1.70920
H	3.22758	4.57397	2.08508
H	4.16346	4.14079	0.65000
H	4.94318	4.13962	2.24586
C	3.64321	2.17867	3.42917
H	3.41818	1.14444	3.69405
H	2.96191	2.83699	3.97039
H	4.65334	2.39179	3.80012
C	4.73401	1.54258	1.32359
H	5.69537	1.78716	1.79156
H	4.85440	1.66820	0.24415
H	4.52616	0.48892	1.52005
C	0.99235	3.59352	-2.14547
C	1.83744	4.88172	-2.03275
H	1.52892	5.47300	-1.16304
H	1.71875	5.50049	-2.93192
H	2.90168	4.64782	-1.91861
C	1.48825	2.79295	-3.35556
H	2.53719	2.50278	-3.24117
H	1.41180	3.39569	-4.26952
H	0.89319	1.88743	-3.49488
C	-0.46605	4.00582	-2.37882
H	-1.11796	3.13485	-2.46806
H	-0.54610	4.58393	-3.30730
H	-0.83909	4.63771	-1.56428
C	2.65798	-1.55177	-1.68706
C	1.56692	-2.48965	-1.51676
C	1.48772	-2.75857	-0.12292
H	0.78675	-3.43632	0.33585
C	2.49373	-2.07978	0.58415
C	3.17566	-1.30024	-0.38178
H	4.04195	-0.68768	-0.18188
C	3.46003	-1.08286	-2.91221
C	4.23178	0.20953	-2.58585
H	4.73666	0.58081	-3.48526
H	5.00177	0.05620	-1.82342
H	3.55297	0.98625	-2.22908
C	4.51871	-2.15610	-3.24453
H	4.06983	-3.11345	-3.51483
H	5.16695	-2.32611	-2.37743
H	5.14638	-1.82573	-4.08275
C	2.61568	-0.77766	-4.15645
H	1.84383	-0.03487	-3.93060
H	2.12698	-1.66323	-4.56324
H	3.25260	-0.36737	-4.94937
C	0.72914	-3.32074	-2.50428
C	1.62269	-4.13825	-3.45380
H	2.16190	-3.51659	-4.16942
H	1.00754	-4.83962	-4.03164
H	2.35795	-4.71948	-2.88610
C	-0.26033	-2.46299	-3.30456
H	-1.00022	-2.05930	-2.60990
H	-0.79063	-3.06758	-4.05186
H	0.21373	-1.62345	-3.81456

C	-0.12270	-4.35169	-1.73607
H	0.50235	-5.08486	-1.21428
H	-0.75919	-4.89846	-2.44231
H	-0.77846	-3.87323	-1.00194
C	2.89726	-2.32927	2.03244
C	4.43177	-2.36845	2.12889
H	4.84481	-3.13107	1.45852
H	4.73951	-2.60733	3.15443
H	4.88837	-1.41003	1.86536
C	2.35796	-3.68579	2.51133
H	1.26432	-3.69655	2.53812
H	2.70953	-3.88507	3.53119
H	2.70127	-4.50187	1.86470
C	2.33995	-1.23859	2.95189
H	2.56366	-0.24293	2.55574
H	2.76609	-1.30390	3.96178
H	1.25438	-1.33012	3.03637
C	-1.81328	-1.09593	3.67210
H	-1.87908	-0.01422	3.70156
C	-2.24023	-1.83721	4.77260
H	-2.61739	-1.31762	5.65127
C	-2.19240	-3.23046	4.75339
H	-2.51841	-3.80617	5.61609
C	-1.73635	-3.87522	3.60253
H	-1.71345	-4.96214	3.55802
C	-1.32141	-3.13502	2.49984
H	-1.00031	-3.64462	1.59520
C	-1.32873	-1.72658	2.51442
C	-0.85995	-1.00378	1.32316
C	-1.54476	-0.98646	0.15089
C	-2.92805	-1.45668	-0.00116
C	-3.94253	-0.89223	0.79758
H	-3.66662	-0.14436	1.53533
C	-5.27461	-1.26152	0.64627
H	-6.03465	-0.79159	1.26679
C	-5.63946	-2.22539	-0.29608
H	-6.68031	-2.51794	-0.41070
C	-4.64942	-2.80357	-1.08934
H	-4.91354	-3.55922	-1.82671
C	-3.31781	-2.41263	-0.95486
H	-2.56658	-2.86339	-1.59411
C	-1.83908	0.39361	-2.39632
H	-1.95648	-0.42961	-3.11582
C	-3.08433	0.95400	-1.90965
C	-3.12765	1.94854	-0.92249
H	-2.19818	2.31791	-0.51451
C	-4.33933	2.40826	-0.43989
H	-4.38071	3.16416	0.33750
C	-5.52015	1.85637	-0.94814
C	-5.50522	0.86416	-1.92756
H	-6.43440	0.43380	-2.28374
C	-4.28175	0.41565	-2.40400
H	-4.25372	-0.38295	-3.13994
Cl	-7.04517	2.39085	-0.30860
O	-0.68831	0.81242	-2.16218
Th	0.65747	0.00350	-0.22921

3	C	0.73302	-1.99266	-2.11086
	C	2.08345	-2.17292	-1.62256
	C	1.95515	-2.71169	-0.30611
	H	2.78935	-3.04007	0.30030
	C	0.60345	-2.94590	0.01834
	C	-0.13777	-2.45928	-1.07729
	H	-1.21786	-2.46191	-1.12349
	C	0.15968	-1.66122	-3.49895
	C	0.43193	-2.85018	-4.43991
	H	-0.03663	-2.67951	-5.41763
	H	0.01948	-3.77344	-4.01729
	H	1.50029	-3.00880	-4.60540
	C	0.68860	-0.35883	-4.11438
	H	0.43081	0.49470	-3.48437
	H	0.22374	-0.19225	-5.09426
	H	1.76463	-0.35114	-4.25738
	C	-1.36916	-1.48422	-3.41553
	H	-1.62971	-0.69300	-2.70244
	H	-1.88383	-2.40365	-3.11817
	H	-1.75903	-1.19393	-4.39802
	C	3.47590	-2.29309	-2.27996
	C	3.68319	-3.79525	-2.58277
	H	2.91974	-4.16602	-3.27459
	H	3.61864	-4.39219	-1.66706
	H	4.66836	-3.96541	-3.03620
	C	3.73462	-1.52083	-3.57862
	H	3.64842	-0.43913	-3.44223
	H	3.07452	-1.82743	-4.39109
	H	4.76071	-1.72153	-3.90964
	C	4.57255	-1.84133	-1.29773
	H	5.56142	-1.96091	-1.75600
	H	4.57612	-2.41122	-0.36531
	H	4.44272	-0.78583	-1.04369
	C	0.09938	-3.79872	1.17453
	C	0.60016	-5.23571	0.92377
	H	0.23959	-5.60787	-0.04199
	H	0.23663	-5.91014	1.70974
	H	1.69544	-5.28029	0.91504
	C	0.64349	-3.31393	2.52633
	H	1.73820	-3.29388	2.53974
	H	0.31435	-3.97779	3.33509
	H	0.27014	-2.30693	2.74952
	C	-1.43008	-3.80621	1.23006
	H	-1.81589	-2.79690	1.38019
	H	-1.77439	-4.43461	2.06001
	H	-1.86647	-4.20643	0.30812
	C	2.69936	0.71762	2.20365
	C	1.60049	1.65244	2.26606
	C	1.63352	2.38812	1.03941
	H	0.95047	3.17825	0.76785
	C	2.72979	1.98434	0.24576
	C	3.34306	0.93231	0.94586
	H	4.24560	0.42691	0.63482
	C	3.45800	-0.13183	3.23910
	C	4.09969	-1.35756	2.55880
	H	4.61232	-1.97480	3.30574
	H	4.84169	-1.08501	1.80341



H	3.33866	-1.97438	2.07318
C	4.59713	0.74731	3.80025
H	4.20292	1.64165	4.29280
H	5.26635	1.07635	2.99769
H	5.18951	0.18518	4.53390
C	2.63740	-0.66687	4.41500
H	1.76421	-1.23007	4.07671
H	2.30410	0.13185	5.07919
H	3.25924	-1.34139	5.01568
C	0.65101	2.09001	3.39942
C	1.47152	2.82614	4.47578
H	2.19092	2.16474	4.96549
H	0.80676	3.22736	5.25165
H	2.02866	3.66115	4.03538
C	-0.16542	0.95895	4.05772
H	-0.59185	0.29289	3.30535
H	-0.98467	1.39316	4.64373
H	0.42326	0.35385	4.74309
C	-0.37722	3.09807	2.84740
H	0.09641	4.02232	2.49871
H	-1.08103	3.37629	3.63991
H	-0.94819	2.67088	2.01662
C	3.14949	2.54559	-1.10284
C	4.65163	2.33173	-1.33144
H	5.24011	2.78369	-0.52521
H	4.95635	2.79060	-2.27961
H	4.91116	1.26905	-1.38660
C	2.83851	4.04613	-1.17900
H	1.76506	4.23832	-1.09388
H	3.16817	4.45144	-2.14345
H	3.35538	4.59088	-0.38077
C	2.36225	1.81358	-2.19478
H	2.52340	0.72460	-2.13592
H	2.67163	2.10742	-3.20561
H	1.29103	2.03799	-2.12339
C	-1.18810	2.50082	-2.96827
H	-1.36968	1.51633	-3.38780
C	-1.09428	3.60233	-3.81661
H	-1.18201	3.45947	-4.89164
C	-0.89697	4.88066	-3.29489
H	-0.81599	5.73984	-3.95592
C	-0.82552	5.04362	-1.91085
H	-0.69837	6.03652	-1.48467
C	-0.92356	3.94117	-1.06569
H	-0.89804	4.08136	0.01179
C	-1.08596	2.63879	-1.57390
C	-1.11492	1.47709	-0.65616
C	-2.20621	1.33509	0.14405
C	-3.43308	2.17690	0.09826
C	-4.14603	2.33983	-1.09869
H	-3.78444	1.84671	-1.99596
C	-5.29657	3.12118	-1.14613
H	-5.83348	3.23320	-2.08524
C	-5.76156	3.75702	0.00591
H	-6.65953	4.36907	-0.03066
C	-5.06727	3.59962	1.20480
H	-5.41947	4.09286	2.10799

C	-3.91834	2.81213	1.25115
H	-3.38059	2.70873	2.19024
C	-2.22975	0.23976	1.19026
H	-2.40513	0.69280	2.17998
C	-3.32752	-0.78257	0.95696
C	-3.59954	-1.24164	-0.33339
H	-3.08696	-0.78326	-1.17295
C	-4.50636	-2.27233	-0.55400
H	-4.71030	-2.63173	-1.55805
C	-5.15832	-2.83961	0.54020
C	-4.92679	-2.38326	1.83526
H	-5.45161	-2.83137	2.67326
C	-4.00919	-1.35283	2.03189
H	-3.80806	-1.00285	3.04226
Cl	-6.29516	-4.14461	0.27905
O	-0.97987	-0.41001	1.22323
Th	0.81002	-0.10178	0.09802

Table S5. Frequencies of the stationary points optimized for 2+*p*-ClPhCHO, obtained with B3PW91-PCM+D3 method.

Species	Frequencies (cm ⁻¹)
2	19 22 28 33 40 42 48 55 59 64 66 72 77 86 86 98 99 104 107 109 121 134 142 144 151 161 176 182 183 192 197 203 207 208 214 217 229 232 246 250 251 255 257 259 262 269 274 278 279 287 288 296 297 312 316 324 326 328 329 337 340 359 359 365 372 372 380 384 390 395 397 402 407 410 414 414 416 420 438 440 446 451 469 471 472 487 489 497 553 563 563 566 566 583 584 591 606 607 608 631 634 659 660 689 692 693 697 698 710 711 771 783 795 797 810 834 835 837 838 841 842 850 851 861 861 902 914 939 939 939 946 946 948 948 953 953 957 957 959 959 964 964 969 970 971 971 976 978 979 979 987 987 1014 1015 1030 1030 1051 1051 1056 1057 1059 1059 1060 1060 1061 1062 1063 1063 1068 1069 1113 1113 1156 1157 1178 1193 1194 1206 1206 1210 1211 1213 1215 1229 1229 1236 1236 1244 1245 1250 1250 1253 1253 1264 1265 1275 1280 1280 1282 1284 1323 1325 1330 1333 1371 1373 1397 1397 1412 1413 1414 1414 1417 1417 1420 1422 1423 1423 1427 1427 1435 1435 1449 1450 1451 1451 1459 1460 1466 1466 1484 1486 1497 1497 1498 1499 1505 1505 1506 1508 1508 1509 1513 1513 1514 1514 1520 1520 1521 1522 1522 1524 1524 1526 1527 1532 1533 1534 1536 1536 1537 1537 1541 1543 1547 1549 1551 1552 1561 1561 1563 1564 1597 1632 1633 1662 1663 2989 2991 3048 3049 3051 3051 3052 3052 3055 3055 3056 3057 3060 3060 3061 3061 3072 3072 3086 3086 3121 3121 3125 3125 3125 3125 3127 3127 3129 3129 3131 3131 3132 3133 3139 3139 3142 3143 3144 3144 3145 3145 3145 3146 3146 3147 3151 3151 3168 3168 3180 3180 3188 3188 3195 3195 3205 3205 3208 3208 3213 3213 3219 3219 3270 3271 3298 3299
<i>p</i> -ClPhCHO	86 172 187 307 315 361 421 494 551 635 711 714 832 848 851 968 988 1031 1038 1117 1146 1206 1245 1329 1371 1434 1464 1537 1636 1660 1805 2926 3193 3219 3232 3234
COM3	17 24 28 39 40 43 50 55 59 61 68 70 82 85 86 89 94 95 100 108 112 113 116 120 125 131 134 142 146 147 150 154 166 181 185 189 192 196 200 206 210 216 219 222 235 237 241 243 252 255 256 261 268 274 277 280 281 289 292 296 302 303 313 321 324 325 328 330 331 348 356 358 366 368 370 380 384 386 387 394 396 403 406 408 410 411 417 419 422 423 427 437 444 451 455 464 474 480 486 488 494 507 549 552 561 562 565 572 577 579 583 597 606 609 630 634 638 658 663 664 685 686 690 706 712 715 716 717 761 785 795 802 807 822 834 836 840 843 846 850 853 858 858 860 862 865 880 912 921 939 941 941 942 945 947 953 954 956 957 959 960 962 963 965 969 970 971 975 976 978 979 980 984 985 987 992 1012 1013 1030 1033 1034 1054 1056 1058 1058 1061 1062 1063 1063 1063 1065 1066 1068 1068 1070 1112 1114 1119 1150 1153 1159 1180 1194 1195 1202 1209 1210 1212 1214 1215 1218 1226 1230 1235 1241 1244 1245 1250 1252 1252 1257 1260 1262 1263 1266 1280 1280 1283 1284 1321 1330 1332 1332 1333 1371 1372 1380 1395 1398 1410 1413 1415 1416 1418 1418 1419 1419 1421 1422 1425 1427 1429 1431 1433 1447 1448 1452 1453 1456 1459 1460 1461 1468 1483 1485 1498 1501 1503 1504 1504 1505 1506 1509 1510 1510 1514 1515 1516 1517 1518 1520 1523 1523 1524 1525 1526 1527 1530 1531 1532 1532 1533 1536 1537 1537 1538 1542 1543 1545 1550 1556 1557 1560 1562 1563 1566 1615 1625 1632 1642 1650 1660 1663 1670 3044 3045 3046 3046 3048 3049 3049 3049 3051 3053 3054 3060 3062 3062 3063 3064 3066 3068 3070 3118 3118 3119

	3121 3121 3122 3122 3123 3123 3126 3127 3127 3129 3132 3135 3137 3138 3138 3139 3142 3143 3144 3150 3155 3161 3162 3164 3169 3169 3170 3176 3179 3182 3183 3186 3188 3189 3194 3198 3202 3207 3212 3215 3224 3227 3232 3237 3249 3250 3257 3261 3292 3304 3310
TS3	-113 21 29 30 39 43 48 54 62 66 71 75 80 82 84 91 93 95 102 104 110 112 115 120 125 128 137 141 143 144 152 155 159 164 180 184 192 197 199 204 206 208 219 226 232 235 241 250 254 255 258 267 274 277 280 284 286 293 298 303 305 309 315 317 321 327 330 332 333 338 345 354 358 365 372 373 383 386 390 393 396 399 405 411 412 413 416 419 422 423 428 442 449 452 457 469 476 483 486 489 489 504 548 551 559 561 565 567 577 579 585 601 606 607 632 634 637 658 662 670 684 686 693 700 705 711 716 718 765 783 799 808 812 816 830 835 838 839 847 849 850 858 860 863 865 870 889 911 928 938 942 943 944 949 951 955 955 956 957 958 959 961 963 966 970 972 973 976 978 980 981 981 984 985 986 1008 1013 1014 1029 1034 1037 1055 1056 1057 1060 1061 1063 1063 1064 1065 1065 1066 1068 1071 1073 1113 1114 1121 1147 1154 1161 1186 1193 1193 1198 1210 1213 1214 1216 1216 1219 1226 1232 1234 1240 1243 1246 1248 1251 1255 1256 1260 1262 1264 1267 1279 1280 1283 1284 1321 1330 1330 1333 1333 1372 1373 1383 1398 1398 1410 1413 1416 1416 1418 1419 1419 1419 1421 1424 1426 1427 1431 1433 1437 1448 1449 1451 1454 1457 1459 1461 1464 1469 1483 1485 1498 1501 1503 1504 1505 1505 1506 1509 1509 1511 1515 1516 1517 1518 1518 1521 1521 1524 1524 1526 1527 1528 1531 1531 1532 1533 1533 1537 1538 1539 1540 1544 1544 1547 1550 1556 1557 1563 1563 1566 1567 1567 1623 1631 1633 1651 1661 1664 1675 3042 3044 3046 3047 3049 3050 3050 3051 3054 3055 3056 3060 3060 3062 3064 3068 3068 3069 3071 3116 3118 3121 3121 3121 3121 3122 3124 3124 3126 3128 3128 3130 3131 3134 3136 3138 3143 3144 3147 3147 3147 3151 3157 3165 3167 3175 3176 3176 3178 3178 3179 3180 3182 3186 3186 3187 3192 3193 3203 3206 3212 3215 3216 3230 3236 3241 3244 3247 3262 3294 3300 3307 3314
3	19 23 24 31 39 45 46 48 58 60 65 68 72 75 79 84 88 93 94 104 106 109 114 116 123 134 135 136 143 151 155 160 175 183 185 191 197 202 205 208 210 217 221 228 233 241 252 252 259 261 263 266 269 276 283 285 292 294 302 304 315 317 320 323 329 333 333 343 349 357 363 366 368 378 383 387 389 393 396 399 404 407 408 411 415 416 420 422 426 438 443 451 453 461 472 475 478 488 491 493 517 557 558 564 566 567 580 586 590 605 609 613 628 632 638 650 661 662 686 687 691 695 708 712 718 722 742 765 793 801 808 826 835 837 839 843 843 844 848 855 858 862 863 867 868 912 924 929 940 942 943 946 951 953 954 954 958 960 962 963 964 968 970 972 974 975 977 978 979 981 982 983 989 994 1014 1016 1029 1030 1031 1043 1054 1055 1056 1057 1060 1061 1062 1064 1065 1065 1067 1068 1070 1072 1110 1114 1118 1126 1145 1157 1159 1194 1197 1204 1206 1209 1212 1214 1216 1222 1228 1228 1229 1237 1242 1243 1246 1248 1249 1250 1251 1258 1264 1264 1275 1279 1281 1285 1287 1300 1321 1323 1331 1339 1343 1365 1371 1377 1386 1396 1403 1411 1413 1414 1416 1417 1418 1421 1421 1423 1423 1426 1426 1432 1435 1448 1450 1452 1452 1457 1458 1460 1461 1465 1484 1488 1498 1500 1503 1504 1504 1506 1507 1509 1509 1511 1513 1515 1516 1517 1518 1518 1522 1524 1525 1528 1530 1530 1531 1533 1534 1536 1536 1537 1539 1540 1540 1542 1543 1547 1550 1554 1559 1562 1563 1564 1566 1608 1633 1644 1646 1664 1666 1671 2996 3002 3042 3047 3048 3048 3048 3049 3052 3052 3055 3056 3062 3064 3064 3069 3069 3070 3071 3089 3118 3120 3120 3121 3123 3124 3125 3125 3126 3126 3126 3130 3131 3134 3136 3136

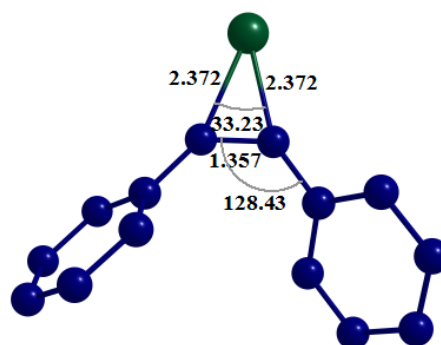
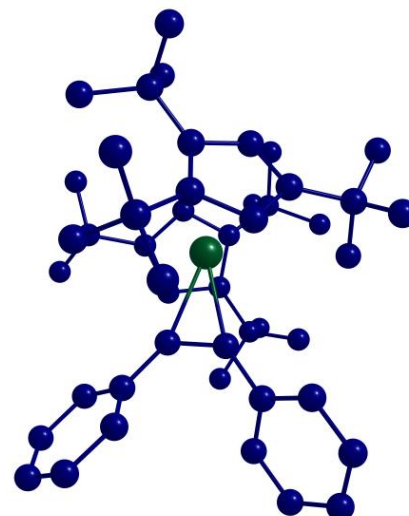
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Table S6. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for 2+*p*-ClPhCHO, obtained with B3PW91-PCM+D3 method

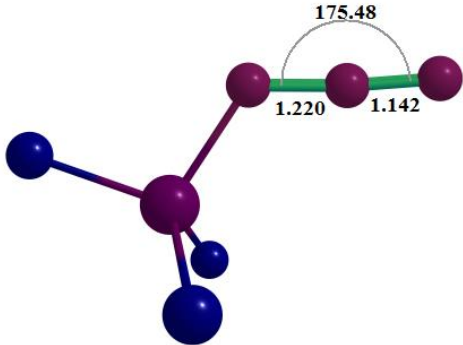
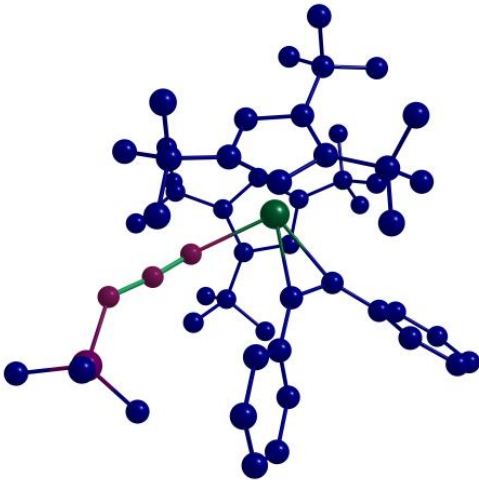
species	E	H	G (gas)	G (sol)
2	-1905.54960	-1904.45059	-1904.59029	-1904.58050
<i>p</i> -ClPhCHO	-804.98785	-804.87859	-804.91974	-804.90800
2 + <i>p</i> -ClPhCHO	-2710.53745(0.0)	-2709.32918(0.0)	-2709.51003(0.0)	-2709.48850(0.0)
COM3	-2710.56005(-14.2)	-2709.34821(-11.9)	-2709.50346(4.1)	-2709.49369(-3.3)
TS3	-2710.55170(-8.9)	-2709.34033(-7.0)	-2709.49264(10.9)	-2709.48289(3.5)
3	-2710.63157(-59.1)	-2709.41835(-56.0)	-2709.57331(-39.7)	-2709.56350(-47.1)

Table S7. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for 2+Me₃SiN₃, obtained with B3PW91-PCM+D3 method.

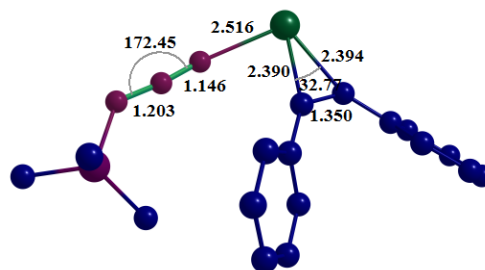
Species	Cartesian coordinates		
2	C	-0.53212	2.71815 -0.92729
	C	-1.90839	2.38559 -0.62165
	C	-2.29546	1.38139 -1.56277
	H	-3.28872	0.95948 -1.63411
	C	-1.23991	1.09915 -2.45075
	C	-0.15960	1.90595 -2.03722
	H	0.81069	1.91970 -2.50878
	C	0.43027	3.79898 -0.40412
	C	-0.13267	5.19692 -0.71985
	H	-1.05428	5.41313 -0.17594
	H	-0.34782	5.28910 -1.79077
	H	0.59877	5.96923 -0.45034
	C	0.74806	3.66566 1.09549
	H	1.40706	4.48342 1.41307
	H	1.27657	2.72599 1.29177
	H	-0.13938	3.69607 1.72551
	C	1.78692	3.69204 -1.12812
	H	2.48285	4.42591 -0.70591
	H	1.69816	3.89911 -2.20055
	H	2.22787	2.69848 -0.99659
	C	-3.03395	3.07202 0.17685
	C	-3.69324	4.09956 -0.76955
	H	-4.54878	4.58218 -0.27930
	H	-4.05053	3.60872 -1.68140
	H	-2.98532	4.87907 -1.06657
	C	-2.63930	3.79360 1.47109
	H	-1.90599	4.58344 1.31090
	H	-2.24523	3.10306 2.22144
	H	-3.53007	4.26462 1.90398
	C	-4.10635	2.03578 0.57398
	H	-3.65698	1.19652 1.11556
	H	-4.64117	1.62627 -0.28796
	H	-4.85543	2.50006 1.22569
	C	-1.22949	0.09539 -3.59282
	C	-0.50754	0.68816 -4.81141
	H	-1.00960	1.59979 -5.15411
	H	-0.49833	-0.03348 -5.63747
	H	0.53245	0.94103 -4.58210
	C	-2.65856	-0.28562 -3.99779
	H	-3.18846	-0.79455 -3.18556
	H	-2.63880	-0.97014 -4.85401
	H	-3.23848	0.60028 -4.27990
	C	-0.48658	-1.16505 -3.12705
	H	0.56465	-0.96422 -2.89627
	H	-0.51733	-1.96657 -3.87570
	H	-0.96964	-1.58996 -2.23034
	C	1.91367	0.21176 0.64311
	C	3.05846	0.55972 1.48650
	C	4.08939	1.39841 1.02024
	H	4.04953	1.75736 -0.00399
	C	5.15079	1.75869 1.84448
	H	5.93088	2.41297 1.46072



C	5.22734	1.27448	3.15243
H	6.06068	1.55210	3.79329
C	4.22363	0.42980	3.62712
H	4.27237	0.04083	4.64210
C	3.14823	0.09058	2.80910
H	2.36643	-0.56209	3.18774
Th	-0.35949	0.00016	-0.00110
C	1.91366	-0.21042	-0.64611
C	3.05889	-0.55773	-1.48934
C	4.09812	-1.38354	-1.01848
H	4.06469	-1.73308	0.00925
C	5.15973	-1.74303	-1.84281
H	5.94638	-2.38730	-1.45551
C	5.22802	-1.27070	-3.15557
H	6.06152	-1.54766	-3.79651
C	4.21589	-0.43887	-3.63506
H	4.25808	-0.05939	-4.65391
C	3.14047	-0.10071	-2.81664
H	2.35183	0.54160	-3.19874
C	-0.52765	-2.71715	0.92666
C	-1.90475	-2.38645	0.62288
C	-2.29165	-1.38236	1.56435
H	-3.28554	-0.96221	1.63756
C	-1.23503	-1.09834	2.45051
C	-0.15446	-1.90408	2.03555
H	0.81651	-1.91646	2.50568
C	0.43485	-3.79744	0.40294
C	-0.12472	-5.19516	0.72569
H	-1.04945	-5.41383	0.18809
H	-0.33345	-5.28443	1.79814
H	0.60593	-5.96752	0.45413
C	0.74655	-3.66780	-1.09825
H	1.40318	-4.48710	-1.41680
H	1.27565	-2.72924	-1.29832
H	-0.14340	-3.69807	-1.72464
C	1.79432	-3.68591	1.12098
H	2.48986	-4.41958	0.69775
H	1.71066	-3.89035	2.19431
H	2.23273	-2.69186	0.98475
C	-3.03140	-3.07497	-0.17257
C	-3.69186	-4.09665	0.77940
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H	-4.04863	-3.60078	1.68871
H	-2.98444	-4.87517	1.08040
C	-2.63920	-3.80476	-1.46307
H	-1.90643	-4.59438	-1.29932
H	-2.24599	-3.11958	-2.21872
H	-3.53128	-4.27755	-1.89130
C	-4.10164	-2.03873	-0.57520
H	-3.65054	-1.20493	-1.12373
H	-4.63373	-1.62113	0.28452
H	-4.85319	-2.50547	-1.22231
C	-1.22407	-0.09715	3.59484
C	-0.51094	-0.69790	4.81486
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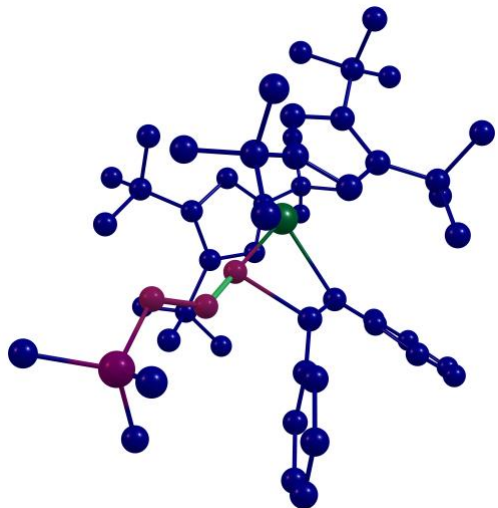
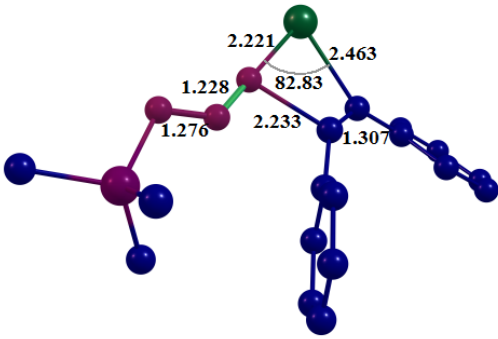
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Me ₃ SiN ₃	N -2.85894 -1.29095 -0.11696 N -3.98243 -1.69939 0.12579 N -1.77500 -0.98118 -0.30155 Si -5.46827 -0.84147 -0.37560 C -5.46791 -0.70982 -2.24914 H -6.36744 -0.18969 -2.60078 H -4.59724 -0.14683 -2.60613 H -5.44540 -1.70106 -2.71553 C -6.85900 -1.91585 0.26362 H -6.80920 -2.01486 1.35363 H -7.83211 -1.48113 0.00634 H -6.81037 -2.92010 -0.17174 C -5.45868 0.86306 0.41311 H -5.42850 0.79338 1.50619 H -4.58919 1.44565 0.08595 H -6.35914 1.42375 0.13358	
COM10	C 1.91511 -0.34543 -2.46559 C 2.48075 -1.50020 -1.79673 C 1.40648 -2.42804 -1.62583 H 1.51858 -3.42534 -1.21988 C 0.22865 -1.94656 -2.22887 C 0.53790 -0.64780 -2.68511 H -0.16061 0.00341 -3.18879 C 2.53328 0.91219 -3.10465 C 3.41694 0.49540 -4.29609 H 3.76045 1.38375 -4.84161 H 2.85143 -0.13616 -4.99111 H 4.30330 -0.06165 -3.98438 C 3.33543 1.79230 -2.13305 H 2.68493 2.19019 -1.34825 H 3.76269 2.64750 -2.67185 H 4.15848 1.26132 -1.65799 C 1.42001 1.81655 -3.66975 H 0.69188 2.07365 -2.89416 H 0.89172 1.34571 -4.50648 H 1.86106 2.74856 -4.04115 C 3.90388 -2.07796 -1.65148 C 4.18432 -2.87987 -2.94379 H 4.19296 -2.22880 -3.82291 H 3.41220 -3.64072 -3.10087 H 5.15830 -3.38294 -2.88038 C 5.06052 -1.09195 -1.45342 H 4.98401 -0.54757 -0.51041 H 5.13876 -0.36822 -2.26482 H 6.00465 -1.64969 -1.42824 C 3.95275 -3.06692 -0.46718 H 4.98821 -3.36197 -0.26168 H 3.39101 -3.98515 -0.66332 H 3.53869 -2.61375 0.43864	

	C	-0.93642	-2.80718	-2.69461
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	H	0.41642	-4.23563	-3.65863
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	C	-2.13019	-1.95805	-3.14980
	H	-2.47010	-1.27100	-2.37464
	H	-2.97243	-2.60126	-3.42930
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	H	-2.93179	-0.78685	2.49169
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	H	-0.46236	2.27491	4.31327
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	H	-1.02137	2.43175	2.62999
	C	3.59417	0.39286	2.50391
	C	4.61858	-0.74318	2.59108
	H	4.48912	-1.32053	3.51384
	H	5.63692	-0.33664	2.58222
	H	4.53361	-1.43189	1.74615
	C	3.83303	1.35759	3.67781
	H	3.15558	2.21705	3.63828
	H	4.86012	1.74282	3.65023
	H	3.68005	0.85031	4.63712
	C	3.77569	1.15281	1.18491
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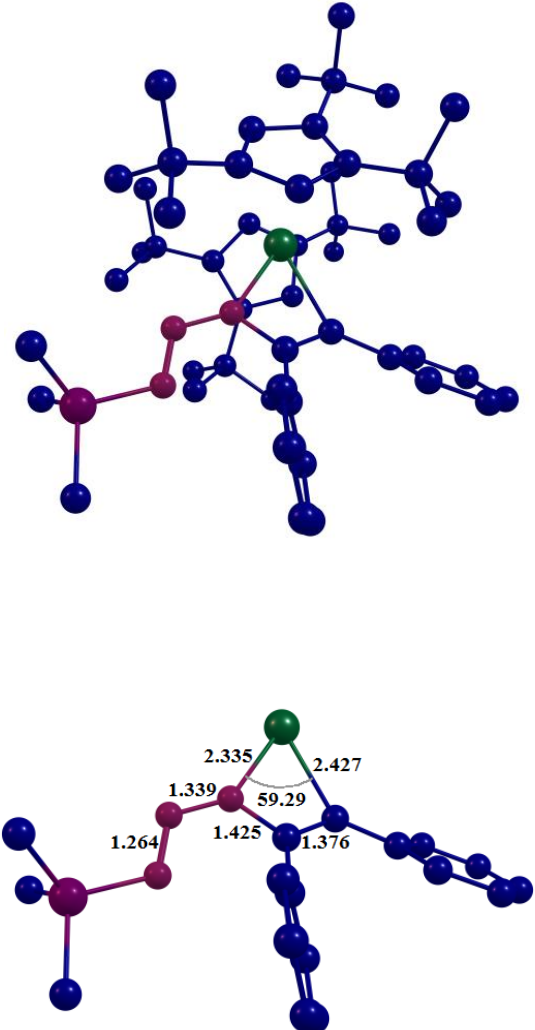


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TS10a	C 2.05108 -0.02167 -2.40042 C 2.56441 -1.27034 -1.87946 C 1.45870 -2.18021 -1.86968 H 1.53097 -3.22794 -1.60502 C 0.31582 -1.59000 -2.44321 C 0.67338 -0.25139 -2.70145 H 0.00291 0.48555 -3.12016 C 2.72133 1.29027 -2.84766 C 3.63909 1.00847 -4.05279 H 4.02743 1.95039 -4.46088 H 3.08298 0.49506 -4.84564 H 4.49644 0.38542 -3.79007 C 3.50353 2.01077 -1.73927 H 2.83196 2.32004 -0.93196	

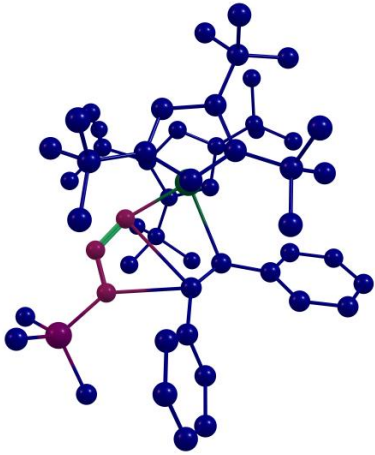
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	H	0.90726	2.48075	-2.55360
	H	1.14226	1.94565	-4.23425
	H	2.13398	3.24897	-3.56826
	C	3.96530	-1.90866	-1.77470
	C	4.25461	-2.54841	-3.15298
	H	4.31136	-1.79024	-3.93978
	H	3.46203	-3.25294	-3.42667
	H	5.20839	-3.09181	-3.13155
	C	5.14894	-0.99879	-1.42556
	H	5.07989	-0.59836	-0.41266
	H	5.26093	-0.16604	-2.11975
	H	6.07447	-1.58509	-1.47592
	C	3.95089	-3.04016	-0.72496
	H	4.97058	-3.39436	-0.53499
	H	3.36562	-3.90637	-1.04748
	H	3.52782	-2.68997	0.22171
	C	-0.87496	-2.34730	-3.00982
	C	-0.33906	-3.11709	-4.23837
	H	0.10423	-2.42841	-4.96712
	H	-1.15227	-3.66543	-4.73147
	H	0.43173	-3.83875	-3.94466
	C	-1.45205	-3.36102	-2.01581
	H	-0.68761	-4.07658	-1.69177
	H	-2.25766	-3.93588	-2.48968
	H	-1.87992	-2.87011	-1.13676
	C	-1.97885	-1.40016	-3.49104
	H	-2.38096	-0.80140	-2.67413
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	H	-1.61114	-0.72496	-4.27323
	C	0.21017	-1.79947	2.51120
	C	-0.19446	-0.46415	2.88409
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	H	1.02922	1.37295	3.11819
	C	2.12235	-0.46195	2.57893
	C	1.63104	-1.75758	2.32446
	H	2.24652	-2.62383	2.11729
	C	-0.48119	-3.17185	2.49300
	C	0.11492	-4.04338	1.36725
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	C	-1.99401	-3.14694	2.25812
	H	-2.26016	-2.65157	1.31798
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	H	-2.36875	-4.17671	2.20365
	C	-1.46973	0.12063	3.52805
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	H	-2.01365	-1.66961	4.68410
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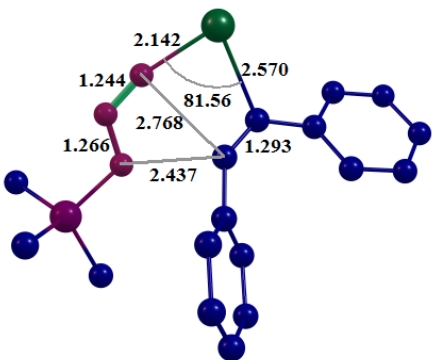



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C	-1.24784	1.60306	3.89441
H	-0.46071	1.73608	4.64513
H	-2.17500	2.01052	4.31417
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C	3.56148	0.02059	2.64091
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C	3.84576	0.89637	1.41734
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Si	-5.28557	-0.99246	-0.55256
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H	-4.99773	0.16424	-2.72942
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H	-6.01922	-2.71660	1.08561
H	-7.30562	-2.38958	-0.09245

	H -5.91930 -3.40117 -0.54477 C -5.73414 0.52025 0.46862 H -5.62385 0.30952 1.53856 H -5.06325 1.34863 0.21958 H -6.76496 0.84746 0.28662	
INT10a	C -1.69374 1.76170 1.94846 C -2.47851 0.58884 2.27757 C -1.56867 -0.36446 2.82362 H -1.85672 -1.32757 3.22741 C -0.27172 0.17679 2.91642 C -0.35233 1.45469 2.32772 H 0.48839 2.12331 2.21531 C -2.05867 3.19327 1.50153 C -2.96832 3.85484 2.55328 H -3.10048 4.91820 2.31712 H -2.52238 3.77934 3.55158 H -3.96199 3.40474 2.59385 C -2.71312 3.27747 0.11128 H -2.01591 2.95181 -0.66995 H -2.97990 4.31603 -0.11891 H -3.62056 2.67954 0.03069 C -0.78471 4.05607 1.41959 H -0.05555 3.62714 0.72693 H -0.31138 4.18062 2.39994 H -1.04380 5.05237 1.04423 C -3.97988 0.32198 2.45467 C -4.38116 0.78853 3.87082 H -4.22917 1.86269 4.00217 H -3.78018 0.27175 4.62714 H -5.43969 0.56695 4.06028 C -4.88185 1.01021 1.43113 H -4.59776 0.74859 0.40811 H -4.85997 2.09663 1.51948 H -5.92274 0.69601 1.57440 C -4.26816 -1.19338 2.37978 H -5.34966 -1.36916 2.35811 H -3.87324 -1.73316 3.24587 H -3.83310 -1.64363 1.48118 C 0.83859 -0.36404 3.80437 C 0.32074 -0.25692 5.25563 H 0.05853 0.77898 5.50070 H 1.09125 -0.59368 5.96118 H -0.57215 -0.87466 5.40488 C 1.15526 -1.83404 3.50227 H 0.26074 -2.46132 3.59304 H 1.89815 -2.21818 4.21274 H 1.56694 -1.93702 2.49341 C 2.11423 0.47611 3.68919 H 2.52652 0.43600 2.67989 H 2.87709 0.09233 4.37591 H 1.92475 1.52295 3.95588 C -0.83965 -2.89464 -0.98499 C -0.31068 -2.09725 -2.07393 C -1.38415 -1.26332 -2.50412 H -1.33037 -0.58395 -3.34152 C -2.57465 -1.55737 -1.80494 C -2.21448 -2.52572 -0.84474	

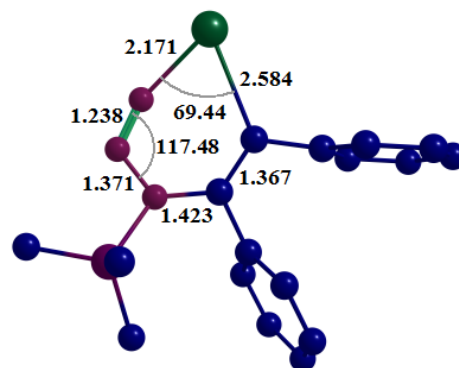
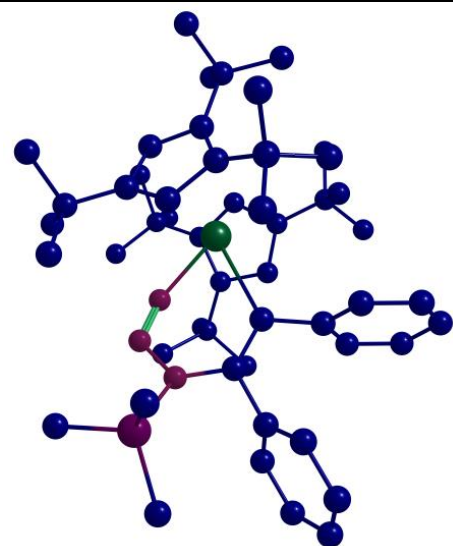
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H	-0.87090	-3.31528	1.77089
C	-0.71428	-5.39168	-0.98676
H	-0.25431	-5.41843	-1.97671
H	-1.80073	-5.44125	-1.12285
H	-0.39551	-6.28793	-0.43875
C	1.18342	-4.11741	0.06167
H	1.50756	-3.18704	0.54123
H	1.76171	-4.24248	-0.85502
H	1.44654	-4.95038	0.72477
C	0.95627	-2.19965	-2.95352
C	1.00105	-3.60733	-3.57883
H	1.25609	-4.37245	-2.84200
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H	0.03670	-3.87156	-4.02809
C	2.29157	-1.90802	-2.25848
H	2.40185	-0.84194	-2.05445
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C	0.87896	-1.19120	-4.11790
H	0.04561	-1.39907	-4.79895
H	1.80414	-1.25330	-4.70277
H	0.79078	-0.16337	-3.74668
C	-3.97345	-1.18038	-2.27464
C	-5.04864	-1.66112	-1.29500
H	-5.01677	-2.74979	-1.17257
H	-6.04480	-1.39770	-1.66952
H	-4.93419	-1.20775	-0.30865
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H	-3.47280	-1.56969	-4.37251
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C	-1.06128	3.58899	-3.93509
H	-1.76214	3.45816	-4.75690
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C	1.60618	1.09952	-0.62057
C	2.84046	1.93091	-0.64167
C	3.29736	2.53039	0.53787
H	2.78941	2.31740	1.47394
C	4.40374	3.37532	0.51492

	H 4.75302 3.83178 1.43853 C 5.06323 3.63441 -0.68788 H 5.92924 4.29162 -0.70613 C 4.59821 3.05162 -1.86846 H 5.10173 3.25548 -2.81068 C 3.48830 2.21286 -1.84780 H 3.11736 1.76174 -2.76399 N 2.59581 -0.75388 0.65384 N 3.72504 -0.47494 0.15887 N 1.54238 -0.05610 0.21071 Th -0.78348 -0.21582 0.08150 Si 5.08145 -1.42144 0.81278 C 5.08948 -1.37601 2.69735 H 5.92713 -1.95169 3.11016 H 5.16984 -0.34608 3.06307 H 4.15644 -1.79655 3.08779 C 6.61166 -0.58458 0.11346 H 6.62463 -0.65665 -0.98023 H 6.60423 0.48101 0.37143 H 7.53683 -1.02977 0.49835 C 4.93455 -3.20531 0.21801 H 4.02049 -3.65974 0.61762 H 4.88006 -3.25052 -0.87555 H 5.78788 -3.81282 0.54382	
TS10b	C 1.23833 -2.37635 1.40521 C 2.22907 -1.50037 1.99097 C 1.51169 -0.54286 2.77339 H 1.97542 0.21691 3.39009 C 0.13471 -0.83670 2.78347 C -0.02690 -1.91491 1.89054 H -0.97906 -2.36843 1.65809 C 1.32522 -3.71658 0.64202 C 2.03245 -4.77106 1.51448 H 1.94390 -5.76202 1.05100 H 1.57773 -4.81724 2.51058 H 3.09723 -4.56456 1.63902 C 2.01675 -3.64083 -0.73214 H 1.46645 -2.98546 -1.41493 H 2.04255 -4.63377 -1.19672 H 3.04205 -3.27774 -0.67037 C -0.09518 -4.25426 0.38013 H -0.70724 -3.52713 -0.15967 H -0.60903 -4.51611 1.31174 H -0.03741 -5.15871 -0.23595 C 3.74605 -1.59726 2.20860 C 3.98831 -2.45607 3.47005 H 3.62750 -3.47936 3.34173 H 3.46603 -2.02412 4.33088 H 5.06070 -2.49805 3.70252 C 4.53928 -2.19753 1.04480 H 4.34259 -1.66822 0.10930 H 4.31058 -3.25265 0.88999 H 5.61483 -2.12726 1.24724 C 4.32983 -0.19886 2.50558 H 5.42513 -0.23717 2.49870 H 4.02883 0.17199 3.49015 H 4.00854 0.53729 1.76271	

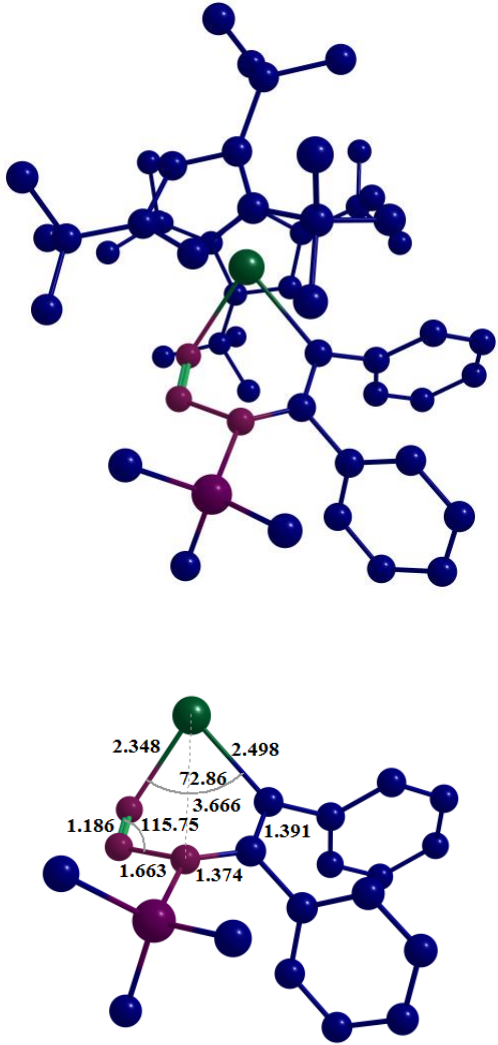
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	H	0.23506	1.43989	4.39681	
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	H	-1.07245	1.71571	3.22944	
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	C	1.69812	1.71051	-2.14495	
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	C	2.86910	1.52537	-1.38221	
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	H	2.64415	3.21948	2.28024	
	H	1.02935	2.51021	2.47766	
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	H	1.69023	5.66306	-0.42026	
	H	3.03799	4.96828	0.49055	
	H	1.84407	5.99301	1.31746	
	C	-0.33745	4.41437	1.04352	
	H	-0.97697	3.56455	1.29055	
	H	-0.74010	4.90890	0.15851	
	H	-0.39742	5.13594	1.86800	
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	C	-0.11347	4.68600	-2.55368	
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	H	-2.00133	1.91860	-1.61150	
	H	-2.52868	3.47464	-2.27890	
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	H	0.41124	2.69581	-4.30427	
	H	-1.33680	2.93055	-4.22845	
	H	-0.63563	1.43587	-3.59470	
	C	4.17300	0.97553	-1.93948	
	C	5.28136	0.95685	-0.88340	
	H	5.46877	1.96203	-0.48854	
	H	6.21655	0.59136	-1.32395	
	H	5.03399	0.30645	-0.04405	
	C	4.61966	1.92085	-3.07565	
	H	3.87650	1.95471	-3.87968	
	H	5.57220	1.58327	-3.50463	
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	C	3.98179	-0.42963	-2.52598	
	H	3.58110	-1.12930	-1.78336	

	H 4.93325 -0.83497 -2.89172 H 3.28127 -0.41730 -3.36701 C -1.04400 -3.09021 -2.74750 H -1.85766 -3.39212 -2.09743 C -0.55542 -3.98431 -3.69347 H -0.99366 -4.97706 -3.76661 C 0.49084 -3.61803 -4.54378 H 0.87255 -4.32227 -5.27877 C 1.03715 -2.34058 -4.44144 H 1.84826 -2.03599 -5.09876 C 0.55334 -1.45054 -3.48480 H 0.98652 -0.46311 -3.39191 C -0.48605 -1.80361 -2.61196 C -0.92150 -0.85169 -1.56482 C -2.04089 -0.83474 -0.91864 C -3.30883 -1.52709 -0.88324 C -3.81597 -2.10605 0.29022 H -3.28114 -1.95767 1.22065 C -4.99854 -2.83719 0.26174 H -5.37832 -3.27835 1.18031 C -5.69962 -3.00113 -0.93609 H -6.62689 -3.56797 -0.95429 C -5.20313 -2.42712 -2.10730 H -5.74376 -2.54337 -3.04358 C -4.01906 -1.69513 -2.08557 H -3.62733 -1.25171 -2.99659 N -2.27493 1.45732 0.97018 N -3.20756 0.92544 0.29865 N -1.09765 1.07154 0.85275 Th 0.71209 0.18774 0.12485 Si -4.85305 1.56045 0.59194 C -5.46206 0.89530 2.24579 H -6.48546 1.22469 2.46409 H -5.44932 -0.20069 2.23445 H -4.81122 1.23191 3.06069 C -5.92553 0.92369 -0.80752 H -5.48438 1.16304 -1.78137 H -6.04035 -0.16334 -0.75118 H -6.92309 1.37775 -0.76293 C -4.78763 3.44251 0.60250 H -4.06919 3.79042 1.35335 H -4.46017 3.82003 -0.37270 H -5.76700 3.88081 0.83059	
INT10b	C 1.65507 -2.25052 -1.42869 C 2.90450 -1.71549 -0.93587 C 2.86792 -1.87268 0.48456 H 3.69575 -1.64836 1.14554 C 1.69859 -2.54842 0.88948 C 0.93655 -2.71667 -0.28203 H -0.03851 -3.18239 -0.30972 C 1.15679 -2.62356 -2.83571 C 2.04846 -3.74826 -3.39675 H 1.64557 -4.11364 -4.35021 H 2.09007 -4.59001 -2.69608 H 3.07249 -3.41317 -3.57670 C 1.10367 -1.45476 -3.82932 H 0.43110 -0.67103 -3.47600	

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H	2.46759	-4.91133	3.25004
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C	-0.72190	3.05328	2.42325
C	-0.25511	4.26433	3.25635
H	0.48004	3.98719	4.01424
H	-1.10926	4.71453	3.77806
H	0.19442	5.02863	2.61183

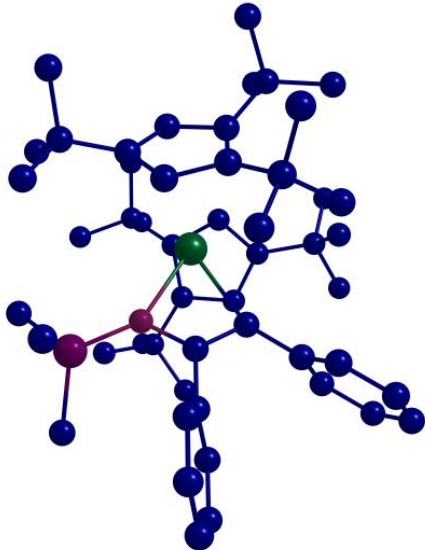
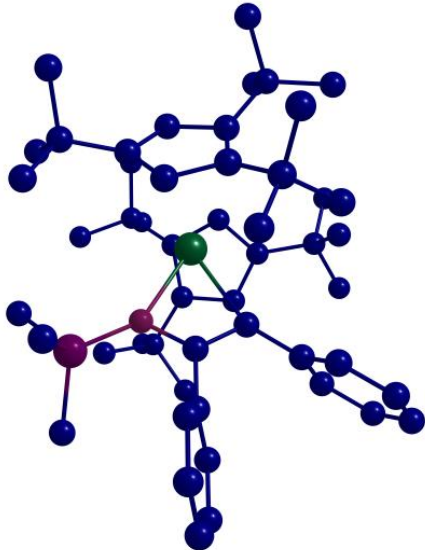
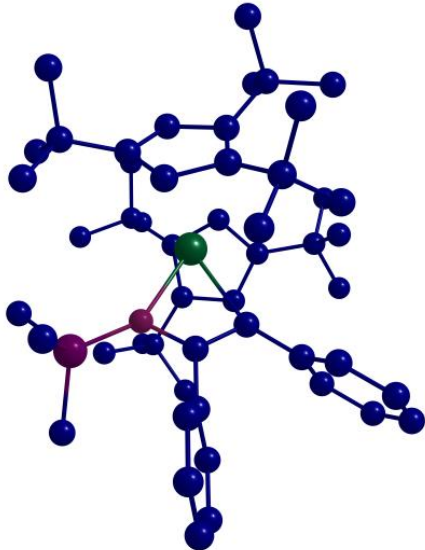
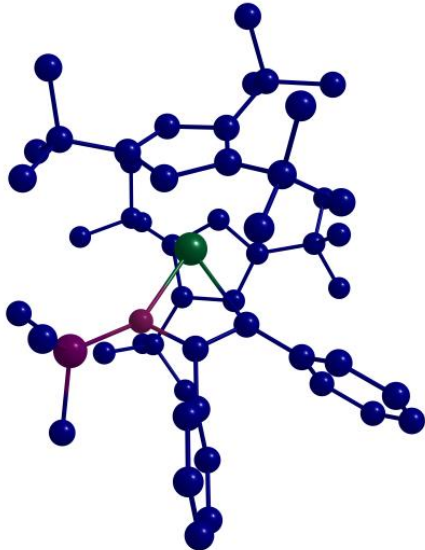
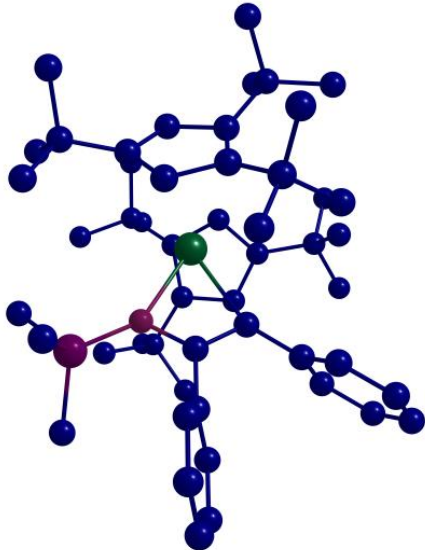
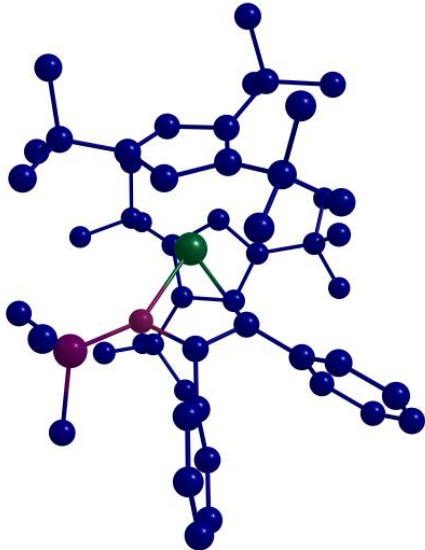
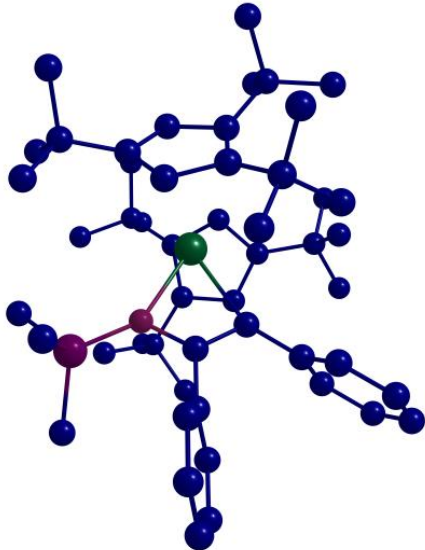
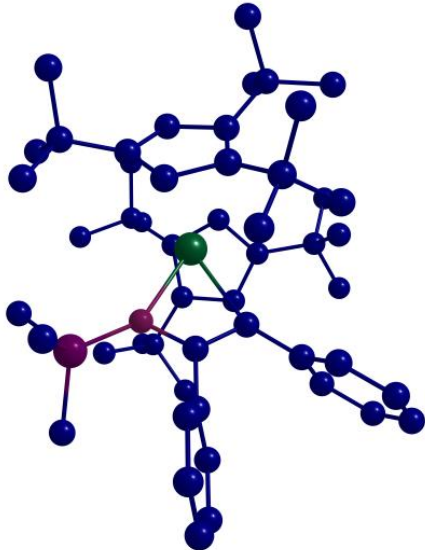
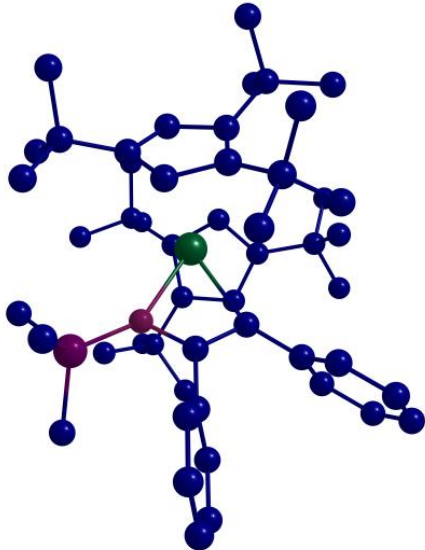
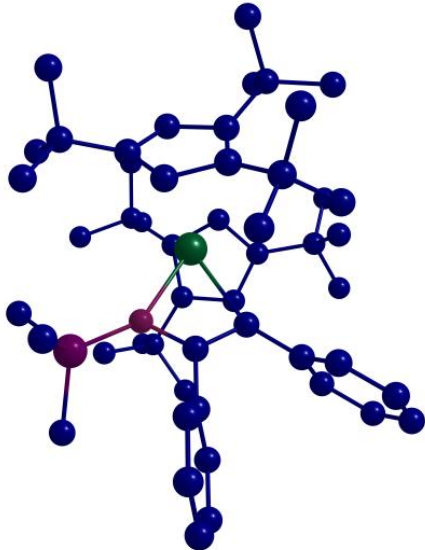
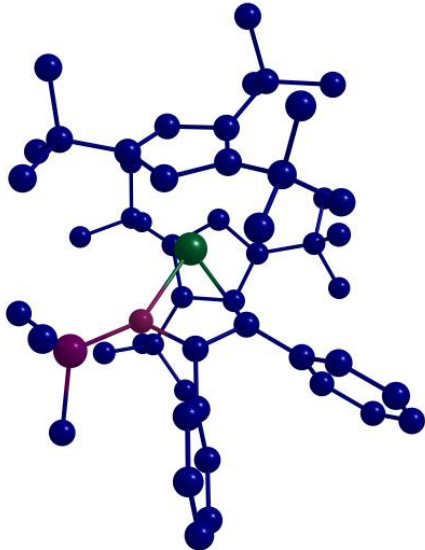
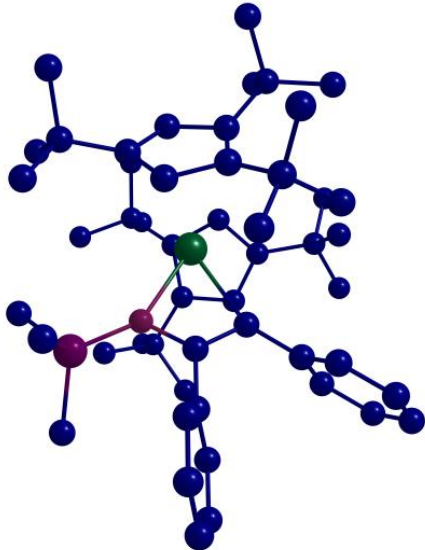
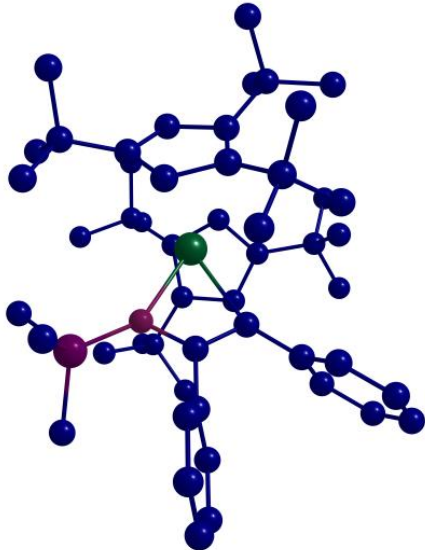
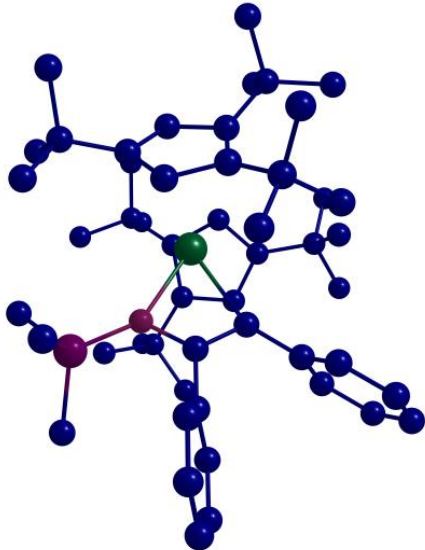
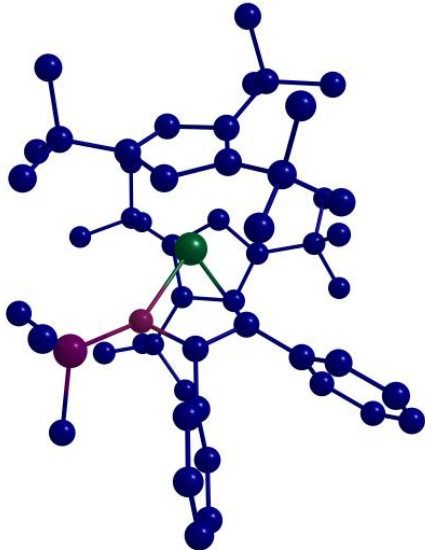


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H	-2.00850	1.33865	2.80019
H	-1.85161	2.44173	4.17234
H	-0.55402	1.30145	3.77158
C	-1.92032	3.53543	1.58494
H	-1.68328	4.41092	0.96982
H	-2.74113	3.81355	2.25701
H	-2.28374	2.73021	0.93788
C	1.91362	2.97439	-1.99354
C	3.41553	3.20358	-2.19984
H	3.77359	4.04192	-1.59178
H	3.62182	3.42970	-3.25276
H	4.00232	2.31732	-1.93545
C	1.14134	4.20600	-2.49039
H	0.05984	4.04590	-2.43489
H	1.39080	4.41185	-3.53884
H	1.39336	5.09042	-1.89452
C	1.47183	1.75353	-2.80936
H	1.98488	0.84234	-2.46307
H	1.72716	1.84786	-3.87220
H	0.38662	1.60650	-2.75437
C	-1.88777	0.19515	-3.27087
H	-1.68573	-0.86932	-3.30713
C	-2.08853	0.89336	-4.45984
H	-2.01716	0.36476	-5.40810
C	-2.38225	2.25609	-4.43730
H	-2.52845	2.80646	-5.36322
C	-2.51361	2.89497	-3.20383
H	-2.78201	3.94850	-3.16073
C	-2.31561	2.19091	-2.01880
H	-2.46208	2.69501	-1.07018
C	-1.95987	0.82880	-2.01763
C	-1.62960	0.09319	-0.76612
C	-2.70083	-0.30224	-0.01450
C	-4.09929	0.03818	-0.41618
C	-4.70634	-0.54299	-1.53505
H	-4.15431	-1.27738	-2.11440
C	-5.99852	-0.17853	-1.90826
H	-6.46093	-0.64289	-2.77596
C	-6.69463	0.78352	-1.17552
H	-7.70131	1.07046	-1.46934
C	-6.09152	1.37866	-0.06636
H	-6.62660	2.13234	0.50659
C	-4.80597	1.00318	0.31313
H	-4.33719	1.45130	1.18560
N	-1.59568	-1.05156	2.05636
N	-2.68949	-0.98904	1.23225
N	-0.56261	-0.48333	1.67872
Th	0.80682	0.08545	0.09328
Si	-3.88573	-2.29038	1.68007
C	-3.61281	-3.64434	0.40405
H	-4.25581	-4.51153	0.59681
H	-3.83125	-3.27644	-0.60453
H	-2.56906	-3.97900	0.42454
C	-5.67942	-1.73481	1.70404
H	-5.81017	-0.83906	2.31982
H	-6.08551	-1.52415	0.71144

	H -6.26959 -2.54351 2.15606 C -3.45848 -2.86311 3.41476 H -2.47712 -3.33822 3.47573 H -3.46201 -2.01657 4.10977 H -4.21826 -3.58232 3.74736	
TS10c	C -0.53896 -2.47239 1.39863 C -1.94271 -2.15758 1.56961 C -2.52343 -2.24386 0.26738 H -3.58375 -2.15609 0.06309 C -1.57301 -2.66987 -0.68359 C -0.34629 -2.73760 0.00993 H 0.60190 -2.99225 -0.44393 C 0.57442 -2.80084 2.40257 C 0.21129 -4.10099 3.14561 H 1.03413 -4.40017 3.80721 H 0.03933 -4.91071 2.42699 H -0.68779 -4.00622 3.75661 C 0.86091 -1.65254 3.37584 H 1.29063 -0.82558 2.80533 H 1.59229 -1.95818 4.13479 H -0.02543 -1.28401 3.88842 C 1.90395 -3.07108 1.67124 H 2.19254 -2.22329 1.04411 H 1.85702 -3.96808 1.04400 H 2.69677 -3.23180 2.41182 C -2.93307 -2.17301 2.75862 C -3.53300 -3.59915 2.79225 H -2.75321 -4.35008 2.95419 H -4.03150 -3.83802 1.84716 H -4.26888 -3.68878 3.60172 C -2.39789 -1.87033 4.16559 H -2.02312 -0.84978 4.26450 H -1.61043 -2.55525 4.47910 H -3.22062 -1.97802 4.88268 C -4.08577 -1.17707 2.51567 H -4.80468 -1.22901 3.34184 H -4.63781 -1.37752 1.59360 H -3.71522 -0.14863 2.46356 C -1.91256 -3.34397 -2.00605 C -2.66331 -4.64373 -1.64362 H -2.05751 -5.26947 -0.97832 H -2.88713 -5.21994 -2.55070 H -3.60923 -4.42698 -1.13425 C -2.81089 -2.47882 -2.88626 H -3.68685 -2.11310 -2.33944 H -3.16847 -3.04583 -3.75458 H -2.25193 -1.61559 -3.25485 C -0.65540 -3.71177 -2.79364 H -0.05861 -2.82566 -3.02243 H -0.93306 -4.19242 -3.73961 H -0.02677 -4.41401 -2.23758 C -2.81276 1.91233 -1.11706 C -1.54823 2.56198 -1.36326 C -0.98364 2.85082 -0.08274 H -0.04427 3.36203 0.07579 C -1.85915 2.44835 0.94396 C -2.95183 1.82440 0.30181	

H	-3.81138	1.41301	0.81216
C	-4.00585	1.55648	-2.02214
C	-5.03677	0.72301	-1.23268
H	-5.86482	0.44706	-1.89484
H	-5.46795	1.27439	-0.39078
H	-4.59018	-0.20187	-0.84768
C	-4.70501	2.86912	-2.42879
H	-4.06104	3.48283	-3.06423
H	-4.97340	3.46019	-1.54570
H	-5.62158	2.65243	-2.99242
C	-3.65263	0.74362	-3.29428
H	-2.63702	0.35143	-3.25159
H	-3.73858	1.34148	-4.20470
H	-4.32948	-0.10691	-3.41340
C	-0.91192	3.22264	-2.59823
C	-1.40418	4.68636	-2.63538
H	-2.48976	4.74689	-2.75623
H	-0.93847	5.22280	-3.47228
H	-1.14280	5.20590	-1.70660
C	-1.21661	2.56512	-3.94497
H	-0.91505	1.51330	-3.95032
H	-0.65552	3.08183	-4.73288
H	-2.27158	2.63629	-4.20757
C	0.62105	3.25887	-2.46165
H	0.94014	3.91976	-1.65202
H	1.06539	3.64797	-3.38525
H	1.02798	2.26000	-2.27464
C	-1.66464	2.60957	2.44168
C	-3.01146	2.86617	3.13195
H	-3.49199	3.76218	2.72376
H	-2.86106	3.01512	4.20813
H	-3.70472	2.02684	3.01035
C	-0.71885	3.77971	2.73413
H	0.26457	3.63204	2.28221
H	-0.56986	3.88514	3.81525
H	-1.13907	4.71653	2.35073
C	-1.05924	1.30882	2.98078
H	-1.71361	0.45152	2.77111
H	-0.90923	1.33044	4.06718
H	-0.06718	1.12852	2.54995
C	2.24934	1.74698	2.57669
H	2.02703	0.84083	3.12884
C	2.72350	2.85211	3.28197
H	2.83249	2.78832	4.36260
C	3.05874	4.02726	2.61329
H	3.41994	4.89341	3.16191
C	2.93920	4.06454	1.22329
H	3.22242	4.96021	0.67423
C	2.47725	2.95133	0.52715
H	2.43791	2.97303	-0.55511
C	2.09483	1.76377	1.17905
C	1.60399	0.59284	0.38280
C	2.61845	-0.06867	-0.30179
C	4.04814	0.30135	-0.04220
C	4.64934	-0.00546	1.18342
H	4.06297	-0.51518	1.94279
C	5.98063	0.32368	1.42078

	H 6.43872 0.06905 2.37370 C 6.72817 0.97414 0.43758 H 7.76862 1.23031 0.62217 C 6.13092 1.30135 -0.78051 H 6.70174 1.82275 -1.54555 C 4.79907 0.96700 -1.01711 H 4.32527 1.22735 -1.96026 N 1.26737 -0.83215 -2.41404 N 2.46501 -1.02475 -1.27677 N 0.31249 -0.22425 -2.05906 Th -0.80316 0.05210 -0.01113 Si 3.69192 -2.10044 -1.99752 C 4.48906 -1.34395 -3.53046 H 4.99835 -2.12232 -4.11286 H 3.72613 -0.88777 -4.17148 H 5.22699 -0.57915 -3.27009 C 2.81301 -3.67642 -2.52859 H 2.29756 -4.15076 -1.68615 H 2.08175 -3.49262 -3.31947 H 3.55427 -4.39020 -2.91048 C 5.01078 -2.61138 -0.75284 H 5.76596 -1.83658 -0.59486 H 4.57117 -2.85798 0.21961 H 5.51113 -3.51154 -1.13382	
10	C 1.13539 -2.24338 1.52423 C 2.41903 -1.95693 0.92145 C 2.85202 -0.71929 1.48837 H 3.82397 -0.27775 1.31125 C 1.96195 -0.28242 2.48641 C 0.87973 -1.18644 2.45267 H 0.00696 -1.11843 3.08642 C 0.23730 -3.48953 1.52374 C 0.93420 -4.60539 2.32673 H 0.27468 -5.47825 2.41603 H 1.17960 -4.25561 3.33635 H 1.86208 -4.93784 1.85580 C -0.13628 -3.98942 0.12270 H -0.66017 -3.20830 -0.43069 H -0.80845 -4.85334 0.19720 H 0.72562 -4.29478 -0.46449 C -1.09117 -3.18346 2.24349 H -1.58904 -2.31926 1.79132 H -0.95010 -2.98725 3.31212 H -1.76171 -4.04643 2.15784 C 3.53252 -2.81633 0.27661 C 4.42083 -3.30174 1.44788 H 3.84605 -3.91438 2.15001 H 4.83305 -2.45533 2.00697 H 5.25688 -3.90545 1.07110 C 3.13698 -4.05844 -0.53133 H 2.54689 -3.81298 -1.41612 H 2.58861 -4.79040 0.06245 H 4.05100 -4.55345 -0.88154 C 4.40080 -1.95486 -0.65813 H 5.19471 -2.56513 -1.10483 H 4.88540 -1.11909 -0.14599 H 3.79361 -1.54260 -1.46597	

	C	2.31429	0.68871	3.60177	
	C	3.40850	0.00909	4.45290	
	H	3.05428	-0.95318	4.83937	
	H	3.68337	0.64442	5.30508	
	H	4.31060	-0.17827	3.85974	
	C	2.87017	2.00863	3.06244	
	H	3.77445	1.85057	2.46533	
	H	3.12921	2.68740	3.88418	
	H	2.13967	2.51988	2.43003	
	C	1.10891	0.96663	4.50044	
	H	0.28468	1.39482	3.93070	
	H	1.37767	1.67512	5.29282	
	H	0.74774	0.05000	4.97975	
	C	1.86825	2.02144	-1.71787	
	C	0.46683	2.18054	-2.05750	
	C	0.08604	0.97255	-2.70678	
	H	-0.89015	0.77900	-3.11380	
	C	1.17803	0.09518	-2.84169	
	C	2.25461	0.73207	-2.19404	
	H	3.26308	0.34798	-2.14405	
	C	2.97249	2.99275	-1.27487	
	C	4.13120	2.22990	-0.59988	
	H	4.87523	2.94090	-0.22248	
	H	4.64896	1.55522	-1.28805	
	H	3.76956	1.63587	0.24448	
	C	3.55148	3.67561	-2.53176	
	H	2.79456	4.25341	-3.06735	
	H	3.94678	2.92341	-3.22359	
	H	4.36953	4.35470	-2.25758	
	C	2.51287	4.05987	-0.28034	
	H	2.03854	3.60931	0.59751	
	H	1.80789	4.76440	-0.72336	
	H	3.37275	4.64224	0.07200	
	C	-0.50610	3.37909	-2.06905	
	C	0.05888	4.50472	-2.95366	
	H	0.93592	4.97933	-2.50826	
	H	-0.69785	5.28637	-3.09769	
	H	0.34515	4.11901	-3.93874	
	C	-0.85628	3.92774	-0.68013	
	H	-1.38813	3.16464	-0.10741	
	H	-1.51019	4.80460	-0.76932	
	H	0.01691	4.22262	-0.10202	
	C	-1.85461	2.95578	-2.68658	
	H	-1.75751	2.66082	-3.73719	
	H	-2.55298	3.79961	-2.64292	
	H	-2.30129	2.12512	-2.12744	
	C	1.19460	-1.19155	-3.65505	
	C	2.61453	-1.48334	-4.16008	
	H	3.00978	-0.63856	-4.73601	
	H	2.60812	-2.36801	-4.80810	
	H	3.30768	-1.68867	-3.33968	
	C	0.27265	-1.04804	-4.87781	
	H	-0.77355	-0.92964	-4.58161	
	H	0.33369	-1.94975	-5.49963	
	H	0.56054	-0.18639	-5.49114	
	C	0.69997	-2.36268	-2.79979	
	H	1.27545	-2.42599	-1.86955	

H	0.81291	-3.32205	-3.32184
H	-0.35435	-2.24149	-2.53899
C	-3.15576	-2.70457	-0.86612
H	-2.96139	-2.98033	0.16465
C	-4.00107	-3.49532	-1.63974
H	-4.44592	-4.38751	-1.20356
C	-4.28745	-3.14604	-2.95967
H	-4.94662	-3.76414	-3.56434
C	-3.72626	-1.98291	-3.48606
H	-3.95328	-1.67921	-4.50601
C	-2.87889	-1.19702	-2.70853
H	-2.47854	-0.27783	-3.12281
C	-2.55784	-1.54025	-1.38305
C	-1.64694	-0.70594	-0.57974
C	-2.18067	0.10603	0.40609
C	-3.64950	0.07967	0.68445
C	-4.13354	-0.54726	1.83661
H	-3.43283	-1.01032	2.52525
C	-5.50164	-0.57942	2.10178
H	-5.86557	-1.06861	3.00236
C	-6.40006	0.00895	1.21157
H	-7.46717	-0.01257	1.41871
C	-5.92369	0.61417	0.04733
H	-6.61950	1.06475	-0.65638
C	-4.55735	0.64360	-0.21741
H	-4.18348	1.10811	-1.12465
N	-1.37820	0.97887	1.16218
Th	0.48848	0.16828	-0.00194
Si	-2.00248	2.06723	2.39836
C	-2.35164	1.17083	4.03580
H	-2.09238	1.80392	4.89333
H	-3.41579	0.92211	4.10821
H	-1.78286	0.23934	4.12538
C	-3.58377	2.99223	1.93104
H	-3.54151	3.38902	0.91084
H	-4.47784	2.36797	2.01480
H	-3.69372	3.84360	2.61703
C	-0.68529	3.41116	2.64641
H	-0.52364	3.63714	3.70646
H	0.27940	3.12825	2.21703
H	-1.00197	4.33498	2.15034

Table S8. Frequencies of the stationary points optimized for 2+Me₃SiN₃, obtained with B3PW91-PCM+D3 method.

Species	Frequencies (cm ⁻¹)
2	19 22 28 33 40 42 48 55 59 64 66 72 77 86 86 98 99 104 107 109 121 134 142 144 151 161 176 182 183 192 197 203 207 208 214 217 229 232 246 250 251 255 257 259 262 269 274 278 279 287 288 296 297 312 316 324 326 328 329 337 340 359 359 365 372 372 380 384 390 395 397 402 407 410 414 414 416 420 438 440 446 451 469 471 472 487 489 497 553 563 563 566 566 583 584 591 606 607 608 631 634 659 660 689 692 693 697 698 710 711 771 783 795 797 810 834 835 837 838 841 842 850 851 861 861 902 914 939 939 939 946 946 948 948 953 953 957 957 959 959 964 964 969 970 971 971 976 978 979 979 987 987 1014 1015 1030 1030 1051 1051 1056 1057 1059 1059 1060 1060 1061 1062 1063 1063 1068 1069 1113 1113 1156 1157 1178 1193 1194 1206 1206 1210 1211 1213 1215 1229 1229 1236 1236 1244 1245 1250 1250 1253 1253 1264 1265 1275 1280 1280 1282 1284 1323 1325 1330 1333 1371 1373 1397 1397 1412 1413 1414 1414 1417 1417 1420 1422 1423 1423 1427 1427 1435 1435 1449 1450 1451 1451 1459 1460 1466 1466 1484 1486 1497 1497 1498 1499 1505 1505 1506 1508 1508 1509 1513 1513 1514 1514 1520 1520 1521 1522 1522 1524 1524 1526 1527 1532 1533 1534 1536 1536 1537 1537 1541 1543 1547 1549 1551 1552 1561 1561 1563 1564 1597 1632 1633 1662 1663 2989 2991 3048 3049 3051 3051 3052 3052 3055 3055 3056 3057 3060 3060 3061 3061 3072 3072 3086 3086 3121 3121 3125 3125 3125 3125 3127 3127 3129 3129 3131 3131 3132 3133 3139 3139 3142 3143 3144 3144 3145 3145 3145 3146 3146 3147 3151 3151 3168 3168 3180 3180 3188 3188 3195 3195 3205 3205 3208 3208 3213 3213 3219 3219 3270 3271 3298 3299
Me ₃ SiN ₃	86 172 187 307 315 361 421 494 551 635 711 714 832 848 851 968 988 1031 1038 1117 1146 1206 1245 1329 1371 1434 1464 1537 1636 1660 1805 2926 3193 3219 3232 3234
COM10	18 28 31 37 42 44 47 51 56 58 62 69 71 78 80 82 86 88 91 94 99 106 109 111 115 121 132 136 140 142 145 152 160 163 173 177 184 186 190 191 194 196 199 202 206 210 211 220 222 227 235 237 240 249 252 254 257 260 265 266 269 275 280 287 291 294 296 297 307 312 314 318 328 330 334 350 355 359 361 368 372 377 384 386 393 396 405 406 412 414 417 418 419 426 439 442 448 451 469 471 472 489 491 495 503 552 556 564 567 567 575 579 581 584 605 605 606 608 630 633 660 661 663 687 687 689 691 695 702 710 710 713 714 772 784 786 790 799 805 807 831 834 835 839 842 846 850 859 860 861 879 888 893 899 914 932 935 936 937 947 948 949 953 957 958 959 961 963 964 967 970 971 973 976 979 980 981 983 986 990 1013 1014 1028 1031 1053 1054 1056 1058 1059 1060 1060 1061 1062 1062 1063 1064 1069 1069 1110 1114 1157 1158 1179 1193 1194 1206 1207 1209 1212 1214 1216 1227 1229 1231 1234 1237 1245 1248 1249 1250 1256 1264 1264 1272 1279 1281 1284 1286 1315 1320 1321 1326 1328 1330 1332 1371 1373 1393 1400 1411 1412 1415 1415 1417 1419 1420 1421 1421 1423 1425 1426 1434 1436 1447 1448 1451 1452 1452 1457 1459 1461 1467 1468 1475 1477 1479 1483 1485 1486 1493 1498 1499 1500 1500 1504 1505 1506 1508 1509 1510 1512 1513 1516 1519 1520 1521 1522 1523 1524 1524 1525 1526 1528 1529 1532 1534 1534 1536 1537 1538 1541 1543 1548 1549 1551 1554 1561 1562 1566 1569 1616 1629 1632 1659 1662 2340 3035 3042 3046 3047 3048 3049 3049 3051 3055 3055 3056 3058 3060 3061 3061 3061 3063 3064 3066 3072

	3073 3098 3119 3119 3120 3122 3123 3124 3125 3125 3126 3126 3128 3128 3131 3133 3136 3138 3138 3140 3141 3142 3142 3145 3146 3148 3149 3151 3152 3154 3155 3158 3160 3162 3163 3167 3169 3179 3180 3181 3187 3188 3194 3198 3200 3205 3206 3210 3211 3212 3218 3218 3221 3256 3257 3291 3318
TS10a	-136 21 25 30 33 35 40 43 48 52 58 62 71 75 82 84 85 88 91 96 101 105 106 108 113 123 124 133 137 138 145 151 153 160 164 168 175 183 187 189 194 197 202 204 207 210 216 220 228 230 237 244 249 253 256 261 262 265 269 274 277 279 288 294 296 300 309 312 315 319 322 327 331 339 347 354 358 367 368 371 378 382 387 390 396 402 406 407 413 415 415 417 420 427 440 445 446 449 451 453 472 474 488 490 500 522 554 559 565 567 568 569 576 582 584 605 607 630 632 634 660 664 664 687 688 689 693 697 701 702 708 712 742 767 775 777 786 793 801 818 834 836 837 841 848 849 856 860 862 863 877 880 885 890 926 934 936 942 945 946 947 951 954 958 958 960 961 966 969 972 972 973 975 979 980 981 982 984 994 1000 1016 1017 1028 1030 1054 1057 1058 1059 1060 1060 1061 1062 1062 1063 1063 1065 1066 1068 1114 1115 1156 1158 1179 1196 1198 1204 1204 1209 1212 1214 1217 1227 1229 1233 1239 1242 1244 1246 1250 1251 1258 1263 1264 1275 1280 1280 1284 1286 1292 1303 1309 1316 1320 1323 1335 1339 1374 1378 1397 1403 1411 1413 1416 1416 1418 1419 1421 1422 1423 1425 1427 1430 1434 1436 1448 1451 1452 1456 1460 1461 1462 1468 1474 1479 1480 1485 1485 1487 1488 1496 1498 1499 1502 1503 1504 1505 1506 1508 1508 1509 1513 1514 1516 1516 1519 1520 1522 1523 1524 1527 1527 1528 1529 1530 1532 1534 1536 1537 1538 1538 1541 1543 1546 1549 1554 1556 1559 1561 1564 1566 1576 1636 1637 1663 1664 1757 3041 3043 3045 3047 3048 3048 3050 3050 3051 3051 3052 3055 3055 3058 3059 3060 3060 3061 3062 3065 3074 3109 3114 3118 3119 3121 3121 3123 3124 3124 3124 3126 3128 3129 3130 3130 3130 3134 3134 3134 3135 3136 3137 3137 3143 3147 3148 3151 3151 3152 3153 3155 3155 3156 3159 3162 3164 3167 3175 3186 3192 3195 3199 3201 3202 3210 3211 3213 3218 3222 3230 3231 3237 3252 3257 3280 3303
INT10a	24 28 38 40 45 46 52 59 63 67 79 80 82 86 89 97 99 106 112 115 118 124 129 132 134 137 143 144 146 153 164 169 173 178 180 183 187 192 195 200 201 205 206 210 212 217 221 226 230 240 245 253 263 264 264 266 273 278 281 287 293 296 299 303 309 312 316 322 325 328 331 335 340 343 348 354 366 367 369 373 377 388 392 394 399 405 407 409 410 415 420 422 425 429 435 438 444 449 452 478 481 488 494 503 535 551 564 569 569 574 578 579 604 606 606 625 631 652 661 663 682 688 690 692 693 696 699 703 709 711 714 745 771 772 783 794 811 824 837 837 839 840 851 852 856 858 863 865 870 877 880 888 913 923 938 943 945 946 948 949 959 960 960 962 963 964 967 969 971 973 974 975 978 980 981 982 984 988 994 1014 1016 1027 1031 1055 1055 1056 1058 1059 1061 1062 1063 1063 1064 1066 1067 1070 1071 1090 1115 1120 1152 1158 1179 1193 1195 1203 1207 1211 1213 1214 1220 1227 1230 1233 1239 1240 1242 1245 1246 1248 1249 1253 1263 1265 1278 1279 1282 1289 1300 1303 1307 1316 1320 1326 1340 1341 1372 1375 1389 1398 1411 1412 1415 1417 1418 1419 1420 1421 1421 1423 1427 1429 1433 1434 1448 1450 1451 1454 1460 1460 1464 1466 1475 1478 1480 1485 1486 1488 1490 1494 1496 1499 1502 1503 1505 1505 1506 1506 1509 1509 1511 1512 1514 1515 1516 1517 1519 1519 1520 1521 1524 1527 1528 1530 1533 1533 1535 1536 1537 1539 1539 1540 1542 1545 1546 1551 1553 1558 1561 1563 1565 1567 1630 1645 1663 1668 3041 3044 3045 3046 3049 3049

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INT10b	8 19 32 37 38 45 48 52 59 59 65 68 76 83 85 87 93 95 101 104 107 116 117 121 125 133 138 141 149 151 161 162 174 175 178 183 186 193 196 200 202 206 208 213 217 223 226 230 238 247 250 258 260 263 263 267 275 278 281 283 287 293 295 297 304 307 311 319 322 328 328 331 344 349 351 355 360 365 368 378 388 389 393 399 401 404 407 410 416 417 424 424 430 434 441 446 446 452 474 476 489 490 492 512 527 556 558 564 566 567 576 586 595 605 608 625 631 633 647 660 662 684 686 690 693 698 700 707 712 716 722 736 775 787 795 798 799 813 833 834 838 839 842 846 849 860 861 864 866 879 882 890 921 930 939 943 943 946 950 950 953 958 958 960 963 965 968 972 974 974 976 979 980 981 983 985 986 991 994 1015 1017 1029 1031 1054 1055 1056 1058 1059 1060 1060 1061 1062 1063 1065 1067 1069 1073 1075 1111 1115 1125 1152 1158 1193 1197 1204 1205 1209 1211 1214 1215 1228 1228 1229 1238 1241 1244 1246 1248 1248 1251 1256 1263 1264 1278 1280 1281 1284 1286 1309 1318 1320 1323 1326 1326 1341 1369 1376 1399 1400 1411 1412 1414 1415 1416 1418 1420 1421 1422 1423 1426 1426 1432 1433 1448 1450 1451 1451 1459 1460 1468 1471 1474 1477 1483 1483 1488 1490 1497 1498 1500 1503 1504 1505 1506 1507 1509 1509 1510 1512 1515 1517 1519 1519 1519 1522 1522 1525 1525 1527 1529 1530 1533 1535 1535 1535 1536 1536 1538 1540 1543 1547 1549 1552 1555 1560 1561

	1562 1563 1566 1597 1631 1644 1662 1670 3007 3041 3047 3048 3048 3048 3049 3050 3050 3052 3052 3052 3054 3055 3056 3058 3060 3064 3065 3066 3070 3090 3115 3116 3118 3121 3121 3122 3123 3124 3125 3126 3127 3129 3130 3130 3132 3134 3135 3136 3137 3138 3138 3140 3140 3145 3146 3146 3147 3148 3158 3160 3162 3162 3163 3170 3171 3173 3179 3181 3184 3184 3186 3189 3194 3205 3210 3212 3220 3229 3232 3236 3239 3252 3274 3279 3312
TS10c	-339 17 32 40 42 49 50 56 58 60 63 69 74 78 80 84 85 92 92 98 102 107 115 118 120 132 135 140 144 150 156 165 169 174 175 179 182 187 197 199 199 207 212 214 217 219 223 225 228 233 242 246 248 254 260 262 264 268 273 277 280 285 288 295 299 303 309 314 315 323 325 329 332 335 339 344 358 362 367 369 376 380 385 387 390 393 397 409 413 416 420 423 425 428 431 439 450 454 460 470 472 485 488 496 503 525 550 554 567 568 570 578 593 599 604 613 625 634 635 638 661 665 683 688 692 693 696 698 700 716 717 721 736 776 783 788 798 801 826 831 836 839 843 848 855 857 860 864 865 868 877 882 884 919 932 937 943 948 948 950 954 956 957 958 965 969 970 971 972 974 976 979 980 982 983 987 991 993 994 998 1018 1018 1028 1030 1053 1054 1056 1059 1060 1061 1062 1063 1064 1066 1069 1070 1073 1076 1114 1114 1156 1156 1159 1193 1196 1205 1207 1209 1212 1214 1219 1228 1230 1231 1233 1236 1244 1248 1248 1255 1256 1257 1265 1266 1278 1282 1286 1289 1303 1308 1316 1320 1322 1323 1332 1341 1369 1376 1392 1403 1406 1412 1413 1416 1416 1420 1421 1422 1423 1427 1429 1430 1434 1436 1441 1450 1451 1452 1457 1461 1462 1463 1469 1477 1482 1482 1483 1489 1491 1495 1498 1500 1500 1502 1504 1505 1506 1507 1507 1510 1510 1511 1513 1515 1515 1516 1519 1522 1524 1526 1527 1529 1531 1532 1533 1535 1536 1537 1538 1539 1540 1543 1543 1545 1546 1551 1553 1560 1561 1562 1565 1633 1644 1662 1668 1801 3034 3043 3048 3049 3050 3050 3051 3052 3052 3053 3054 3055 3056 3059 3060 3062 3065 3065 3066 3075 3083 3107 3118 3120 3120 3122 3123 3125 3126 3126 3128 3128 3129 3129 3131 3131 3131 3133 3135 3135 3136 3137 3138 3147 3147 3148 3150 3154 3155 3156 3157 3160 3162 3164 3167 3169 3173 3174 3179 3180 3183 3188 3189 3191 3196 3199 3203 3210 3210 3217 3217 3235 3246 3252 3278 3278 3279
N₂	2473
10	22 29 32 43 45 50 61 63 69 76 81 86 89 94 95 101 109 112 115 118 120 126 133 140 144 150 152 158 162 162 172 174 183 184 186 187 194 196 198 202 211 215 220 224 227 240 243 248 249 253 254 260 266 271 276 276 278 286 289 290 297 299 302 307 310 319 323 330 332 335 339 341 346 354 358 366 370 385 387 389 395 399 405 407 412 414 417 419 420 425 427 440 444 451 454 474 476 481 490 492 510 540 550 565 566 568 579 580 585 605 606 626 629 635 642 661 665 683 684 685 687 689 698 702 714 716 727 728 771 777 785 794 805 809 811 835 837 839 840 846 851 852 859 861 864 870 873 883 912 930 936 943 944 947 950 952 954 958 959 960 964 965 969 971 972 972 975 976 980 981 981 983 985 987 994 1017 1019 1028 1034 1054 1056 1056 1059 1059 1061 1062 1063 1066 1066 1067 1068 1070 1073 1113 1115 1130 1157 1160 1193 1197 1205 1210 1211 1215 1216 1218 1226 1231 1235 1243 1244 1244 1245 1251 1254 1255 1259 1264 1266 1279 1282 1285 1286 1306 1308 1311 1320 1322 1328 1330 1342 1369 1376 1395 1396 1412 1413 1415 1417 1418 1419 1420 1421 1423 1424 1425 1427 1435 1435 1448 1451 1452 1452 1459 1459 1463 1468 1477 1478 1480 1484 1488 1490 1492 1495 1497 1499 1500 1502 1503 1504 1504 1505 1508 1509 1511 1514 1515 1517 1517

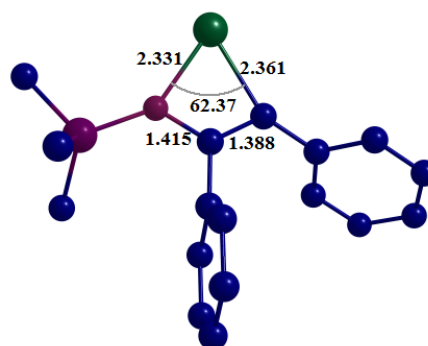
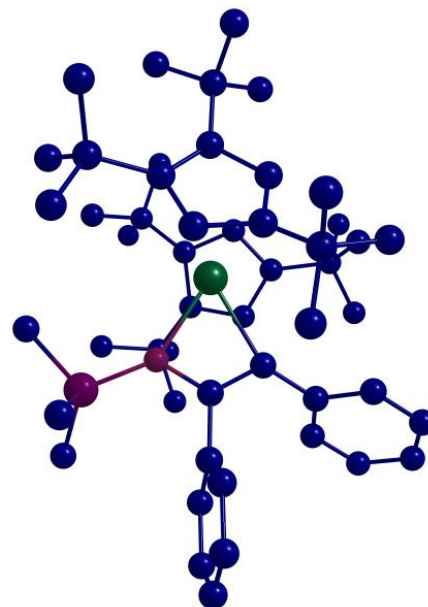
	1519 1519 1522 1523 1524 1524 1526 1528 1531 1533 1534 1536 1537 1539
	1540 1541 1543 1546 1547 1549 1553 1554 1561 1563 1563 1567 1633 1645
	1665 1670 3043 3044 3044 3047 3048 3049 3049 3052 3052 3053 3053 3058
	3058 3060 3063 3063 3065 3066 3067 3069 3073 3114 3119 3120 3121 3122
	3123 3124 3125 3126 3126 3127 3128 3129 3131 3133 3134 3135 3135 3137
	3141 3144 3145 3148 3150 3151 3152 3153 3154 3157 3161 3162 3162 3164
	3165 3167 3169 3178 3179 3180 3186 3186 3195 3196 3200 3207 3209 3216
	3218 3224 3227 3233 3237 3257 3282 3285 3342

Table S9. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for $2+\text{Me}_3\text{SiN}_3$, obtained with B3PW91-PCM+D3 method

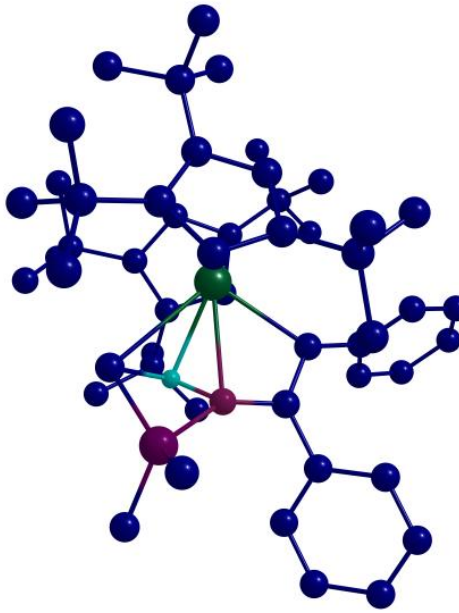
species	E	H	G (gas)	G (sol)
2	-1905.54960	-1904.45059	-1904.59029	-1904.58050
Me_3SiN_3	-573.34499	-573.20819	-573.25567	-573.24550
$2+\text{Me}_3\text{SiN}_3$	-2478.89459(0.0)	-2477.65878(0.0)	-2477.84596(0.0)	-2477.82600(0.0)
COM10	-2478.91990(-15.9)	-2477.68097(-13.9)	-2477.84293(1.9)	-2477.83326(-4.6)
TS10a	-2478.89972(-3.2)	-2477.66327(-2.8)	-2477.82368(14.0)	-2477.81396(7.6)
INT10a	-2478.93724(-26.8)	-2477.69820(-24.7)	-2477.85374(-4.9)	-2477.84414(-11.4)
TS10b	-2478.87762(10.7)	-2477.64058(11.4)	-2477.79685(30.8)	-2477.78719(24.4)
INT10b	-2478.94116(-29.2)	-2477.70202(-27.1)	-2477.86102(-9.5)	-2477.85137(-15.9)
TS10c	-2478.93127(-23.0)	-2477.69362(-21.9)	-2477.85036(-2.8)	-2477.84064(-9.2)
N_2	-109.47454	-109.46560	-109.48736	-109.48168
10	-2369.53682	-2368.30780	-2368.45856	-2368.44875
10+N₂	-2479.01136(-73.3)	-2477.77340(-71.9)	-2477.94592(-62.7)	-2477.93043(-65.5)

Table S10. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for 1,5-H shift of **10**, obtained with B3PW91-PCM+D3 method.

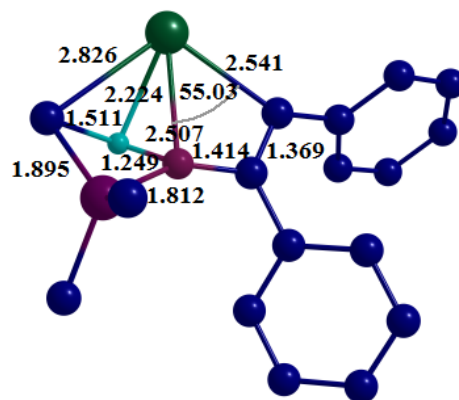
Species	Cartesian coordinates		
10	C	0.556780	8.684880
	C	1.282309	8.265353
	C	0.623429	7.494008
	C	-0.722134	7.160956
	C	-1.433482	7.585962
	C	-0.787777	8.347261
	C	2.751685	8.552603
	C	3.707593	7.640609
	C	3.375663	6.527332
	C	2.875678	6.783551
	C	2.603479	5.758045
	C	2.821576	4.428246
	C	3.315793	4.147772
	C	3.590881	5.177125
	N	3.146116	9.742613
	Si	2.027296	10.987551
	C	0.823590	11.702231
	Th	5.365437	9.048435
	C	3.089877	12.461302
	C	7.652799	9.553960
	C	6.980017	10.809098
	C	5.736385	10.553390
	C	5.738330	9.158709
	C	6.929019	8.541718
	C	4.705630	11.472788
	C	3.386260	10.714212
	C	7.705269	12.112878
	C	7.025935	12.822253
	C	7.447672	7.152098
	C	8.903371	7.277651
	C	4.322397	12.736877
	C	5.242793	11.860104
	C	7.843427	13.080314
	C	9.154165	11.812413
	C	7.412146	6.197255
	C	6.608806	6.547784
	C	0.990606	10.385424
	C	5.064221	8.403312
	C	5.553655	7.204345
	C	6.908768	7.466624
	C	7.309115	8.746909
	C	6.122370	9.346489
	C	4.949624	5.820376
	C	5.658836	4.742761
	C	8.824672	8.999021
	C	9.263537	10.462709
	C	5.910674	10.546659
	C	6.254243	11.915130
	C	9.283937	8.227571
	C	9.625093	8.414860
	C	6.715836	10.340903
	C	4.437850	10.623253



C	3.437637	5.788748	5.757056
C	5.190506	5.483454	7.497171
H	8.643814	9.425459	2.250600
H	4.974784	8.656162	0.155680
H	2.647635	11.394423	-0.315957
H	2.986364	10.330223	1.064079
H	3.507576	9.881453	-0.575084
H	5.152966	13.425176	1.294462
H	3.907097	12.476316	2.118864
H	3.550416	13.287146	0.591430
H	4.502005	12.468432	-1.570414
H	5.433523	10.961370	-1.632329
H	6.172486	12.428538	-0.989383
H	7.058784	12.189354	4.227206
H	5.982990	13.069469	3.132268
H	7.546627	13.755346	3.581768
H	6.892622	13.491283	0.623838
H	8.316468	12.578293	0.110119
H	8.479315	13.926442	1.245663
H	9.642535	12.744256	2.887496
H	9.737382	11.383732	1.761841
H	9.204939	11.127059	3.431257
H	8.974745	7.964738	-0.536994
H	9.279092	6.299047	-0.008373
H	9.569430	7.644506	1.099956
H	8.035405	6.569640	2.822448
H	7.784262	5.203557	1.726469
H	6.385561	6.070897	2.364918
H	5.568394	6.393135	-0.036604
H	7.019670	5.573240	-0.620134
H	6.622330	7.191559	-1.219918
H	7.594022	6.727780	5.075490
H	4.058757	8.525339	6.724972
H	5.604547	12.135511	6.028859
H	7.287417	11.981353	6.543461
H	6.097132	12.707682	7.620920
H	7.794164	10.407410	8.643424
H	6.494617	9.363646	9.231129
H	6.439361	11.110686	9.520319
H	4.295197	11.513250	8.559375
H	4.149395	9.754549	8.536957
H	3.752623	10.696918	7.090446
H	10.358038	10.513809	6.297602
H	8.912006	10.923388	7.203550
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H	10.361085	8.363280	7.556932
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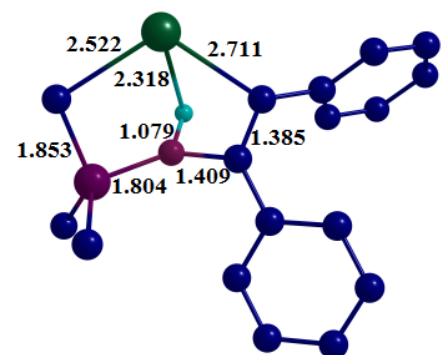
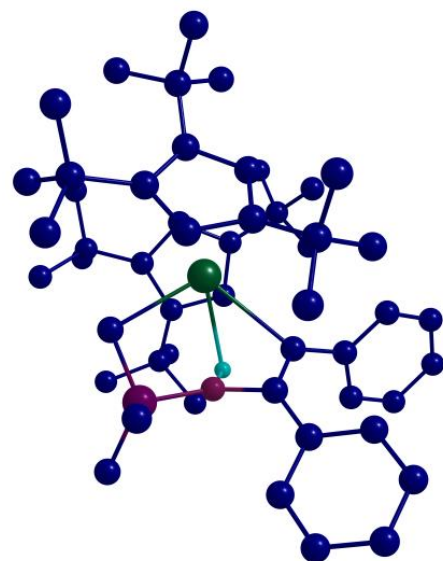
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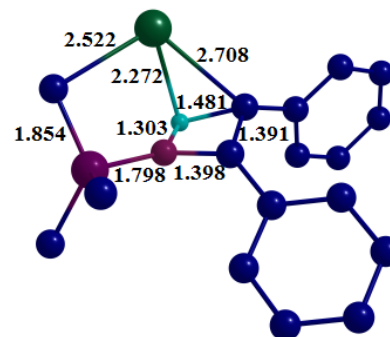
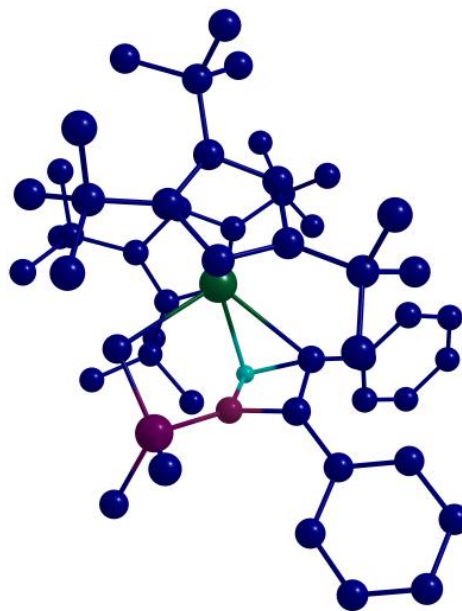
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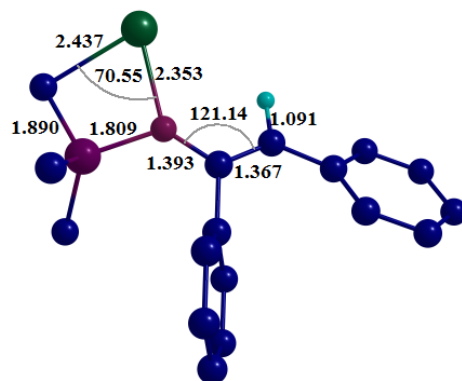
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	H	5.722172	5.216657	7.275222
	H	4.068678	4.709555	7.669938
	H	2.066696	7.581129	-0.070712
	H	1.938948	5.829372	-1.801414

	H 3.224912 3.711300 -1.537896 H 4.623850 3.383607 0.493839 H 4.743041 5.127018 2.215691 H 0.020068 9.392643 3.249198 H -2.184422 8.390820 3.757427 H -2.418619 5.920659 3.911451 H -0.432340 4.470547 3.552076 H 1.769297 5.477692 3.073200 H 1.617211 12.398827 2.236631 H 1.145055 13.056479 3.810534 H 0.207305 11.745788 3.083701 H 1.509720 11.353461 6.416445 H 1.930193 9.638669 6.280964 H 0.422628 10.234712 5.585565 H 4.439078 11.776729 5.206932 H 4.388431 12.072468 3.468107 H 3.462529 9.101037 2.123467	
11	C 6.229615 9.481439 6.759221 C 5.109317 8.619144 6.544891 C 5.502266 7.426132 5.895366 C 6.877216 7.598217 5.603804 C 7.370800 8.821381 6.161324 C 4.742786 6.100420 5.899188 C 5.230932 5.313628 7.136217 C 8.899912 8.957219 6.356902 C 9.669062 8.386161 5.152504 C 6.107336 10.683336 7.723721 C 4.644452 10.876167 8.173888 C 5.019242 5.257234 4.648049 C 3.231541 6.319708 6.029192 C 9.456765 10.372782 6.562565 C 9.281158 8.093617 7.583671 C 6.562462 12.026670 7.124830 C 6.887758 10.391205 9.024282 Th 5.456454 9.365954 3.826531 C 7.142173 8.843649 1.513756 C 7.733417 9.964869 2.138375 C 6.943643 11.144344 1.937478 C 5.776641 10.723897 1.192541 C 5.906993 9.313165 1.005843 C 7.540190 12.534928 2.261081 C 8.907352 12.384916 2.955375 C 4.729390 11.461701 0.326931 C 5.350778 11.670243 -1.075384 C 7.813596 7.516941 1.142905 C 7.651690 7.305067 -0.376306 C 3.174179 7.023547 1.892723 C 2.689393 5.874415 1.125641 C 1.524518 5.142019 1.428556 C 1.148921 4.041299 0.665214 C 1.923744 3.622971 -0.416874 C 3.090986 4.321624 -0.722176 C 3.464882 5.424247 0.038290 C 2.505678 7.940859 2.653684 N 3.191361 8.916064 3.374022 Si 2.474712 10.377900 4.162213 C 1.556941 10.041821 5.795831	

C	1.006910	7.968088	2.652248
C	0.331375	8.277180	1.462880
C	-1.059529	8.326620	1.423776
C	-1.802979	8.056125	2.572538
C	-1.143839	7.735608	3.758257
C	0.249762	7.695920	3.798782
C	1.253599	11.363302	3.095033
C	4.102590	11.285510	4.475507
C	3.477637	10.582351	0.123430
C	4.239690	12.819111	0.849786
C	6.681420	13.396362	3.202414
C	7.821881	13.308507	0.955974
C	9.317741	7.563822	1.447571
C	7.203051	6.312480	1.872796
H	8.711848	9.962626	2.595277
H	5.216377	8.719763	0.422180
H	2.711527	11.157516	-0.407885
H	3.059127	10.243831	1.073292
H	3.685859	9.698762	-0.485819
H	5.033296	13.564885	0.902450
H	3.779232	12.735893	1.837381
H	3.478724	13.213344	0.167048
H	4.616668	12.134599	-1.744960
H	5.646383	10.710654	-1.510811
H	6.235062	12.310340	-1.049174
H	6.587666	12.925537	4.185014
H	5.675553	13.569751	2.823900
H	7.157069	14.373945	3.345390
H	6.911006	13.601337	0.433125
H	8.427288	12.705863	0.270987
H	8.378212	14.226369	1.180143
H	9.293654	13.377327	3.209535
H	9.647494	11.897520	2.313237
H	8.828434	11.816086	3.886104
H	9.802725	8.398228	0.930871
H	9.793902	6.636695	1.110017
H	9.514567	7.662869	2.517545
H	7.317477	6.410977	2.956453
H	7.700666	5.383292	1.571156
H	6.138332	6.194370	1.648835
H	6.600468	7.211625	-0.664348
H	8.164674	6.387485	-0.687254
H	8.079071	8.142628	-0.936738
H	7.507318	6.831983	5.170144
H	4.113555	8.814838	6.914700
H	5.914134	12.315426	6.294443
H	7.585838	12.004109	6.754558
H	6.502918	12.814261	7.885376
H	7.966978	10.344724	8.879088
H	6.565853	9.439422	9.459855
H	6.690774	11.180922	9.758698
H	4.583160	11.755522	8.823916
H	4.280067	10.018713	8.748671
H	3.965883	11.037998	7.333949
H	10.548733	10.319119	6.637378
H	9.099694	10.851128	7.473502
H	9.221582	11.025825	5.717846



H	10.363403	8.135761	7.756260
H	9.003313	7.047784	7.420631
H	8.779857	8.430446	8.493581
H	9.455475	8.957095	4.246183
H	9.441345	7.335003	4.959769
H	10.746294	8.449991	5.340733
H	4.525316	4.283077	4.735416
H	6.088714	5.067509	4.513161
H	4.628780	5.735189	3.744284
H	2.977601	6.823168	6.967989
H	2.709810	5.356637	6.020630
H	2.855947	6.921536	5.198415
H	5.057264	5.882238	8.055487
H	6.302354	5.098646	7.070536
H	4.696513	4.359438	7.217064
H	0.915752	5.430249	2.278084
H	0.244691	3.497426	0.927220
H	1.626612	2.760496	-1.006968
H	3.713098	4.008190	-1.556836
H	4.375842	5.961853	-0.215640
H	0.910832	8.477004	0.566680
H	-1.564064	8.573104	0.493374
H	-2.888605	8.090197	2.542683
H	-1.714773	7.511217	4.655501
H	0.752547	7.435626	4.724550
H	1.669137	11.673060	2.134399
H	0.985705	12.268387	3.653511
H	0.337217	10.797109	2.907640
H	1.573156	10.954751	6.402210
H	2.000799	9.236066	6.385897
H	0.510243	9.787610	5.608580
H	4.111627	11.754628	5.460518
H	4.211473	12.079633	3.728395
H	4.251056	7.179113	1.818575

Table S11. Frequencies of the stationary points optimized for 1,5-H shift of **10**, obtained with B3PW91+D3 method.

Species	Frequencies (cm ⁻¹)
10	15 24 27 32 40 42 47 51 54 55 15 24 62 69 77 79 80 85 89 91 101 62 115 117 119 128 131 133 136 140 157 115 164 168 172 176 180 186 191 194 198 198 203 205 209 213 221 240 242 244 246 251 256 257 260 263 264 265 272 275 276 284 284 302 304 304 310 314 315 316 317 321 328 332 349 351 354 357 367 374 380 383 386 388 391 395 404 407 412 419 424 425 429 434 436 464 466 471 474 477 504 531 535 548 555 555 560 564 575 595 596 622 625 634 637 647 649 670 673 675 682 685 690 702 705 713 720 720 765 770 778 786 801 805 811 826 828 831 834 846 848 852 855 856 861 865 871 874 919 925 927 930 936 937 937 942 942 942 945 947 949 950 955 956 960 961 964 964 970 971 973 976 979 990 997 1012 1015 1018 1020 1039 1041 1042 1043 1046 1047 1048 1049 1051 1054 1054 1056 1059 1064 1103 1108 1114 1137 1142 1181 1184 1189 1193 1199 1202 1204 1208 1215 1219 1220 1222 1228 1232 1234 1236 1237 1241 1244 1254 1255 1265 1267 1269 1271 1287 1288 1291 1303 1312 1317 1321 1333 1365 1368 1382 1383 1391 1392 1394 1396 1396 1397 1398 1399 1400 1403 1404 1405 1415 1418 1426 1428 1430 1431 1435 1438 1452 1455 1456 1464 1466 1468 1469 1475 1477 1478 1479 1480 1482 1484 1485 1485 1486 1487 1488 1490 1491 1492 1493 1495 1498 1502 1502 1503 1504 1505 1506 1507 1509 1510 1511 1512 1515 1516 1517 1521 1523 1525 1528 1528 1533 1533 1538 1538 1539 1543 1546 1630 1640 1661 1664 3039 3042 3047 3050 3050 3052 3053 3053 3053 3054 3056 3056 3057 3058 3059 3062 3064 3064 3065 3066 3070 3116 3118 3123 3124 3126 3126 3126 3127 3128 3128 3129 3130 3132 3134 3134 3137 3137 3137 3139 3140 3140 3141 3142 3144 3155 3161 3163 3164 3165 3167 3167 3169 3173 3173 3174 3174 3176 3180 3182 3183 3185 3191 3193 3193 3201 3204 3213 3215 3225 3230 3232 3252 3264 3272 3284 3285
TS11a	-1527 22 29 36 45 46 51 57 58 59 63 67 70 75 80 82 84 87 91 94 101 103 107 115 121 123 132 137 139 143 147 156 157 161 178 182 184 186 188 191 194 199 204 207 214 223 227 238 241 244 248 249 254 257 260 262 263 269 270 274 283 288 291 293 295 304 308 313 316 321 323 327 333 348 351 355 358 365 367 371 375 381 384 388 394 397 405 411 416 419 425 428 430 432 439 467 468 473 475 477 482 524 532 533 547 552 554 561 566 581 595 598 611 627 633 646 649 666 670 674 675 683 685 694 699 708 714 716 730 764 781 799 800 807 813 827 830 830 831 835 845 852 853 854 859 863 876 884 900 912 930 933 934 935 936 938 941 943 945 946 948 949 954 955 955 957 960 962 963 965 967 970 971 980 988 997 1011 1014 1016 1019 1041 1043 1045 1046 1046 1049 1049 1051 1052 1053 1053 1055 1059 1061 1102 1111 1131 1145 1145 1180 1184 1186 1198 1200 1201 1201 1206 1215 1219 1222 1227 1229 1233 1233 1235 1236 1243 1253 1254 1257 1262 1264 1268 1270 1284 1288 1296 1308 1310 1320 1340 1364 1376 1378 1378 1382 1390 1392 1397 1398 1398 1399 1400 1400 1401 1405 1406 1408 1411 1414 1428 1430 1431 1432 1434 1439 1441 1450 1455 1457 1461 1469 1474 1477 1477 1480 1481 1481 1483 1485 1486 1487 1488 1489 1491 1492 1493 1496 1496 1498 1500 1501 1502 1504 1505 1507 1508 1511 1511 1512 1514 1516 1516 1519 1522 1522 1525 1527 1529 1530 1532 1538 1538 1539 1542 1569 1627 1641 1659 1664 1823 3044 3049 3051 3051 3052 3052 3053 3054 3055 3056 3057 3058 3058 3061 3062 3063 3063 3064 3067 3070 3098 3123 3126 3126 3127 3127 3127 3128 3129 3131 3132 3132 3135 3136 3136 3137 3137 3139 3139 3141 3142 3142 3148 3150 3151 3152 3154 3158 3163 3164 3164 3169 3170 3174 3176 3179 3183 3183 3185 3187 3190 3192 3192 3199 3200 3210 3214 3215 3217 3231 3233 3236 3265 3268 3277 3282

INT11	21 25 32 44 47 51 53 57 58 62 67 72 74 75 79 81 87 91 97 101 103 105 117 124 126 136 139 147 151 153 157 161 171 175 177 179 184 187 188 195 196 201 209 212 230 230 239 240 243 250 254 256 258 262 267 269 271 274 278 279 288 299 300 305 307 313 317 328 328 336 341 346 347 355 359 361 367 369 375 379 389 390 394 396 398 407 411 414 417 418 429 429 435 440 443 462 468 468 473 474 498 531 537 541 552 553 561 564 579 594 596 597 621 629 633 639 647 650 669 670 673 679 689 697 701 710 716 719 743 764 781 786 796 801 807 810 826 827 830 832 846 847 849 851 855 855 856 876 897 907 924 930 931 933 934 935 936 942 943 944 945 946 946 949 955 956 957 961 962 963 967 968 971 977 990 997 1011 1012 1014 1017 1038 1041 1042 1045 1045 1047 1047 1048 1050 1051 1052 1055 1058 1062 1102 1108 1119 1138 1142 1181 1184 1191 1194 1196 1200 1203 1205 1215 1216 1216 1223 1225 1230 1232 1232 1235 1238 1244 1251 1255 1262 1264 1266 1267 1277 1289 1298 1305 1307 1320 1328 1338 1366 1376 1377 1377 1381 1389 1391 1395 1398 1398 1399 1400 1401 1402 1403 1407 1409 1410 1411 1428 1429 1430 1433 1439 1439 1447 1453 1458 1461 1469 1474 1477 1479 1480 1482 1482 1482 1485 1486 1487 1487 1489 1492 1493 1495 1497 1497 1498 1502 1503 1504 1504 1505 1506 1507 1512 1513 1513 1515 1515 1518 1521 1522 1522 1526 1528 1530 1531 1533 1536 1537 1542 1542 1591 1629 1641 1659 1664 3045 3049 3049 3050 3051 3051 3051 3053 3053 3055 3056 3056 3057 3058 3059 3061 3063 3065 3066 3067 3069 3118 3123 3124 3124 3125 3127 3127 3128 3129 3130 3131 3131 3132 3133 3134 3136 3140 3142 3143 3145 3145 3148 3151 3151 3153 3157 3164 3165 3166 3166 3167 3170 3171 3179 3179 3180 3181 3183 3185 3190 3191 3192 3200 3205 3206 3212 3213 3216 3221 3235 3251 3268 3270 3270 3275 3513
TS11b	-1894 18 23 31 37 42 48 55 56 62 63 67 69 74 75 78 82 87 90 95 99 101 107 113 121 127 130 130 139 147 148 153 154 159 173 180 181 185 188 192 196 198 205 208 212 227 234 236 240 246 248 252 256 260 263 265 268 269 275 278 283 288 289 294 300 306 311 317 322 325 335 341 344 345 351 354 359 364 364 377 378 385 386 395 397 402 404 407 416 421 423 429 431 434 439 444 462 464 468 472 475 491 500 531 542 552 553 562 564 564 594 595 620 625 629 632 647 648 663 666 670 671 694 696 704 710 713 720 741 756 771 785 797 800 804 812 828 829 831 834 843 851 852 855 860 866 874 878 892 925 931 932 934 934 934 939 939 942 943 945 948 949 953 955 956 959 960 965 965 967 969 979 980 980 995 1002 1012 1016 1017 1017 1039 1043 1044 1045 1046 1047 1047 1048 1050 1052 1053 1055 1058 1063 1106 1111 1132 1138 1144 1182 1186 1190 1193 1197 1200 1204 1206 1216 1217 1221 1225 1229 1230 1231 1231 1237 1243 1252 1255 1259 1261 1265 1269 1269 1286 1293 1306 1308 1314 1316 1325 1346 1365 1372 1377 1379 1380 1389 1391 1395 1395 1396 1397 1399 1402 1402 1404 1407 1408 1410 1414 1428 1430 1431 1433 1439 1440 1449 1454 1457 1458 1465 1472 1477 1478 1479 1482 1482 1483 1484 1485 1486 1489 1491 1491 1493 1495 1495 1498 1499 1502 1503 1503 1505 1506 1506 1509 1510 1510 1512 1512 1514 1516 1518 1519 1521 1524 1525 1531 1532 1535 1536 1539 1541 1542 1553 1630 1642 1660 1666 1835 3042 3048 3049 3049 3050 3051 3052 3053 3054 3055 3057 3058 3058 3059 3060 3061 3063 3065 3066 3068 3111 3118 3123 3125 3125 3126 3127 3128 3129 3129 3130 3130 3131 3132 3134 3135 3139 3139 3140 3141 3141 3149 3149 3152 3152 3155 3155 3156 3156 3157 3161 3162 3170 3171 3172 3178 3182 3187 3194 3194 3194 3195 3195 3206 3206 3208 3214 3216 3218 3233 3234 3241 3250 3271 3278 3286
11	19 24 29 38 40 42 46 52 55 56 66 68 69 72 73 77 80 83 85 93 96 102 118 119 123 131 139 146 151 157 158 165 168 173 178 184 186 193 194 197 198 202 207 214 219 224 233 242 247 251 252 257 260 262 263 265 268 276 277 280 282 283 288 293 301 307 311 312 314 316 327 331 340 343 345 353 356 360 369 370 374 379 384 388 393 394 401 405 415

418	424	430	435	436	454	463	465	472	475	480	514	526	539	545	553	553
557	561	564	595	597	617	623	630	647	648	659	662	668	675	678	692	692
695	708	710	719	722	757	764	774	787	801	806	810	827	828	828	829	837
841	850	851	852	855	863	865	872	876	909	923	929	931	935	935	936	937
940	940	943	944	948	949	953	954	957	958	960	964	965	968	970	970	981
990	1000	1010	1015	1018	1019	1041	1041	1043	1044	1045	1046	1047	1048			
1050	1050	1052	1053	1058	1062	1107	1109	1127	1134	1142	1182	1184	1184			
1189	1197	1200	1204	1207	1217	1218	1224	1225	1228	1231	1232	1233	1234			
1237	1242	1253	1253	1261	1264	1270	1270	1283	1288	1295	1309	1309	1332			
1342	1367	1369	1374	1380	1381	1389	1392	1394	1396	1396	1396	1396	1397	1399		
1400	1401	1403	1407	1408	1414	1417	1429	1429	1431	1433	1437	1439	1451			
1452	1456	1462	1470	1477	1478	1479	1480	1481	1482	1482	1484	1484	1486			
1488	1489	1491	1492	1493	1493	1495	1498	1501	1501	1502	1504	1506	1506			
1507	1510	1511	1511	1514	1514	1515	1520	1520	1523	1526	1528	1531	1532			
1536	1537	1539	1539	1541	1620	1638	1645	1666	1668	3043	3048	3050	3051			
3052	3052	3053	3053	3055	3056	3057	3059	3059	3060	3060	3061	3061	3065			
3067	3067	3103	3123	3124	3124	3126	3126	3128	3129	3129	3130	3131	3132			
3132	3133	3133	3137	3137	3138	3139	3140	3141	3142	3144	3145	3145	3146			
3147	3157	3161	3162	3163	3165	3166	3166	3166	3174	3176	3177	3179	3180			
3181	3190	3190	3192	3199	3200	3201	3204	3214	3215	3223	3227	3234	3251			
3262	3281	3283														

Table S12. The energies, enthalpies and free energies (in au at 323K) and corresponding relative values (in kcal/mol) for 1,5-H shift of **10**, obtained with B3PW91+D3 method, including PCM for solvent correction to the G value

species	E (gas)	H(gas)	G (gas)	G (sol)
10	-2456.08145618(0.0)	-2454.86066338(0.0)	-2455.01723438(0.0)	-2455.96118538(0.0)
TS11a	-2456.03516428(29.0)	-2454.81971218(25.7)	-2454.97578887(26.0)	-2455.91489348(29.0)
INT11	-2456.06006584(13.4)	-2454.84461374(10.1)	-2455.00069043(10.4)	-2455.93979504(13.4)
TS11b	-2456.03079511(31.8)	-2454.81534301(28.4)	-2454.97141970(28.7)	-2455.91052431(31.8)
11	-2456.08497843(-2.2)	-2454.86952633(-5.6)	-2455.02560303(-5.3)	-2455.96470763(-2.2)