Reaction mechanism for the formation of nitrogen oxides (NO_x) during coke oxidation in fluidized catalytic cracking units

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Supplementary Material

Table S1: The energies (in hartree), molecular geometries (in Å), vibrational frequencies (in cm⁻¹), moments of inertia (in amu) and spin multiplicity of the chemical species (CS) and the transition states (TS) before annihilation obtained using B3LYP/6-311++G(d,p).

Species	Energy (Ha)	Cartesian coordinate (Å)	Vibrational Frequencies (cm ⁻¹)	Moments of inertia (amu)	Multiplicity
CS1	-555.025613	C -5.0710 0.3195 -0.0181	92.1 120.8 231.0 245.8 268.9	821.945	2
		C -4.4289 -0.8700 0.1921	386.0 393.9 404.2 472.2 485.2	3868.906	
		C -3.0089 -0.9671 0.0776	506.0 549.5 583.8 587.0 632.4	4690.851	
		C -2.2590 0.2162 -0.2652	668.4 734.0 757.0 757.4 774.2		
		C -2.9688 1.4366 -0.4760	801.5 821.7 854.5 872.5 899.7		
		C -4.3311 1.4872 -0.3564	906.2 924.7 975.5 978.9 995.9		
		C -0.8633 0.1379 -0.3816	1028.3 1040.9 1116.8 1155.9		
		C -0.1977 -1.0628 -0.1711	1171.0 1186.1 1202.9 1264.8		
		C -0.9370 -2.2514 0.1718	1285.0 1288.8 1352.4 1365.9		
		C -2.3257 -2.1725 0.2874	1406.2 1423.4 1429.1 1485.3		
		C -0.2027 -3.4635 0.3782	1506.3 1558.6 1588.3 1638.1		
		C 1.1588 -3.4820 0.2515	1664.0 1723.1 3152.2 3157.0		
		C 1.7634 -2.2384 -0.0909	3160.4 3165.6 3177.7 3184.3		
		N 1.1833 -1.1393 -0.2864	3189.2 3204.6		
		H -6.1497 0.3797 0.0719			
		H -4.9915 -1.7612 0.4501			
		H -2.4050 2.3267 -0.7338			
		H -4.8564 2.4214 -0.5195			
		H -0.2819 1.0160 -0.6383			
		H -2.8897 -3.0638 0.5455			
CS2	-705.46208704	H -0.7468 -4.3673 0.6371			2
		H 1.7463 -4.3781 0.3998			
		C -2.5198 0.3116 -0.0304	55.3 103.6 107.9 170.0 199.7	927.271	
		C -1.9871 -0.9398 -0.1800	242.8 296.1 323.4 341.3 399.0		
		C -0.5782 -1.1505 -0.0946	413.4 478.0 489.6 512.5 542.7	6615.130	
		C 0.2788 -0.0162 0.1531	558.2 611.0 635.2 643.8 682.1		
		C -0.3192 1.272 0.3030	756.9 762.1 763.0 765.5 775.8	7542.401	
		C -1.6751 1.4309 0.2140	825.7 840.4 858.0 901.9 910.3	7542.40163	

		C 1.6636 -0.2050 0.2398 C 2.2290 -1.4717 0.0905 C 1.3752 -2.6067 -0.1570 C -0.0039 -2.4202 -0.2436 C 2.0059 -3.8801 -0.3019 C 3.3612 -3.9942 -0.2062 C 4.0827 -2.7924 0.04060 N 3.5905 -1.6083 0.1832 H -3.5917 0.4582 -0.0974 H -2.6304 -1.7932 -0.3663 H 0.3249 2.1244 0.4892 H -2.1158 2.4145 0.3297 H 2.3245 0.6336 0.4253 H -0.6463 -3.2754 -0.4301 H 1.3933 -4.7557 -0.4890 H 3.8856 -4.9321 -0.3079 O 5.4861 -2.8012 0.1566 O 6.0482 -3.9900 0.0188	923.2 976.1 979.0 993.5 999.0 1029.5 1087.2 1143.4 1160.8 1172.5 1185.2 1196.7 1223.0 1286.4 1294.2 1310.4 1365.2 1374.8 1410.7 1424.9 1445.3 1487.2 1507.1 1579.0 1591.6 1631.5 1643.8 1667.7 3158.5 3162.3 3167.6 3172.7 3179.4 3187.4 3190.7 3238.1	927.27151 6615.13014 7542.40163	
CS3	-705.459387	C -5.0544 0.4603 0.1189 C -4.4381 -0.6828 -0.3108 C -3.0359 -0.8738 -0.1222 C -2.2763 0.1640 0.5324 C -2.9602 1.3410 0.9651 C -4.3057 1.4846 0.7649 C -0.8999 -0.0067 0.7255 C -0.2490 -1.1629 0.2962 C -1.0061 -2.2020 -0.3582 C -2.3772 -2.033 -0.5513 C -0.2936 -3.3669 -0.7791 C 1.0471 -3.4612 -0.5562 C 1.6687 -2.3601 0.1010 N 1.1031 -1.2822 0.5092 H -6.1198 0.5932 -0.0301 H -5.0079 -1.4638 -0.8030 H -2.3893 2.1209 1.4570 H -4.8119 2.3833 1.09854 H -0.3116 0.7607 1.2148 H -2.9457 -2.8161 -1.0441 H -0.8305 -4.1687 - 1.2745 H 1.6373 -4.3182 -0.8526 O 3.0535 -2.5590 0.2819 O 3.7077 -1.58370 0.8843	53.1 82.4 117.1 155.5 192.8 244.1 263.6 340.4 363.9 398.9 412.3 471.0 476.9 487.5 542.7 571.0 625.0 644.6 646.0 646.2 756.3 760.4 762.3 773.6 786.6 816.6 851.1 856.4 897.9 909.5 923.3 977.8 986.4 986.4 998.2 1029.1 1097.5 1153.7 1157.1 1170.5 1175.7 1192.1 1218.6 1286.3 1292.8 1308.6 1363.7 1374.8 1410.7 1425.2 1448.0 1489.8 1508.1 1581.6 1596.1 1633.5 1640.1 1669.1 3158.0 3161.8 3167.3 3174.2 3179.1 3187.9 3190.4 3209.1	1112.901 6211.309 7324.211	2
CS4	-705.528534	C -4.9313 0.5321 0.0577 C -4.3449 -0.6530 -0.3151 C -2.9548 -0.8664 -0.1198 C -2.1672 0.1750 0.47393 C -2.8067 1.3874 0.8473	61.3 88.7 118.8 194.8 221.3 252.9 333.9 339.0 364.6 394.0 404.5 481.0 490.4 503.8 517.3 541.5 587.8 628.2 641.8 651.7 709.9 722.6 761.6 763.3 791.6	1187.37 8 5432.91 9	2

		C -4.1544 1.5609 0.6441 C -0.7835 -0.0290 0.6717 C -0.1930 -1.2187 0.2977 C -0.9617 -2.2691 -0.2958 C -2.3173 -2.0709 -0.4903 C -0.3000 -3.4946 -0.6700 C 1.0217 -3.6759 -0.4755 C 1.8762 -2.6572 0.1223 N 1.1943 -1.4133 0.5000 H -5.9933 0.6850 -0.0956 H -4.9384 -1.4422 -0.7643 H -2.2119 2.1752 1.2962 H -4.6306 2.4907 0.9333 H -0.1717 0.7437 1.1178 H -2.9068 -2.8634 -0.9401 H -0.8987 -4.2805 -1.1189 H 1.5273 -4.5918 -0.7530 O 3.0618 -2.7631 0.3203 O 1.8889 -0.4946 1.0237	829.6 834.7 862.7 904.6 908.8 915.3 976.5 985.2 996.0 999.5 1039.2 1100.3 1138.4 1170.2 1180.4 1198.0 1220.3 1255.8 1281.7 1291.0 1351.8 1391.91 1396.3 1406.51429.8 1468.9 1498.5 1536.8 1597.4 1623.5 1650.7 1658.4 1762.1 3162.7 3165.0 3168.2 3169.8 3180.9 3191.9 3206.4 3209.6	6620.29 8	
CS5	-705.487481	C -3.7907 0.6024 -0.1785 C -3.1617 -0.6209 -0.2724 C -1.7541 -0.7126 -0.1851 C -0.9839 0.4794 0.0023 C -1.6616 1.7254 0.0955 C -3.0331 1.7822 0.0067 C 0.4135 0.3742 0.0873 C 1.1022 -0.8571 -0.0036 C 0.3114 -2.0637 -0.1939 C -1.0625 -1.9461 -0.2758 C 0.8671 -3.3929 -0.3039 C 2.1443 -3.8054 -0.2616 C 3.3730 -3.0326 -0.0913 O 4.4572 -3.5486 -0.0746 N 2.4340 -0.6513 0.1113 O 3.4008 -1.6364 0.0654 H -4.8706 0.6642 -0.2464 H -3.7421 -1.5263 -0.4145 H -1.080 2.6297 0.2375 H -3.5411 2.7370 0.0789 H 1.0176 1.2621 0.2289 H -1.6486 -2.8488 -0.4177 H 0.1232 -4.1726 -0.4422 H 2.3568 -4.8625 -0.3646	24.2 32.7 101.6 148.96 192.5 234.9 285.7 315.2 342.7 374.2 409.5 428.0 474.0 479.4 514.4 537.0 624.9 631.8 650.4 674.0 708.8 738.7 748.5 758.8 793.7 805.7 832.5 841.9 854.9 884.0 913.1 920.9 971.7 995.3 995.7 1009.9 1039.4 1093.7 1153.6 1163.6 1175.4 1213.6 1231.6 1278.2 1296.5 1319.3 1332.5 1374.9 1409.1 1432.0 1451.8 1481.5 1513.7 1577.3 1602.2 1634.9 1680.9 1788.6 3147.41 3160.6 3164.8 3170.3 3181.9 3192.6 3193.4 3193.7	1001.608 6230.546 7232.154	2
CS6	-575.565429	C -4.9715 0.5418 0.2933 C -4.4843 -0.6594 -0.1792 C -3.1108 -0.9786 -0.0768 C -2.2272 -0.0267 0.5304 C -2.7571 1.1948 1.0045	91.7 107.8 204.9 219.1 245.0 334.9 354.8 391.4 413.3 485.4 522.59 553.1 584.7 626.4 647.2 682.8 712.2 742.3 766.3 778.4 780.6 814.5 834.8 869.8	942.084 3864.779 4806.864	2

		C -4.1026 1.4766 0.8897 C -0.8339 -0.3353 0.6414 C -0.3795 -1.5271 0.1674 C -1.2542 -2.4793 -0.4382 C -2.5896 -2.2213 -0.5623 C -0.4403 -3.6431 -0.8331 C 0.8526 -3.4483 -0.5049 C 1.0048 -2.1105 0.1485 H -6.0278 0.7693 0.2061 H -5.1561 -1.3773 -0.6381 H -2.0852 1.9125 1.4632 H -4.4942 2.4177 1.2581 H -0.1548 0.3770 1.0990 H -3.2669 -2.9352 -1.0204 H -0.8484 -4.5213 -1.3186 H 1.6831 -4.1203 -0.6668 O 2.0251 -1.6076 0.5707	907.2 907.8 938.3 974.1 977.6 996.9 1027.6 1047.8 1072.9 1134.1 1167. 1171.6 1178.0 1226.4 1249.0 1278.9 1340.3 1360.5 1370.3 1447.6 1469.7 1484.7 1547.5 1588.0 1639.1 1646.7 1668.3 1770.0 3159.6 3162.5 3165.5 3171.6 3177.6 3190.0 3193.3 3231.5		
CS7		C -4.8710 0.5734 0.0605 C -4.2474 -0.5862 -0.3781 C -2.8710 -0.7808 -0.1916 C -2.0984 0.2446 0.4649 C -2.771 1.4198 0.9112 C 4.1249 1.5781 0.7100 C -0.7276 0.06704 0.6437 C -0.0344 -1.116 0.1312 C -0.8795 -2.1998 -0.4274 C -2.2141 -1.9864 -0.6058 C -0.2281 -3.4461 -0.7365 C 1.0057 -3.7330 -0.2706 C 1.7072 -2.831 0.6458 N 1.2562 -1.4325 0.7726 H -5.9353 0.7069 -0.0936 H -4.8269 -1.3595 -0.8714 H -2.1956 2.1918 1.4090 H -4.6212 2.4792 1.051 H -0.1148 0.8229 1.1191 H -2.8197 -2.7724 -1.0477 H -0.7744 -4.1779 -1.3239 H 1.4876 -4.6836 -0.4618 O 2.6294 -3.1663 1.3488 O 1.1739 -0.8453 -0.5918	47.7 98.6 117.6 211.9 231.9 241.7 312.6 336.1 378.0 387.9 430.7 456.5 488.3 516.4 524.6 543.4 614.8 618.8 641.9 691.0 700.3 735.3 741.4 761.4 775.3 791.0 813.8 848.7 860.6 869.0 871.2 918.6 926.3 963.7 986.8 998.5 1040.0 1098.9 1136.8 1161.1 1173.7 1183.5 1210.7 1226.9 1259.0 1280.6 1311.9 1352.5 1409.1 1415.6 1432.0 1459.6 1505.1 1556.2 1603.0 1618.5 1636.8 1768.7 3155.1 3160.0 3164.3 3170.4 3182.3 3193.8 3198.6 3199.9	1132.214 5383.697 6178.449	2
CS8	-705.468517	C -4.8292 0.6914 -0.4295 C -4.1984 -0.4969 -0.7080 C -2.8974 -0.7599 -0.2033 C -2.2532 0.2313 0.6026 C -2.9321 1.4471 0.8736 C -4.1903 1.6713 0.3678 C -0.9628 -0.0453 1.1146	43.9 82.9 114.1 175.8 219.2 227.9 300.1 319.0 358.9378.0 416.9 433.0 485.1 503.5 509.6 539.3 599.1 630.8 633.4 684. 718.3 741.8 760.3 763.6 772.8 812.0 829.8 862.3 877.4 904.5 913.0 919.7 975.4 998.2	1129.118 5886.483 6710.608	2

		C -0.3286 -1.2240 0.8184 C -0.9376 -2.2244 0.0062 C -2.2143 -1.9685 -0.4675 C -0.2769 -3.4736 -0.3347 C 1.0452 -3.6989 -0.3390 C 2.1101 -2.7027 -0.0816 N 2.0648 -1.8007 1.0003 H -5.8216 0.8842 -0.8203 H -4.6864 -1.2484 -1.3193 H -2.4429 2.1972 1.4853 H -4.7008 2.6039 0.5790 H -0.4630 0.6665 1.7605 H -2.7047 -2.7224 -1.0748 H -0.9304 -4.2690 -0.6809 H 1.4318 -4.6495 -0.6892 O 3.1540 -2.7297 -0.7127 O 0.8681 -1.4128 1.5201	1006.8 1035.6 1040.3 1086.5 1155.4 1164.8 1178.2 1205.4 1247.9691 1268.1 1289.4 1297.1 1345.0 1388.2 1403.2 1425.1 1467.3 1492.0 1533.4 1599.2 1633.7 1655.6 1661.6 1688.1 3151.4 3163.4 3166.0 3169.7 3180.9 3182.9 3191.8 3193.0		
CS9	-705.364005	C -2.5544 0.2096 0.0057 C -2.0128 -1.0352 -0.2308 C -0.6342 -1.2809 -0.0233 C 0.1939 -0.2061 0.4390 C -0.3928 1.0597 0.6720 C -1.7388 1.2662 0.4607 C 1.5894 -0.4356 0.6510 C 2.0998 -1.6736 0.4118 C 1.2809 -2.7508 -0.0428 C -0.0562 -2.5658 -0.2613 C 2.1418 -3.9348 -0.1826 C 3.4063 -3.6364 0.1560 C 3.5169 -2.1823 0.5499 N 4.5887 -1.4093 -0.0871 H -3.6124 0.3801 -0.1584 H -2.6419 -1.8468 -0.5810 H 0.2369 1.8710 1.0215 H -2.1741 2.2419 0.6434 H 2.2176 0.3779 0.9979 H -0.6892 -3.3747 -0.6114 H 1.7903 -4.9048 -0.5110 H 4.2650 -4.2919 0.1561 O 4.1492 -1.9534 1.8699 O 5.1865 -1.2240 1.1298	67.8 88.6 105.6 186.7 188.4 236.2 309.0 314.3 340.4 407.0 413.3 462.1 484.5 535.0 557.0 571.1 590.0 627.9 714.7 751.1 759.7 773.2 777.7 789.4 807.8 860.7 869.8 891.1 905.1 909.6 924.6 971.3 975.6 980.5 996.3 1024.5 1046.7 1074.9 1086.6 1116.7 1144.3 1171.8 1178.0 1200.5 1242.9 1256.4 1280.2 1340.0 1364.6 1376.4 1445.9 1475.3 1484.8 1545.0 1606.1 1635.9 1649.7 1676.0 3160.2 3164.8 3167.0 3175.2 3177.9 3190.1 3199.3 3234.6	1328.381 5182.057 6278.749	2
CS10	-705.393837	C -2.6330 0.1525 -0.1512 C -2.0306 -1.0754 -0.3246 C -0.6568 -1.2586 -0.0409 C 0.1040 -0.1387 0.4316 C -0.5439 1.1075 0.5990 C -1.8848 1.2529 0.3142 C 1.4935 -0.3028 0.7225	40.8 70.5 101.6 130.9 155.3 219.5 239.1 298.9 315.0 358.0 400.7 416.2 478.2 484.6 555.5 564.4 602.5 626.9 666.3 689.0 704.6 742.4 764.7 776.5 783.7 789.8 817.6 853.8 867.2 906.5 912.0 932.3 972.4 974.4 997.7	1129.948 6289.858 7348.900	2

		C 2.0681 -1.5260 0.5439 C 1.3146 -2.6479 0.0730 C -0.0163 -2.5244 -0.2153 C 2.2303 -3.7902 0.0037 C 3.4752 -3.4283 0.3864 C 3.4600 -1.9979 0.7547 N 4.3544 -1.1991 1.2147 H -3.6870 0.2748 -0.3733 H -2.6083 -1.9209 -0.6831 H 0.0342 1.9528 0.9568 H -2.3672 2.2143 0.4473 H 2.0730 0.5413 1.0794 H -0.5976 -3.3671 -0.5751 H 1.9390 -4.7849 -0.3085 H 4.3459 -4.0612 0.4295 O 5.6688 -1.8096 1.3770 O 6.1298 -2.4292 0.3279	1036.1 1047.1 1098.6 1136.3 1147.4 1172.4 1178.7 1205.9 1246.5 1254.1 1280.5 1346.1 1368.0 1374.6 1444.3 1472.3 1486.1 1543.7 1579.2 1626.8 1637.3 1647.6 1678.0 3160.9 3165.7 3167.8 3178.3 3182.3 3190.8 3205.03263.1		
CS11	-705.332372	C -2.4653 0.4517 -0.4457 C -1.9678 -0.8260 -0.6197 C -0.6507 -1.1537 -0.2309 C 0.1717 -0.1328 0.3525 C -0.3660 1.1634 0.5170 C -1.6591 1.4530 0.1264 C 1.5067 -0.4437 0.7524 C 1.9864 -1.7188 0.5725 C 1.1610 -2.7522 -0.0155 C -0.1237 -2.4718 -0.4055 C 1.9552 -3.9612 -0.0626 C 3.2095 -3.6978 0.4673 C 3.2534 -2.3390 0.8613 N 4.2996 -1.6004 1.4476 H -3.4792 0.6844 -0.7504 H -2.5908 -1.5970 -1.0611 H 0.2561 1.9351 0.9582 H -2.0548 2.4531 0.2603 H 2.1270 0.3289 1.1932 H -0.7551 -3.2360 -0.8480 H 1.6201 -4.9137 -0.4496 H 4.0250 -4.3971 0.5697 O 5.5885 -2.0794 0.9818 O 5.1086 -2.4489 2.3036	15.6 87.4 107.1 121.2 188.1 257.6 279.1 301.1 312.6 396.3 414.4 448.0 476.4 515.5 557.1 573.3 585.7 625.8 666.2 710.3 718.3 759.3 761.1 770.6 771.1 786.1 815.5 840.1 864.5 904.4 913.3 915.6 922.1 970.5 993.1 1013.1 1048.6 1054.8 1089.0 1133.4 1164.5 1180.8 1208.9 1223.7 1250.3 1280.7 1295.0 1361.6 1367.1 1404.4 1411.2 1466.6 1476.7 1487.5 1548.8 1612.7 1625.9 1637.2 3160.3 3163.4 3165.9 3178.1 3180.1 3191.0 3213.9 3247.0	1225.626 5937.749 7042.623	2
CS12	-500.206831	C -2.4357 0.4698 -0.3812 C -1.9620 -0.8044 -0.6165 C -0.6484 -1.1760 -0.2463 C 0.1932 -0.1985 0.3841 C -0.3234 1.0991 0.6111 C -1.6094 1.4296 0.2379 C 1.5214 -0.5516 0.7658	101.7 149.2 257.6 269.8 320.4 391.3 405.3 424.7 474.1 557.4 571.8 579.6 625.3 689.4 721.1 743.8 747.9 758.6 773.1 808.0 856.2 869.0 869.8 896.4 906.7 916.0 967.1 990.4 1030.8 1045.8 1091.7 1154.8 1167.4	699.453 3233.169 3932.622	3

		C 1.9824 -1.8220 0.5268 C 1.1318 -2.8194 -0.1134 C -0.1473 -2.4914 -0.4848 C 1.8989 -4.0433 -0.2231 C 3.1733 -3.8294 0.3218 C 3.2149 -2.5081 0.7649 H -3.4455 0.7356 -0.6722 H -2.5987 -1.5427 -1.0931 H 0.3128 1.8378 1.0876 H -1.9876 2.4291 0.4200 H 2.1525 0.1914 1.2418 H -0.7937 -3.2218 -0.9625 H 1.5431 -4.9692 -0.6556 H 3.9690 -4.5572 0.3833	1179.7 1182.1 1228.0 1244.6 1278.4 1335.4 1355.4 1371.2 1386.0 1433.1 1469.4 1485.3 1541.1 1612.4 1625.9 1640.8 3155.1 3158.0 3162.0 3170.9 3175.6 3188.6 3202.1 3228.7		
CS13	-516.971662	C -7.8595 0.6787 0.0606 C -7.2432 -0.5181 0.4178 C -5.8313 -0.6221 0.4481 C -5.0542 0.5243 0.1051 C -5.6906 1.7474 -0.2600 C -7.1078 1.7987 -0.2745 C -3.6599 2.7866 -0.5716 C -2.9378 1.6447 -0.2308 C -3.6315 0.4662 0.1217 C -2.9989 -0.7498 0.4847 C -3.7602 -1.8645 0.8182 C -5.1520 -1.8137 0.8038 N -4.9898 2.8641 -0.5941 H -7.5773 2.7340 -0.5538 H -8.9421 0.7371 0.0437 H -7.8421 -1.3844 0.6770 H -5.7306 -2.6926 1.0667 H -3.2634 -2.7880 1.0939 H -3.1295 3.6956 -0.8436 H -1.8538 1.6633 -0.2370 H -1.9159 -0.8005 0.4992	156.9 163.7 209.2 286.6 426.5 448.7 476.6 479.5 493.0 493.4 498.6 583.4 631.5 646.8 670.3 759.1 762.3 795.4 806.3 832.9 846.3 852.9 880.6 904.1 976.9 980.0 984.5 1051.0 1055.8 1102.3 1122.5 1135.0 1173.0 1204.4 1227.0 1248.7 1260.2 1301.8 1349.0 1383.2 1411.6 1437.3 1448.9 1491.5 1530.1 1561.2 1568.6 1582.0 1591.6 3141.3 3162.4 3165.0 3173.0 3179.0 3179.9 3186.1 3198.1	1576.782 1629.440 3206.223	2
CS14	-667.298067	C 0.9709 -0.0461 -3.7094 C -0.3916 0.1666 -3.7183 C -1.1324 0.1411 -2.5101 C -0.4466 -0.1080 -1.2838 C 0.9617 -0.3228 -1.3187 C 1.6672 -0.2931 -2.5158 C 0.9260 -0.5995 1.1071 C -0.4164 -0.3962 1.1533 C -1.1655 -0.1401 -0.0476 C -2.5429 0.0751 -0.0574 C -3.2173 0.3201 -1.2637 C -2.5360 0.3537 -2.4628 N 1.5759 -0.5613 -0.0901	65.8 114.7 162.1 193.8 218.5 221.6 281.7 339.6 442.9 445.1 452.9 483.0 496.9 515.4 525.0 601.9 623.7 647.2 671.8 714.7 752.3 764.4 778.5 798.7 825.9 836.4 879.5 883.0 901.6 950.8 979.7 986.7 995.9 1057.9 1085.9 1110.0 1127.3 1174.7 1181.3 1203.1 1218.7 1246.1 1261.1 1337.5 1375.2 1396.1 1422.3 1426.5 1461.2 1491.3 1534.3 1593.3 1600.4 1615.8 1644.3 3165.0 3170.6 3175.3	1632.120 3276.117 4908.237	2

		O 2.9692 -0.7724 -0.1391 O 3.5168 -0.9954 1.0460 H 2.7348 -0.4579 -2.5254 H 1.5262 -0.0241 -4.6399 H -0.9116 0.3558 -4.6504 H -3.0660 0.5438 -3.3894 H -4.2887 0.4849 -1.2494 H 1.5672 -0.7977 1.9534 H -0.9190 -0.4295 2.1112 H -3.0919 0.0518 0.8772	3186.7 3188.2 3198.9 3224.2 3238.0		
CS15	-667.256142	C 0.9067 0.0807 -3.8438 C -0.4688 0.1576 -3.7628 C -1.1244 -0.0312 -2.5239 C -0.3459 -0.2840 -1.3587 C 1.0567 -0.3922 -1.4796 C 1.6742 -0.2155 -2.7070 C 1.2538 -0.5929 0.9705 C -0.2142 -0.6201 1.0655 C -0.9968 -0.4291 -0.0710 C -2.4081 -0.3712 -0.0205 C -3.1603 -0.1440 -1.1737 C -2.5423 0.0330 -2.4008 N 1.8569 -0.7675 -0.3587 O 2.7989 0.2923 -0.0040 O 1.8743 0.7430 1.0888 H 2.7510 -0.3097 -2.7765 H 1.4037 0.2286 -4.7956 H -1.0617 0.3610 -4.6476 H -3.1350 0.2215 -3.2891 H -4.2411 -0.0959 -1.1044 H 1.7480 -1.2535 1.6877 H -0.6659 -0.7524 2.0409 H -2.9022 -0.4899 0.9373	83.0 111.7 169.3 221.1 234.6 313.6 358.2 408.7 447.8 457.8 470.9 509.9 518.6 557.7 604.7 623.8 657.1 683.9 736.1 753.2 769.2 774.1 800.3 814.3 826.4 851.1 864.1 886.2 916.4 926.0 960.9 976.6 988.4 1047.6 1091.7 1103.5 1125.6 1159.4 1184.1 1202.7 1227.6 1246.4 1272.7 1292.8 1352.3 1370.4 1403.8 1411.0 1446.6 1466.8 1481.8 1526.3 1571.6 1595.8 1638.0 3055.6 3165.4 3168.4 3175.2 3183.3 3187.9 3190.2 3196.5	1782.181 2733.660 4296.474	2
CS16	-667.371259	C 0.8736 0.2067 -3.8396 C -0.4979 0.1958 -3.7061 C -1.0960 -0.0039 -2.4349 C -0.2636 -0.1791 -1.2885 C 1.1558 -0.1786 -1.4714 C 1.7099 0.0126 -2.7283 C 1.4715 -0.4836 0.9682 C 0.0173 -0.4865 1.1669 C -0.8639 -0.3737 -0.0154 C -2.2374 -0.4268 0.1054 C -3.0631 -0.2684 -1.0270 C -2.5047 -0.0521 -2.2645 N 1.9972 -0.4088 -0.3715 O 3.2648 -0.5120 -0.5044 O 0.8379 0.6806 1.4688	75.3 143.6 175.0 192.7 266.5 331.0 351.3 397.2 441.3 461.2 469.1 481.7 524.8 554.0 559.8 620.3 625.1 658.1 692.5 764.7 770.5 795.8 817.3 822.1 829.7 867.2 909.3 925.4 981.0 985.2 991.9 1044.2 1070.5 1089.7 1098.9 1141.8 1166.1 1190.9 1201.3 1238.7 1242.6 1269.8 1291.8 1335.0 1372.6 1386.0 1387.6 1425.5 1462.8 1477.5 1485.6 1539.4 1607.0 1620.7 1653.6 3135.9 3164.4 3169.3 3171.9 3178.5 3186.4 3189.2 3218.9	1930.830 2542.218 4316.694	2

		H 2.7864 0.0024 -2.8279 H 1.3222 0.3595 -4.8144 H -1.1370 0.3349 -4.5707 H -3.1377 0.0791 -3.1354 H -4.1402 -0.3087 -0.9142 H 2.1749 -0.9841 1.6236 H -0.3920 -0.9712 2.0489 H -2.6843 -0.5793 1.0820			
CS17	-537.41031	C 2.0108 -1.0346 -2.0939 C 0.9051 -1.7694 -2.4737 C -0.3992 -1.3617 -2.0761 C -0.4714 -0.1956 -1.2962 C 0.6591 0.5638 -0.9134 C 1.9067 0.1470 -1.3057 C 0.1503 1.7372 -0.1309 C -1.3280 1.5958 -0.0562 C -1.6812 0.3399 -0.7952 C -2.8602 -0.3092 -1.0649 C -2.8170 -1.4966 -1.8499 C -1.6359 -2.0126 -2.3453 O -0.7189 2.6004 -0.8991 H 2.8037 0.6936 -1.0362 H 2.9957 -1.3648 -2.4049 H 1.0306 -2.6671 -3.0700 H -1.6482 -2.9235 -2.9346 H -3.7478 -2.0102 -2.0641 H 0.7444 2.2358 0.6271 H -1.9269 1.9802 0.7621 H -3.8130 0.0604 -0.7019	157.8 171.6 178.7 312.1 389.8 427.4 440.5 467.5 511.8 545.2 561.6 627.7 649.1 669.1 690.8 765.6 786.2 813.1 813.4 820.6 854.9 855.9 914.3 924.8 971.0 978.9 987.0 1032.2 1053.0 1064.4 1070.5 1126.0 1179.1 1201.2 1229.3 1230.4 1245.3 1260.4 1294.5 1342.9 1394.8 1398.9 1447.0 1466.2 1496.4 1520.4 1636.0 1651.1 1661.1 3156.8 3160.1 3160.7 3165.5 3171.1 3171.6 3183.7 3184.3	1552.876 1661.121 3093.147	1
CS18	-667.3442	C -7.8577 0.8864 -0.0456 C -7.2385 -0.2218 0.6783 C -5.8622 -0.4368 0.6374 C -4.9844 0.5371 0.0085 C -5.5219 1.6877 -0.5880 C -6.9783 1.8884 -0.7086 C -3.3305 2.4867 -1.0511 C -2.7690 1.3711 -0.5111 C -3.5730 0.3473 0.0555 C -3.0368 -0.8063 0.6654 C -3.8813 -1.7492 1.2466 C -5.2583 -1.5694 1.2447 N -4.7051 2.6621 -1.0967 H -7.3086 2.9096 -0.8542 H -8.8517 1.1985 0.2599 H -7.8711 -0.8936 1.2470 H -5.9006 -2.3050 1.7158 H -3.4585 -2.6305 1.7152 H -2.7836 3.3075 -1.4905	95.3 121.1 161.6 205.0 298.5 311.4 377.8 391.9 430.4 440.2 477.3 518.0 533.4 543.5 576.9 599.2 634.0 675.1 709.2 733.8 739.9 760.1 778.1 801.1 821.1 829.4 846.9 884.2 951.5 976.6 977.3 994.7 1049.9 1065.0 1109.0 1139.8 1146.8 1189.5 1194.1 1212.5 1221.7 1266.21286.9 1322.1 1346.8 1379.1 1400.2 1414.5 1438.4 1461.3 1472.0 1538.7 1550.7 1581.1 1644.4 3140.8 3166.9 3176.2 3179.6 3181.4 3186.5 3190.1 3241.0	2022.864 2454.958 4330.024	2

		H -1.6893 1.2790 -0.5089 H -1.9617 -0.9438 0.6854 O -5.1760 3.7296 -1.6249 O -7.6775 0.9070 -1.4893			
CS19	-667.266658	C -7.7504 0.7619 -0.2552 C -7.1823 -0.3549 0.5097 C -5.8277 -0.5906 0.5158 C -4.9733 0.3998 -0.1000 C -5.3927 1.5460 -0.6918 C -6.8193 1.7841 -0.8951 C -4.1770 2.3632 -1.0370 C -3.0179 1.5055 -0.5828 C -3.5135 0.3540 -0.0072 C -2.9225 -0.7595 0.6342 C -3.7574 -1.7410 1.1950 C -5.1482 -1.6745 1.1667 N -4.0023 3.7234 -0.3229 H -7.1789 2.7976 -1.0449 H -8.7525 1.0858 0.0118 H -7.8549 -0.9657 1.1022 H -5.7323 -2.4537 1.6432 H -3.2943 -2.5860 1.6933 H -4.1157 2.6398 -2.0984 H -1.9857 1.8143 -0.6610 H -1.8456 -0.8496 0.7137 O -4.9155 4.0420 0.3793 O -7.5157 0.7996 -1.6775	44.8 98.8 133.8 163.4 192.9 244.2 289.4 345.6 372.9 437.1 465.2 481.4 493.0 545.5 561.6 566.5 633.8 672.9 684.8 708.0 718.5 727.8 760.8 773.0 802.7 814.8 844.5 863.0 887.6 969.4 979.1 983.1 1026.1 1058.1 1075.4 1099.7 1107.7 1135.5 1152.0 1180.3 1204.7 1214.7 1236.5 1273.4 1311.7 1354.0 1385.0 1399.6 1408.5 1447.5 1485.4 1541.6 1558.5 1642.6 1652.3 3010.5 3129.6 3142.6 3162.9 3171.5 3179.0 3188.8 3228.2	2153.753 2585.910 4185.982	2
CS20	-537.357709	C -7.6895 0.7218 -0.6145 C C -7.2092 -0.3056 0.2976 C C -5.8610 -0.5706 0.4132 C C -4.9455 0.3260 -0.2144 C C -5.2741 1.4774 -0.8974 C C -6.6556 1.7027 -1.2684 C C -4.0435 2.2453 -1.0785 C -2.9966 1.5462 -0.5424 C -3.5307 0.3233 0.0566 C -3.0236 -0.6569 0.8619 C -3.9146 -1.6373 1.4329 C -5.2680 -1.5921 1.2477 H -7.0015 2.6955 -1.5453 H -8.7075 1.0791 -0.4855 H -7.9302 -0.7977 0.9420 H -5.9095 -2.3269 1.7220 H -3.4890 -2.4138 2.0587 H -3.9740 3.1957 -1.5909 H -1.9575 1.8432 -0.5455 H -1.9693 -0.6956 1.1167 O -7.2964 0.6513 -1.9884	134.1 158.9 200.2 281.2 373.5 416.7 444.6 453.2 490.2 512.2 550.4 585.6 618.2 646.1 674.9 710.1 718.8 746.6 767.4 806.6 832.6 856.2 894.8 912.9 939.5 972.9 985.1 1005.4 1027.9 1068.5 1087.5 1104.6 1114.6 1185.7 1202.7 1215.7 1230.7 1269.1 1340.1 1360.2 1382.6 1413.1 1430.8 1464.0 1492.71533.9 1570.1 1615.0 1669.7 3124.1 3132.0 3160.5 3169.3 3171.0 3185.2 3202.9 3226.0	1284.859 1962.074 3114.656	1

CS21	-667.173329	C 0.9271 -0.0068 -3.3717	53.0 101.7 140.2 178.2 243.4	1693.897	2
		C -0.3536 -0.5990 -3.3727	258.4 311.3 335.6 402.7 428.8		
		C -1.1269 -0.6162 -2.1607	476.2 483.5 502.2 521.8 556.4	2877.757	
		C -0.4720 -0.2020 -1.0033	594.8 616.8 656.3 672.8 691.8		
		C 0.9969 0.0497 -0.9035	726.2 740.1 758.3 770.3 806.9	3722.373	
		C 1.5759 0.4075 -2.2256	827.5 841.8 857.3 868.0 903.7		
		C 1.0779 0.9129 0.3497	965.3 967.7 982.1 1005.6		
		C -0.1182 0.9279 0.9703	1043.0 1068.4 1096.7 1113.3		
		C -1.1271 0.2339 0.1470	1140.9 1162.3 1173.9 1190.7		
		C -2.5084 0.0701 0.2363	1234.7 1253.5 1302.3 1340.3		
		C -3.1832 -0.4887 -0.8650	1344.4 1391.0 1423.9 1466.7		
		C -2.5263 -0.8007 -2.0524	1483.0 1523.3 1581.9 1621.5		
		N 1.5814 -1.3060 -0.3331	1629.2 3161.3 3163.5 3175.2		
		O 2.9968 -1.3363 -0.5117	3183.9 3187.0 3196.3 3198.3		
		O 2.1102 -2.1323 -1.3562	3220.8		
		H 2.5549 0.8662 -2.2780			
		H 1.4210 0.1416 -4.3264			
		H -0.7996 -0.9215 -4.3064			
		H -3.0955 -1.1389 -2.9116			
		H -4.2569 -0.6284 -0.8065			
		H 2.0042 1.3249 0.7264			
		H -0.3250 1.4040 1.9204			
		H -3.0637 0.3873 1.1116			
CS22	-462.198558	C 0.7697 -0.0360 -3.5609	158.0 211.1 226.5 373.7 422.4	1192.779	2
		C -0.5900 -0.2882 -3.5614	458.3 470.1 517.9 560.5 577.8		
		C -1.3218 -0.2460 -2.3390	615.2 667.8 669.8 695.4 736.6	1477.071	
		C -0.5833 0.0573 -1.1956	764.0 784.4 817.0 836.7 878.9		
		C 0.8072 0.3181 -1.1753	917.9 930.2 935.6 974.0 982.8	2669.850	
		C 1.4913 0.2708 -2.3718	1026.5 1033.4 1055.1 1101.3		
		C 1.1475 0.5860 0.2322	1112.4 1175.6 1202.9 1222.8		
		C 0.0183 0.4865 0.9879	1245.2 1271.8 1330.6 1383.4		
		C -1.1162 0.1487 0.1120	1417.3 1445.5 1456.0 1486.8		
		C -2.4666 -0.0778 0.2769	1513.0 1534.5 1633.0 1648.6		
		C -3.2529 -0.3903 -0.8689	1657.3 3158.7 3159.2 3168.1		
		C -2.7144 -0.4753 -2.1397	3168.8 3182.1 3182.9 3202.0		
		H 2.5581 0.4601 -2.4306	3221.9		
		H 1.3122 -0.0720 -4.4992			
		H -1.0983 -0.5179 -4.4920			
		H -3.3522 -0.7164 -2.9837			
		H -4.3142 -0.5676 -0.7339			
		H -0.0432 0.6308 2.0580			
		H -2.9424 -0.0245 1.2505			
CS23	-555.012687	C -3.5890 -1.0529 -0.4915	91.4 114.1 234.4 239.5 267.7	806.918	2
		C -2.2225 -1.0984 -0.4868	394.1 408.6 422.7 472.1 480.8		
		C -1.4562 0.1062 -0.4871	517.9 524.2 576.5 612.9 628.0	3870.304	
		C -2.1436 1.3756 -0.4924	656.8 731.1 750.8 758.5 768.0		
		C -3.5726 1.3760 -0.4972	797.6 828.8 867.0 877.1 898.4	4677.223	
		C -4.2695 0.1996 -0.4968	918.5 928.6 968.9 978.3 998.9		

		C -0.0604 0.1230 -0.4824 C -0.1647 2.5506 -0.4885 C 0.6313 1.3349 -0.4829 C 2.0581 1.4257 -0.4783 H 2.6342 0.5064 -0.4742 C 2.6912 2.6374 -0.4790 C 1.9283 3.8534 -0.4845 C 0.5845 3.7494 -0.4888 H 0.4916 -0.8129 -0.4783 H -4.1648 -1.9713 -0.4913 H -1.6997 -2.0493 -0.4828 H -4.0713 2.3376 -0.5012 H -5.3537 0.2122 -0.5005 H 3.7742 2.6937 -0.4755 H 2.4338 4.8134 -0.4850 N -1.5027 2.5536 -0.4930	1023.6 1029.9 1123.6 1156.1 1175.2 1184.2 1189.9 1261.1 1286.5 1318.8 1329.4 1360.6 1392.2 1416.1 1445.3 1483.6 1496.0 1530.3 1572.8 1615.1 1647.5 1668.9 3150.9 3158.3 3159.7 3165.6 3170.6 3182.2 3185.3 3197.8		
CS24	-705.454048	C -3.9091 -0.2872 -0.6831 C -2.5438 -0.3421 -0.6358 C -1.7703 0.8574 -0.6658 C -2.4481 2.1283 -0.7468 C -3.8748 2.1397 -0.7942 C -4.5796 0.9678 -0.7631 C -0.3758 0.8707 -0.6206 C -0.4626 3.2898 -0.7351 C 0.3212 2.0802 -0.6536 C 1.7443 2.1589 -0.6105 H 2.3168 1.2398 -0.5493 C 2.3754 3.3742 -0.6458 C 1.6321 4.5785 -0.7257 C C 0.2643 4.5307 -0.7684 H 0.1731 -0.0643 -0.5594 H -4.4920 -1.2008 -0.6600 H -2.0284 -1.2950 -0.5748 H -4.3657 3.1034 -0.8548 H -5.6630 0.9867 -0.7996 H 3.4569 3.4292 -0.6129 H 2.1251 5.5402 -0.7538 N -1.7946 3.2999 -0.7794 O -0.5291 5.6669 -0.8467 O 0.1267 6.8163 -0.8775	65.3 90.1 113.6 155.2 198.1 259.5 292.9 299.9 353.6 403.0 413.2 481.0 493.4 500.5 537.1 567.6 594.6 607.2 631.5 677.4 743.8 748.1 770.2 783.7 799.2 819.5 866.0 871.2 911.6 928.0 932.5 977.9 980.6 1001.8 1008.6 1025.2 1083.4 1135.9 1151.6 1163.0 1191.2 1192.6 1214.3 1273.0 1292.8 1333.2 1345.0 1380.0 1414.4 1417.8 1461.7 1491.8 1510.1 1537.2 1579.3 1615.4 1648.8 1667.4 3157.8 3161.7 3168.8 3172.5 3186.9 3189.0 3199.6 3220.8	1531.358 4930.828 6462.186	2
CS25	-705.448239	C -3.9105 -0.3050 -0.6842 C -2.5459 -0.3543 -0.6189 C -1.7764 0.8479 -0.6479 C -2.4587 2.1161 -0.7441 C -3.8853 2.1212 -0.8130 C -4.5852 0.9470 -0.7830 C -0.3823 0.8662 -0.6013 C -0.4787 3.2857 -0.7072	74.5 79.7 92.1 153.6 195.5 235.5 272.3 308.6 366.2 406.2 438.6 476.4 480.9 500.5 540.9 543.9 584.2 625.2 648.2 660.4 721.5 748.0 770.0 782.8 796.4 820.8 869.4 879.0 912.4 928.7 932.1 979.3 981.9 1000.9 1023.0 1037.2 1071.9 1115.7	1661.896 4484.786 6067.127	2

		C 0.3105 2.0783 -0.6354 C 1.7353 2.1589 -0.6188 H 2.3080 1.2393 -0.5638 C 2.3664 3.3702 -0.6759 C 1.6097 4.5728 -0.7345 C 0.2473 4.5235 -0.7343 H 0.1699 -0.0672 -0.5435 H -4.4902 -1.2207 -0.6614 H -2.0279 -1.3048 -0.5449 H -4.3788 3.0827 -0.8846 H -5.6681 0.9609 -0.8332 H 3.4481 3.4281 -0.6672 H 2.1022 5.5370 -0.7711 N -1.8098 3.2886 -0.7702 O -0.4358 5.7421 -0.8508 O -1.2816 5.9642 0.1549	1151.4 1163.3 1188.7 1191.6 1218.7 1271.5 1294.5 1330.2 1344.3 1380.4 1412.2 1423.5 1458.8 1496.5 1507.3 1556.0 1585.9 1618.8 1654.0 1671.0 3157.1 3161.4 3167.6 3172.3 3186.5 3186.7 3198.9 3200.0		
CS26	-705.394664	C -3.9112 -0.1599 -0.6488 C -2.5433 -0.2290 -0.4497 C -1.7385 0.9350 -0.3964 C -2.4296 2.1892 -0.5231 C -3.8061 2.2569 -0.7217 C -4.5459 1.0806 -0.7964 C -0.3184 0.8739 -0.2641 C -0.2801 3.2432 -0.4855 C 0.4529 2.0594 -0.3910 C 1.8575 2.2316 -0.5419 H 2.5121 1.3715 -0.4654 C 2.3879 3.4804 -0.8352 C 1.5917 4.6369 -1.0246 C 0.2337 4.4680 -0.8399 H 0.1625 -0.0927 -0.1794 H -4.4941 -1.0725 -0.6941 H -2.0568 -1.1931 -0.3497 H -4.2852 3.2238 -0.8109 H -5.6159 1.1301 -0.9579 H 3.4601 3.5769 -0.9601 H 2.0245 5.5878 -1.3022 N -1.6480 3.3304 -0.3275 O -0.7966 5.3871 -0.9540 O -2.0309 4.5634 -1.0147	73.0 110.9 158.7 211.3 234.4 237.7 295.6 354.8 393.0 416.3 456.8 482.8 516.2 539.8 559.8 564.2 606.4 640.3 667.0 698.1 716.8 720.1 742.4 758.6 772.8 789.7 831.9 841.6 856.5 859.3 928.2 937.8 956.1 973.2 974.7 1048.1 1053.0 1070.2 1139.9 1175.4 1183.5 1189.8 1237.7 1247.5 1271.6 1296.5 1322.3 1345.2 1391.9 1411.1 1462.3 1484.2 1499.6 1507.7 1575.8 1598.0 1610.2 1657.3 3165.1 3173.8 3178.2 3188.2 3189.3 3190.2 3200.8 3216.6	1480.795 4054.216 5486.118	
CS27	-705.453092	C -3.8050 0.0073 -0.3113 C -2.5320 -0.1587 0.2196 C -1.5574 0.8151 -0.0493 C -1.8925 1.9561 -0.8447 C -3.1769 2.1191 -1.3580 C -4.1242 1.1291 -1.0952 C -0.1702 0.8905 0.3074 C -0.7034 2.8170 -0.8817	61.0 82.1 87.7 127.7 171.3 185.0 220.5 246.4 276.9 321.2 383.0 411.3 444.5 489.7 525.2 537.9 553.8 560.0 583.7 635.0 646.4 693.3 704.5 757.7 761.6 800.1 804.5 843.6 873.0 874.5 889.9 970.6 981.3 983.8 999.0 1029.9 1058.1 1077.5 1117.6	1784.498 3722.196 4512.394	2

		C 0.3809 2.0480 -0.2521 C 1.7024 2.5080 -0.3305 H 2.5041 1.9740 0.1662 C 1.9884 3.6399 -1.1254 C 1.0159 4.3156 -1.8342 C -0.3900 3.9233 -1.7995 H 0.3697 0.1473 0.8795 H -4.5668 -0.7403 -0.1206 H -2.2939 -1.0277 0.8231 H -3.4180 2.9882 -1.9571 H -5.1246 1.2258 -1.5013 H 3.0172 3.9785 -1.1932 H 1.2631 5.1702 -2.4530 N -1.3246 3.7713 0.6766 O -1.2796 4.5460 -2.3889 O -1.7002 4.8353 0.4893	1152.8 1166.8 1179.0 1207.2 1254.2 1305.5 1334.9 1354.0 1368.3 1394.4 1416.9 1465.2 1466.5 1503.5 1563.8 1592.5 1614.7 1631.2 1841.8 3160.8 3164.8 3175.9 3183.2 3187.2 3193.1 3203.2 3206.0		
CS28	-575.51751	C -3.6860 -0.1763 -0.2888 C -2.3557 -0.4670 -0.1955 C -1.4042 0.5743 -0.4333 C -1.8693 1.9290 -0.7714 C -3.2585 2.1840 -0.8570 C -4.1306 1.1493 -0.6194 C -0.0257 0.5781 -0.4109 C -0.7431 2.7501 -0.9526 C 0.4148 1.9308 -0.7332 C 1.6818 2.4378 -0.8351 H 2.5524 1.8121 -0.6678 C 1.8604 3.8295 -1.1712 C 0.7900 4.6346 -1.3857 C -0.6184 4.1468 -1.2908 H 0.6246 -0.2592 -0.1958 H -4.4280 -0.9463 -0.1135 H -2.0160 -1.4662 0.0539 H -3.6070 3.1782 -1.1053 H -5.1985 1.3305 -0.6816 H 2.8682 4.2226 -1.2497 H 0.9090 5.6822 -1.6389 O -1.5568 4.9252 -1.4966	83.0 115.9 176.3 179.7 258.7 295.2 392.7 418.4 431.0 478.0 519.3 523.7 541.7 568.8 622.1 635.2 676.7 698.5 747.5 761.7 780.1 806.8 851.7 872.8 873.8 941.2 977.1 983.0 994.4 996.6 1004.0 1023.2 1058.8 1126.1 1163.8 1170.3 1183.6 1215.2 1256.1 1287.4 1361.4 1376.9 1395.6 1412.1 1443.5 1474.3 1548.3 1565.0 1570.9 1632.6 1657.5 1666.2 3163.3 3164.5 3172.1 3176.5 3189.2 3191.5 3207.0 3213.6	1167.807 3175.982 4343.789	1
CS29	-705.323614	C -3.8804 -0.1613 -0.6122 C -2.5128 -0.2342 -0.6346 C -1.7159 0.9467 -0.6374 C -2.3950 2.2056 -0.6127 C -3.8076 2.2694 -0.6033 C -4.5281 1.1001 -0.6010 C -0.3151 0.9220 -0.6920 C -0.2711 3.3649 -0.6251 C 0.4239 2.1040 -0.6933 C 1.8486 2.1535 -0.7673	76.4 82.2 109.4 148.1 226.5 240.7 258.0 280.0 383.2 400.1 418.3 433.9 473.9 488.2 514.7 540.9 566.6 585.6 641.2 657.0 706.3 726.7 730.3 743.7 768.2 836.5 858.7 860.9 882.7 886.2 905.2 956.6 978.0 979.6 981.4 999.5 1038.4 1045.2 1128.0 1167.5 1180.4 1197.6 1224.9 1268.4 1292.1 1316.9 1336.6	1673.879 3994.460 5652.860	2

		H 2.3962 1.2204 -0.8326 C 2.5034 3.3565 -0.7519 C 1.7834 4.5855 -0.6314 C 0.4205 4.5798 -0.5628 H 0.1974 -0.0328 -0.7449 H -4.4742 -1.0674 -0.6090 H -2.0090 -1.1940 -0.6510 H -4.2947 3.2336 -0.5982 H -5.6108 1.1437 -0.5942 H 3.5869 3.3806 -0.8093 H 2.3386 5.5168 -0.5733 N -1.6338 3.3405 -0.6040 O -1.5430 5.6085 -0.9675 O -2.3254 4.5366 -0.5253	1369.3 1403.7 1414.4 1442.4 1470.0 1502.2 1527.2 1585.6 1598.5 1626.0 1656.7 3148.2 3163.3 3169.6 3173.1 3183.2 3183.8 3195.8 3230.4		
CS30	-705.225321	C -3.7977 0.4162 -1.0211 C -2.7498 0.1483 -0.2069 C -1.6277 1.0543 -0.2064 C -1.8397 2.4754 -0.7224 C -2.8315 2.5192 -1.8558 C -3.7808 1.5696 -1.9188 C -0.3132 0.8470 0.0450 C -0.4259 2.9829 -0.8974 C 0.4689 2.0102 -0.3783 C 1.8393 2.2500 -0.3625 H 2.5249 1.5106 0.0360 C 2.3293 3.4606 -0.8697 C 1.4604 4.4289 -1.3871 C 0.1062 4.1414 -1.3683 H 0.1159 -0.0655 0.4410 H -4.6356 -0.2688 -1.0784 H -2.7042 -0.7702 0.3678 H -2.8129 3.3674 -2.5292 H -4.5530 1.6323 -2.6785 H 3.3969 3.6528 -0.8672 H 1.8447 5.3604 -1.7869 N -2.6040 3.1997 0.4116 O -2.3849 4.6003 0.3400 O -1.7199 3.7899 1.3558	71.0 83.8 104.2 128.3 196.1 210.8 244.8 307.8 353.1 403.4 413.7 440.3 477.3 522.8 532.0 554.0 567.4 610.0 632.0 656.6 708.5 726.6 733.0 758.1 769.5 793.1 847.8 855.5 866.8 880.7 899.7 910.6 967.1 970.0 977.4 997.4 1013.6 1067.0 1087.9 1137.0 1160.3 1172.8 1175.6 1182.1 1203.4 1241.2 1260.3 1328.5 1353.5 1392.1 1435.5 1445.9 1464.0 1563.1 1579.2 1617.2 1637.1 1674.9 3161.6 3161.8 3169.8 3175.8 3184.8 3187.9 3193.5 3193.9	1789.998 3670.116 4283.670	2
CS31	-500.219205	C -3.8247 0.1467 -0.9126 C -2.5019 -0.2888 -0.9845 C -1.4710 0.6533 -0.8729 C -1.7854 2.0363 -0.6883 C -3.1027 2.4570 -0.6184 C -4.1234 1.5016 -0.7320 C -0.0468 0.5077 -0.9081 C -0.5151 2.7623 -0.6077 C 0.5481 1.7951 -0.7464 C 1.8889 2.2108 -0.7074	101.8 138.1 217.0 274.0 299.5 421.7 427.0 442.9 495.6 502.6 538.3 559.2 624.1 651.9 689.4 710.0 746.6 749.8 769.6 785.4 849.9 873.5 878.1 880.4 951.9 953.0 981.9 999.2 1036.3 1059.7 1102.5 1108.9 1155.8 1170.0 1178.5 1215.5 1254.7 1270.8 1318.7 1349.4 1369.0 1422.7 1453.8 1481.7 1496.4	761.528 3093.493 3855.022	1

		H 2.6881 1.4851 -0.8115 C 2.1891 3.5606 -0.5342 C 1.1629 4.5163 -0.3974 C -0.1426 4.0651 -0.4415 H 0.4908 -0.4228 -1.0361 H -4.6322 -0.5716 -0.9975 H -2.2762 -1.3404 -1.1247 H -3.3447 3.5046 -0.4786 H -5.1590 1.8179 -0.6789 H 3.2230 3.8866 -0.5034 H 1.4027 5.5650 -0.2629	1544.8 1600.5 1601.8 1617.5 3161.0 3162.5 3170.2 3172.3 3179.8 3183.7 3189.8 3204.7		
CS33	-897.223856	C -3.5990 0.1614 0.9919 C -3.0030 -0.9574 0.4499 C -1.6203 -0.9523 0.1553 C -0.8571 0.2152 0.4287 C -1.5013 1.3446 1.0013 C -2.8605 1.3234 1.2747 C 0.6600 2.5882 0.9370 C 1.2869 1.4489 0.3649 C 0.5379 0.2563 0.1188 C 2.6663 1.5138 0.0281 C 3.3777 2.7131 0.2609 C 2.7344 3.8046 0.8046 C 1.3727 3.7584 1.1498 C 1.1670 -0.8667 -0.4528 C 0.3873 -2.0357 -0.7042 C -0.9465 -2.0770 -0.4162 C 2.5569 -0.7876 -0.7687 C 3.2745 0.3513 -0.5414 N -0.6818 2.4376 1.3043 H -4.6608 0.1559 1.2105 H -3.5864 -1.8468 0.2412 H -3.3505 2.1868 1.7017 H 0.8763 -2.9009 -1.1398 H -1.5223 -2.9732 -0.6204 H 4.4294 2.7644 0.0036 H 3.2817 4.7245 0.9759 H 0.8918 4.6268 1.5768 H 3.0396 -1.6564 -1.2040 H 4.3285 0.3925 -0.7938 O -1.3428 3.6079 1.7520 O -1.7891 4.3461 0.7541	-22.4 26.5 64.2 99.2 180.3 208.8 213.5 255.7 284.4 298.7 303.7 356.3 399.5 439.1 448.7 452.5 480.5 520.0 530.3 534.5 545.0 568.7 604.7 617.2 643.6 660.9 682.1 695.5 748.6 761.0 763.5 767.0 785.2 796.5 823.7 842.7 846.2 850.0 878.7 883.0 953.3 963.9 972.2 974.8 978.1 984.8 1050.4 1058.4022 1088.4 1125.2 1142.8 1173.0 1174.1 1202.1 1205.5 1227.3 1238.5 1254.9 1274.2 1314.1 1325.6 1378.9 1383.7 1401.1 1416.5 1436.7 1449.0 1458.2 1481.1 1523.0 1523.4 1551.5 1610.2 1634.1 1636.8 1642.9 1662.4 3158.2 3160.4 3169.0 3169.1 3177.0 3178.3 3185.5 3185.7 3216.7 3217.1	4034.763 4762.112 8654.417	2
CS34	-897.193354	C -3.4772 0.4588 0.9578 C -2.9521 -0.6782 0.4382 C -1.5285 -0.9196 0.3124 C -0.6636 0.1225 0.7411 C -1.1804 1.1987 1.4331 C -2.6188 1.4946 1.6082	69.2 96.6 121.3 186.7 212.2 255.0 263.4 279.5 286.3 350.9 390.9 395.9 406.2 451.1 466.9 478.8 500.6 512.9 537.6 548.0 558.1 571.6 607.8 617.3 644.5 665.9 688.3 697.9 713.0 749.9	3630.103 4864.237 8331.320	2

		C 0.8020 2.5348 1.0579 C 1.4254 1.3768 0.5041 C 0.7019 0.1578 0.3413 C 2.7578 1.4701 0.0185 C 3.4256 2.7107 0.0954 C 2.7844 3.8224 0.6128 C 1.4716 3.7469 1.1036 C 1.2626 -0.9525 -0.3206 C 0.4200 -2.0658 -0.5998 C -0.9409 -2.0264 -0.3271 C 2.6313 -0.8580 -0.7314 C 3.3424 0.2965 -0.5651 N -0.4742 2.3576 1.6208 H -4.5504 0.6006 0.9974 H -3.6278 -1.4391 0.0592 H -2.9064 1.6681 2.6547 H 0.8438 -2.9329 -1.0941 H -1.5710 -2.8518 -0.6427 H 4.4431 2.7890 -0.2713 H 3.3034 4.7732 0.6509 H 0.9818 4.6186 1.5177 H 3.0949 -1.7163 -1.2063 H 4.3722 0.3514 -0.9019 O -1.4410 3.4396 1.5875 O -2.6458 2.8381 0.9692	759.9 765.4 787.5 793.1 814.3 837.8 845.1 875.1 892.9 898.8 945.1 951.7 974.1 976.8 982.7 984.9 1009.6 1068.9 1094.5 1119.0 1154.3 1167.3 1192.8 1196.2 1214.4 1231.0 1243.2 1261.5 1293.5 1302.7 1344.7 1360.3 1384.8 1390.5 1403.6 1418.6 1427.3 1448.2 1457.7 1512.3 1530.6 1550.8 1566.4 1601.5 1627.8 1630.7 1651.2 2978.3 3156.2 3158.9 3159.9 3168.1 3176.6 3178.9 3184.3 3188.5 3203.9		
CS35	-897.277358	C -3.5938 0.6125 1.0368 C -2.9740 -0.6269 0.5695 C -1.6474 -0.6623 0.1794 C -0.7883 0.4880 0.3729 C -1.2961 1.6703 0.9382 C -2.7342 1.8148 1.2349 C 0.8954 2.6753 0.9167 C 1.4267 1.5080 0.3202 C 0.5923 0.3943 0.0494 C 2.8175 1.4594 0.0076 C 3.6162 2.5821 0.2964 C 3.0632 3.7147 0.8800 C 1.7052 3.7741 1.1969 C 1.1370 -0.7867 -0.5117 C 0.2682 -1.9004 -0.7217 C -1.0523 -1.8445 -0.3817 C 2.5237 -0.8158 -0.8246 C 3.3329 0.2625 -0.5800 N -0.4869 2.7318 1.2244 H -4.5065 0.5343 1.6200 H -3.5770 -1.5265 0.5222 H -2.9997 2.5729 1.9610 H 0.6801 -2.8078 -1.1505	69.4 83.3 132.7 150.2 197.7 234.9 273.4 289.7 324.6 369.7 381.6 387.8 424.9 436.7 446.6 481.5 487.2 511.7 538.2 545.8 572.5 583.7 612.5 629.4 660.1 687.4 696.8 711.3 722.7 740.1 747.0 773.9 781.4 803.8 813.9 823.5 849.7 863.0 923.0 928.2 945.5 969.4 979.5 992.7 1003.8 1031.1 1055.6 1083.3 1099.6 1144.0 1159.3 1161.5 1185.7 1194.3 1236.1 1242.0 1251.7 1263.6 1268.6 1293.7 1345.6 1365.8 1373.0 1389.8 1397.4 1420.2 1442.0 1445.8 1458.4 1474.4 1506.4 1522.8 1550.4 1583.8 1600.8 1619.7 1649.7 3138.5 3161.4 3163.3 3168.8 3177.4 3179.8 3181.1 3183.4 3186.2 3227.8	3424.142 5377.518 8645.244	2

		H -1.6899 -2.7079 -0.5370 H 4.6741 2.5529 0.0595 H 3.6932 4.5699 1.0955 H 1.2580 4.6471 1.6503 H 2.9394 -1.7175 -1.2616 H 4.3885 0.2189 -0.8252 O -0.9551 3.7968 1.7572 O -3.6141 1.7260 0.1041			
CS36	-767.281227	C -3.4236 0.9527 0.6974 C -2.9616 -0.4159 0.4589 C -1.7156 -0.6430 -0.0726 C -0.8493 0.4872 -0.1795 C -1.0606 1.7881 0.2481 C -2.4212 2.1508 0.6020 C 0.2681 2.4569 0.2813 C 1.2016 1.4739 -0.1604 C 0.5342 0.2828 -0.4242 C 2.5883 1.5627 -0.1814 C 3.1062 2.8342 0.1984 C 2.2292 3.8373 0.5882 C 0.8127 3.6721 0.6546 C 1.1539 -0.9236 -0.6394 C 0.2496 -2.0696 -0.6493 C -1.0829 -1.9319 -0.3670 C 2.5879 -0.8552 -0.7135 C 3.2696 0.3363 -0.5077 H -4.2817 1.0773 1.3530 H -3.5922 -1.2315 0.7970 H -2.6239 3.0323 1.2049 H 0.6459 -3.0606 -0.8454 H -1.7088 -2.8182 -0.3498 H 4.1747 3.0215 0.2054 H 2.6396 4.7968 0.8836 H 0.2058 4.4956 1.0154 H 3.1594 -1.7565 -0.9103 H 4.3535 0.3324 -0.5623 O -3.4192 1.8881 -0.3864	70.5 105.9 156.1 216.1 244.5 252.7 280.8 326.4 407.9 418.3 436.3 453.0 481.4 489.3 528.9 540.8 559.5 577.7 595.4 613.5 641.7 655.0 660.5 670.8 726.7 748.8 762.7 774.5 788.5 804.8 825.1 842.7 854.8 884.9 921.0 926.9 962.4 966.0 978.9 983.6 984.2 1033.3 1047.8 1076.7 1100.7 1147.2 1150.3 1163.672 1195.1 1206.2 1216.4 1228.6 1244.6 1268.4 1297.9 1353.6 1379.5 1397.9 1403.0 1419.8 1430.4 1450.6 1459.1 1489.4 1508.1 1537.5 1582.7 1600.5 1625.9 1655.1 1699.0 3121.7 3130.1 3156.9 3157.6 3159.7 3169.5 3170.0 3174.0 3175.4 3182.7	2726.319 4422.286 6994.254	1
CS37	-897.070777	1 C1 -3.8463 -0.0564 0.2373 C 2 C2 -3.0777 -1.1840 0.0399 C 3 C3 -1.6645 -1.1189 - 0.0132 C 4 C4 -1.0009 0.1402 0.1878 C 5 C5 -1.8586 1.2272 0.3382 C 6 C6 -3.2176 1.2022 0.3879	40.4 63.2 73.3 116.6 132.9 161.9 176.0 207.4 250.4 269.5 325.6 343.5 382.3 427.2 439.7 449.8 469.8 502.5 521.3 528.7 537.2 555.2 577.7 599.7 632.8 666.7 695.7 707.9 741.5 749.0 752.3 759.6 768.7 786.0 808.8 825.5 834.4 845.0 852.4 890.7 919.7 930.0 967.6 971.4 975.7 980.2 985.1 1045.7 1069.9 1100.9 1129.6 1138.2 1171.6	3702.928 5512.960 8471.680	2

		C	1177.9 1187.1 1190.6 1217.5		
		7 C7 0.7814 2.5643 1.1724	1225.0 1245.3 1252.9 1281.1		
		C	1340.6 1357.5 1375.8 1392.7		
		8 C8 1.2134 1.4328 0.4133	1407.7 1435.7 1449.5 1459.4		
		C	1500.0 1520.5 1537.9 1575.5		
		9 C9 0.4449 0.2302 0.1234	1628.8 1641.7 1643.3 1664.1		
		C	3156.5 3158.7 3163.3 3166.8		
		10 C10 2.5762 1.4919 -	3169.1 3176.9 3180.3 3182.3		
		0.0318 C	3188.9 3207.3		
		11 C11 3.3392 2.6731			
		0.1108 C			
		12 C12 2.8281 3.7782			
		0.7470 C			
		13 C13 1.5510 3.7018			
		1.3183 C			
		14 C14 1.1416 -0.9191 -			
		0.3221 C			
		15 C15 0.4590 -2.1627 -			
		0.4974 C			
		16 C16 -0.8843 -2.2718 -			
		0.3174 C			
		17 C17 2.5275 -0.8465 -			
		0.6534 C			
		18 C18 3.2002 0.3295 -			
		0.5763 C			
		19 N19 -0.5199 2.5853			
		1.8096 N			
		20 H20 -4.9284 -0.1275			
		0.2675 H			
		21 H21 -3.5535 -2.1491 -			
		0.0971 H			
		22 H22 -3.8028 2.1040			
		0.5325 H			
		23 H23 1.0452 -3.0272 -			
		0.7901 H			
		24 H24 -1.3857 -3.2251 -			
		0.4480 H			
		25 H25 4.3526 2.6801 -			
		0.2754 H			
		26 H26 3.4154 4.6820			
		0.8546 H			
		27 H27 1.1670 4.5263			
		1.9039 H			
		28 H28 3.0204 -1.7435 -			
		1.0121 H			
		29 H29 4.2372 0.3987 -			
		0.8856 H			
		30 O30 -0.4482 3.2270			

		3.0864 O 31 O31 -0.5194 1.7742 2.9970 O			
CS38	-897.096184	C -3.4874 0.4741 -0.0183 C -2.9964 -0.8155 -0.1843 C -1.6042 -1.0587 -0.0731 C -0.8393 0.0642 0.2377 C -1.3006 1.3879 0.3669 C -2.6584 1.5977 0.2544 C -0.0555 2.2680 0.6763 C 1.0710 1.2865 0.4498 C 0.5675 0.0089 0.2928 C 2.3848 1.5706 0.1091 C 2.6665 2.9438 -0.1803 C 1.5883 3.8577 -0.2898 C 0.2743 3.5616 0.0103 C 1.3155 -1.1155 -0.0505 C 0.5316 -2.2979 -0.3061 C -0.8493 -2.2712 -0.3060 C 2.7136 -0.8652 -0.2107 C 3.2166 0.4269 -0.1546 N -0.1810 2.3955 2.2321 H -4.5543 0.6399 -0.1187 H -3.6817 -1.6233 -0.4186 H -3.1053 2.5809 0.3483 H 1.0360 -3.2300 -0.5395 H -1.3883 -3.1861 -0.5296 H 3.6685 3.2618 -0.4443 H 1.8114 4.8539 -0.6583 H -0.4973 4.3096 -0.1184 H 3.3873 -1.6812 -0.4509 H 4.2664 0.5885 -0.3767 O 0.5210 3.5228 2.7316 O -0.9294 3.5612 2.5650	48.7 78.7 86.0 134.8 157.5 207.3 240.7 256.1 277.7 304.6 325.5 388.6 414.7 436.7 457.2 462.9 471.2 508.9 526.6 541.6 558.3 575.0 593.7 630.4 643.9 665.2 673.9 698.3 712.7 749.4 760.4 770.1 773.2 781.4 822.2 830.4 843.5 848.4 857.1 879.2 927.9 936.0 967.2 969.6 974.1 976.1 986.5 1041.8 1046.5 1055.4 1115.2 1141.4 1158.7 1169.2 1179.5 1190.7 1206.4 1226.8 1239.9 1252.3 1267.2 1315.5 1347.2 1380.1 1395.3 1421.0 1433.2 1447.3 1467.0 1476.1 1501.4 1520.6 1530.1 1616.6 1630.6 1653.5 1661.1 3157.8 3159.1 3159.7 3162.3 3174.6 3175.3 3175.9 3183.7 3186.8 3198.1	3817.120 4805.035 7527.365	2
CS39	-692.117298	C -3.4860 0.4663 0.0878 C -3.0182 -0.8390 -0.0127 C -1.6190 -1.0747 -0.0987 C -0.8426 0.0771 -0.0715 C -1.2730 1.4282 0.0297 C -2.6398 1.6142 0.1112 C -0.0138 2.2539 0.0129 C 1.0517 1.3193 -0.0967 C 0.5504 0.0172 -0.1469 C 2.4168 1.5718 -0.1524 C 2.7597 2.9499 -0.0896 C 1.7509 3.9005 0.0179 C 0.3616 3.5825 0.0710 C 1.3025 -1.1320 -0.2528	68.5 118.8 183.6 244.1 275.9 294.0 294.2 424.4 433.9 443.4 444.4 460.7 511.9 548.1 562.3 576.7 578.3 601.6 639.9 648.7 670.1 674.8 750.6 759.5 771.5 775.2 782.5 800.3 829.3 841.5 876.9 922.2 926.1 945.6 965.8 970.7 978.1 980.3 981.8 1040.0 1040.8 1069.7 1147.2 1156.3 1158.9 1185.4 1209.4 1215.0 1233.6 1250.8 1261.2 1305.6 1349.0 1395.3 1400.5 1423.6 1435.4 1449.7 1454.0 1481.9 1492.2 1512.0 1537.0	2418.356 3842.427 6260.783	1

		C 0.5131 -2.3415 -0.2828 C -0.8694 -2.3079 -0.2095 C 2.7256 -0.8906 -0.3121 C 3.2470 0.3914 -0.2641 H -4.5567 0.6266 0.1526 H -3.7251 -1.6620 -0.0242 H -3.0898 2.5978 0.1920 H 1.0065 -3.3046 -0.3645 H -1.4118 -3.2477 -0.2364 H 3.7958 3.2699 -0.1244 H 2.0317 4.9470 0.0645 H -0.3596 4.3882 0.1553 H 3.4107 -1.7281 -0.3962 H 4.3243 0.5138 -0.3124	1623.7 1624.1 1650.1 1675.0 1698.8 3155.3 3155.7 3158.8 3159.1 3169.7 3170.5 3172.4 3173.3 3181.9 3182.6		
CS40	-594.34853	C -5.2729 0.4962 0.0187 C -4.5952 -0.6923 0.0058 C -3.1648 -0.7509 0.0094 C -2.4286 0.4961 0.0305 C -3.2153 1.6609 0.0368 C -4.5614 1.7421 0.0366 C -1.0156 0.4992 0.0331 C -0.3130 -0.7313 0.0292 C -1.0567 -1.9661 -0.0143 C -2.4565 -1.9533 -0.0212 C -0.3273 -3.1946 -0.0452 C 1.0400 -3.2149 -0.0213 C 1.7711 -1.9985 0.0458 C 1.1116 -0.7982 0.0725 N -0.3469 1.7115 0.0915 H -6.3577 0.5096 0.0158 H -5.1434 -1.6281 -0.0077 H -5.0967 2.6847 0.0505 H -2.9984 -2.8926 -0.0525 H -0.8887 -4.1222 -0.0854 H 1.5720 -4.1594 -0.0442 H 2.8540 -2.0239 0.0858 H 1.6929 0.1129 0.1530 H 0.5705 1.7545 -0.3230 H -0.9125 2.5253 -0.1030	79.1 114.8 154.3 231.3 235.7 294.6 303.4 339.3 396.5 418.4 429.9 473.8 501.6 525.5 545.9 554.4 565.2 619.4 632.6 652.0 705.0 713.8 740.2 756.1 792.3 830.7 851.6 858.9 872.8 874.6 913.6 961.4 968.5 988.1 1024.4 1038.8 1106.0 1122.3 1146.6 1175.6 1186.5 1205.2 1211.9 1267.7 1302.8 1347.8 1368.6 1387.4 1394.6 1441.4 1456.1 1476.4 1498.5 1542.8 1582.5 1609.1 1646.9 1654.1 1659.1 3157.3 3158.5 3163.8 3167.3 3170.7 3178.1 3181.3 3189.5 3568.0 3674.1	1235.262 3997.218 5230.613	2
CS41	-744.787475	C -5.2565 0.5226 0.0713 C -4.5498 -0.6530 0.0388 C -3.1240 -0.6681 0.0349 C -2.3912 0.5792 0.0614 C -3.1984 1.7733 0.1023 C -4.5776 1.7530 0.1051 C -0.9698 0.5446 0.0601 C -0.2925 -0.7178 0.0075 C -1.0489 -1.9372 0.0055	51.4 74.3 113.5 122.2 191.1 208.0 281.3 291.9 300.1 307.8 349.4 394.8 409.5 433.8 482.3 484.0 507.1 539.9 557.1 579.7 599.6 615.8 636.5 648.2 710.9 726.5 745.3 779.7 793.9 803.2 838.9 861.0 869.5 911.4 916.0 960.6 980.0 981.2 990.9 1022.5 1045.7 1086.9 1128.4	1803.003 5287.756 7089.072	2

		C -2.4459 -1.8874 0.0178 C -0.3536 -3.1831 -0.0186 C 1.0135 -3.2343 -0.0545 C 1.7632 -2.0320 -0.0797 C 1.1265 -0.8159 -0.0519 N -0.2166 1.6914 0.0714 H -6.3400 0.5129 0.0717 H -5.0687 -1.6047 0.0157 H -5.1042 2.6960 0.1330 H -3.0150 -2.8100 0.0114 H -0.9386 -4.0966 -0.0117 H 1.5259 -4.1893 -0.0739 H 2.8451 -2.0731 -0.1306 H 1.7390 0.0758 -0.1026 H 0.7474 1.6323 0.3474 H -0.6707 2.5767 0.2214 O -2.5254 2.9748 0.1346 O -3.2539 4.0964 0.2190	1143.0 1167.7 1183.2 1192.5 1209.8 1229.6 1272.9 1307.7 1365.0 1381.2 1393.2 1405.6 1441.1 1458.9 1475.1 1516.5 1529.4 1580.2 1599.3 1625.9 1653.8 1664.0 3162.1 3169.5 3170.9 3174.5 3182.2 3189.0 3192.8 3227.2 3603.6 3721.4		
CS42	-744.782125	C -5.2111 0.5634 0.1803 C -4.5228 -0.6200 0.0407 C -3.1065 -0.6205 0.0050 C -2.3730 0.6044 0.0949 C -3.1293 1.7990 0.2462 C -4.5230 1.7759 0.2900 C -0.9014 0.5810 0.0037 C -0.2353 -0.7489 0.0123 C -1.0126 -1.9394 -0.0783 C -2.4202 -1.8513 -0.1070 C -0.3574 -3.1979 -0.1223 C 1.0158 -3.2845 -0.0539 C 1.7815 -2.1122 0.0654 C 1.1593 -0.8733 0.0961 N -0.2609 1.7028 -0.1056 H -6.2947 0.5677 0.2116 H -5.0490 -1.5644 -0.0355 H -5.0609 2.7028 0.4090 H -3.0026 -2.7630 -0.1845 H -0.9610 -4.0958 -0.2029 H 1.5048 -4.2515 -0.0837 H 2.8611 -2.1743 0.1376 H 1.7791 0.0100 0.1999 H 0.7430 1.5475 -0.1871 O -2.4326 2.9669 0.3563 O -3.3512 4.0726 0.6299 H -2.7288 4.7936 0.4596	25.8 68.8 113.6 120.9 156.6 182.3 203.9 275.7 292.8 298.9 333.1 369.6 383.6 427.4 476.5 494.4 514.9 555.2 591.7 602.3 606.6 647.8 655.8 701.4 708.1 747.7 767.7 788.7 808.1 817.9 829.9 869.6 874.9 884.9 887.6 910.2 961.7 976.3 989.4 1051.0 1067.6 1102.7 1133.3 1167.2 1174.0 1193.6 1198.7 1223.4 1253.0 1269.4 1293.0 1318.6 1350.6 1374.8 1407.2 1424.5 1456.8 1468.3 1492.8 1521.0 1543.0 1577.3 1582.8 1609.5 1631.2 3161.3 3166.2 3168.1 3171.4 3178.6 3186.8 3191.0 3246.3 3483.2 3790.9	1767.152 5435.016 7178.252	2
CS43	-668.998193	C -5.1826 0.6675 -0.0029 C -4.6599 -0.6094 0.0005 C -3.2414 -0.8049 0.0057	84.6 121.3 221.1 225.6 228.7 257.0 309.2 380.3 419.8 432.0 496.4 500.3 528.8 553.4 589.9	1477.322 4148.171	1

		C -2.4924 0.3915 0.0036 C -3.0401 1.6813 0.0109 C -4.3972 1.8653 0.0019 C -1.1172 0.4858 -0.0028 C -0.3317 -0.6774 -0.0064 C -1.0676 -1.9317 0.0159 C -2.4796 -1.9812 0.0157 C -0.2928 -3.1325 0.0305 C 1.0764 -3.1067 0.0179 C 1.7803 -1.8726 -0.0170 C 1.0903 -0.6891 -0.0290 N -0.7700 1.8545 -0.0908 H -6.2613 0.7829 -0.0076 H -5.3246 -1.4653 -0.0046 H -4.8611 2.8418 0.0051 H -2.9654 -2.9508 0.0237 H -0.8184 -4.0814 0.0502 H 1.6339 -4.0366 0.0285 H 2.8638 -1.8727 -0.0405 H 1.6256 0.2535 -0.0714 H -0.2008 2.2083 0.6754 O -2.0245 2.6033 0.0175	608.4 614.1 638.0 679.5 707.9 733.9 750.8 752.1 766.5 789.2 836.3 841.2 854.6 872.7 875.7 932.6 966.1 967.9 989.5 990.0 1033.9 1039.2 1079.3 1110.8 1165.3 1175.5 1192.6 1203.0 1242.8 1279.9 1306.9 1353.9 1366.4 1383.0 1393.0 1417.8 1459.3 1479.4 1485.3 1510.2 1566.3 1604.4 1641.3 1662.8 1670.4 3158.9 3164.0 3164.7 3170.1 3177.0 3184.2 3189.5 3211.9 3489.7	5621.124	
CS44	-668.883635	C -5.0315 0.6981 -0.0248 C -4.4493 -0.5398 -0.0338 C -3.0281 -0.6791 -0.0119 C -2.2195 0.5256 0.0202 C -2.8892 1.7896 0.0281 C -4.2517 1.8871 0.0065 C -0.8542 0.3491 0.0407 C -0.1698 -0.8487 0.0340 C -0.9904 -2.0467 0.0018 C -2.3849 -1.9223 -0.0200 C -0.3274 -3.3120 -0.0063 C 1.0378 -3.3929 0.0156 C 1.8365 -2.2135 0.0472 C 1.2527 -0.9770 0.0561 N -2.6323 4.0959 0.0673 H -6.1114 0.7887 -0.0418 H -5.0592 -1.4362 -0.0579 H -4.7210 2.8601 0.0134 H -2.9907 -2.8224 -0.0440 H -0.9318 -4.2129 -0.0303 H 1.5232 -4.3623 0.0090 H 2.9166 -2.3035 0.0641 H 1.8533 -0.0755 0.0801 H -1.8042 4.7035 0.0906 O -2.0306 2.8749 0.0592	62.3 88.2 104.3 145.8 200.4 246.7 280.6 286.8 341.2 390.3 405.3 480.5 481.9 492.6 512.4 538.8 566.0 599.0 620.4 633.0 663.8 738.4 739.2 755.2 760.4 797.1 797.7 854.5 869.2 886.9 911.5 925.0 974.1 978.3 993.9 996.8 1025.9 1075.9 1124.4 1150.9 1172.1 1192.1 1197.3 1217.9 1257.7 1285.1 1318.3 1357.6 1374.6 1390.5 1407.8 1457.0 1483.0 1497.2 1514.8 1558.0 1566.9 1618.0 1657.9 1665.3 3158.3 3163.1 3166.9 3170.4 3182.3 3184.9 3192.8 3226.7 3391.5	1518.632 5088.885 6607.517	3
CS45	-668.921513	C -5.1092 0.6701 -0.0152	57.7 90.3 102.7 154.9 204.1	1515.685	1

		C -4.4906 -0.5497 -0.0005 C -3.0656 -0.6525 -0.0013 C -2.2742 0.5548 -0.0180 C -2.9901 1.7891 -0.0327 C -4.3499 1.8719 -0.0317 C -0.8796 0.4704 -0.0190 C -0.2292 -0.7686 -0.0041 C -1.0125 -1.9793 0.0125 C -2.4078 -1.8864 0.0135 C -0.3319 -3.2357 0.0276 C 1.0342 -3.2934 0.0263 C 1.8082 -2.0974 0.0098 C 1.1957 -0.8749 -0.0050 N -2.6886 4.1231 -0.0628 H -6.1908 0.7354 -0.0144 H -5.0761 -1.4623 0.0121 H -4.8315 2.8408 -0.0434 H -2.9989 -2.7968 0.0260 H -0.9218 -4.1461 0.0402 H 1.5383 -4.2531 0.0378 H 2.8902 -2.1639 0.0090 H 1.7839 0.0364 -0.0175 H -0.2901 1.3787 -0.0315 O -2.1635 2.9475 -0.0487	251.2 288.8 289.6 342.3 392.9 404.8 480.6 481.0 499.8 537.7 566.0 591.9 602.4 635.5 665.6 729.2 741.0 758.9 771.4 791.0 801.6 855.0 859.1 894.4 912.1 915.9 925.5 976.4 976.9 979.8 996.0 1028.2 1074.0 1127.3 1164.4 1172.5 1185.5 1194.5 1220.4 1269.3 1289.4 1297.3 1336.6 1374.8 1403.6 1416.6 1428.2 1467.7 1484.5 1510.2 1570.7 1589.7 1620.1 1666.0 1671.2 3158.9 3161.1 3165.4 3169.5 3177.6 3187.3 3189.0 3193.1 3206.6	5007.861 6523.546	
CS46	-538.971356	C -5.1160 0.6747 -0.0152 C -4.4943 -0.5435 -0.0006 C -3.0678 -0.6576 -0.0013 C -2.2706 0.5564 -0.0180 C -3.0049 1.7587 -0.0322 C -4.3465 1.8872 -0.0319 C -0.8755 0.4698 -0.0190 C -0.2243 -0.7682 -0.0041 C -1.0099 -1.9786 0.0125 C -2.4066 -1.8890 0.0135 C -0.3289 -3.2348 0.0275 C 1.0373 -3.2946 0.0262 C 1.8127 -2.0996 0.0098 C 1.2006 -0.8769 -0.0049 H -6.1988 0.7389 -0.0144 H -5.0831 -1.4544 0.0119 H -4.8429 2.8513 -0.0434 H -2.9940 -2.8024 0.0260 H -0.9195 -4.1449 0.0401 H 1.5400 -4.2552 0.0378 H 2.8947 -2.1670 0.0090 H 1.7900 0.0339 -0.0174 H -0.2910 1.3832 -0.0315	89.4 121.1 233.0 234.9 263.0 389.8 394.5 399.9 472.0 485.5 511.3 525.0 571.4 616.1 637.2 654.2 721.5 752.7 761.4 767.2 777.4 821.1 849.9 869.0 899.5 899.9 905.3 924.7 968.7 975.7 993.4 1022.7 1029.9 1110.8 1161.8 1172.8 1176.4 1192.8 1241.4 1284.7 1291.1 1322.1 1359.1 1378.5 1398.1 1422.6 1445.1 1478.9 1499.0 1544.5 1583.4 1618.2 1656.6 1665.6 3153.1 3158.0 3158.5 3163.2 3168.5 3173.6 3176.2 3181.1 3187.8	811.060 3984.755 4795.815	2
CS47	-668.913137	C -5.4215 0.3934 0.0485	58.2 103.8 121.0 170.6 191.6	1768.062	3

		C -4.6937 -0.7698 0.0108 C -3.2676 -0.7554 0.0162 C -2.5934 0.5190 0.0623 C -3.4043 1.6575 0.0988 C -4.7627 1.6566 0.0942 C -1.1718 0.5542 0.0683 C -0.3992 -0.6499 0.0296 C -1.1024 -1.9045 -0.0161 C -2.5058 -1.9314 -0.0218 C -0.3476 -3.1139 -0.0551 C 1.0219 -3.1011 -0.0499 C 1.7140 -1.8668 -0.0049 C 1.0222 -0.6801 0.0336 N -0.5448 1.7723 0.1122 H -6.5059 0.3584 0.0436 H -5.1986 -1.7290 -0.0239 H -5.3381 2.5755 0.1239 H -3.0128 -2.8901 -0.0566 H -0.8878 -4.0539 -0.0893 H 1.5789 -4.0303 -0.0799 H 2.7977 -1.8572 -0.0007 H 1.5983 0.2376 0.0673 H 0.4733 1.7930 0.1161 O -1.1299 2.9064 0.1492	239.3 241.2 297.1 380.4 403.5 414.5 428.1 475.0 497.1 531.8 542.7 563.4 599.1 606.2 649.6 668.8 713.5 729.7 741.6 757.2 768.9 835.4 864.8 865.7 880.6 889.4 952.7 963.1 973.1 988.5 1041.8 1048.0 1082.1 1120.2 1173.1 1184.8 1204.6 1205.2 1226.7 1289.7 1324.2 1343.3 1363.1 1378.6 1388.3 1411.7 1446.1 1469.5 1495.2 1508.0 1528.5 1577.6 1598.6 1636.7 1650.5 3156.4 3159.8 3162.8 3166.7 3168.7 3179.6 3180.4 3192.1 3467.6	4089.533 5857.595	
CS48	-668.9838	C -5.4668 0.3155 -0.0052 C -4.7058 -0.8179 -0.0361 C -3.2797 -0.7385 0.0049 C -2.6363 0.5460 0.0795 C -3.4701 1.7043 0.1095 C -4.8348 1.5868 0.0684 C -1.2103 0.6148 0.1201 C -0.4120 -0.5709 0.0880 C -1.0915 -1.8419 0.0130 C -2.4899 -1.8870 -0.0259 C -0.3384 -3.0519 -0.0214 C 1.0290 -3.0290 0.0158 C 1.7012 -1.7856 0.0895 C 1.0134 -0.5952 0.1247 N -0.7434 1.9492 0.1922 H -6.5483 0.2533 -0.0364 H -5.1681 -1.7976 -0.0922 H -5.4469 2.4815 0.0924 H -2.9767 -2.8563 -0.0823 H -0.8761 -3.9923 -0.0779 H 1.5967 -3.9519 -0.0106 H 2.7851 -1.7688 0.1190 H 1.5500 0.3363 0.1808 O 0.4662 2.1491 0.2330	54.2 99.5 107.8 171.2 238.5 240.3 263.3 296.7 371.2 399.1 405.3 437.5 477.2 503.8 531.3 540.4 605.8 607.5 655.1 679.1 719.7 754.2 755.5 776.3 795.6 868.3 875.4 882.5 889.1 931.2 960.9 983.0 987.2 1012.8 1019.1 1035.3 1039.6 1051.3 1128.0 1174.4 1177.0 1190.0 1207.2 1248.4 1257.4 1306.5 1331.9 1364.3 1392.4 1412.8 1420.1 1466.2 1478.0 1506.6 1531.8 1562.0 1593.5 1609.5 1650.8 1662.4 3155.7 3163.2 3164.3 3172.8 3173.2 3188.9 3189.1 3229.3 3265.2	1801.317 4060.289 5861.606	1

		H	-3.0019	2.6757	0.1653			
CS49	-538.971077	C	-5.4543	0.3542	-0.0033	87.5 117.0 231.5 232.5 260.0	812.772	2
		C	-4.7254	-0.8026	-0.0361	382.7 390.5 397.4 472.2 500.4		
		C	-3.2976	-0.7761	0.0028	501.0 536.0 578.8 612.6 636.2	4014.808	
		C	-2.6427	0.5191	0.0783	656.9 741.4 744.4 758.2 766.4		
		C	-3.4415	1.7035	0.1103	770.7 828.2 847.7 861.0893.5	4827.581	
		C	-4.8056	1.6209	0.0706	904.9 931.5 971.7 973.9 992.4		
		C	-1.2643	0.4922	0.1135	993.0 1023.4 1026.7 1122.9		
		C	-0.4428	-0.6151	0.0854	1164.4 1166.3 1187.7 1196.3		
		C	-1.1176	-1.9000	0.0099	1233.6 1266.7 1290.7 1321.9		
		C	-2.5166	-1.9377	-0.0287	1360.5 1371.8 1388.1 1411.1		
		C	-0.3108	-3.0786	-0.0218	1471.9 1481.0 1506.8 1561.1		
		C	1.0541	-3.0012	0.0177	1568.6 1617.5 1655.4 1661.7		
		C	1.7093	-1.7380	0.0917	3156.4 3157.8 3161.4 3169.2		
		C	0.9851	-0.5787	0.1247	3169.4 3181.2 3181.4 3191.5		
		H	-6.5372	0.3137	-0.0337	3191.9		
		H	-5.2234	-1.7652	-0.0924			
		H	-5.4047	2.5240	0.0953			
		H	-3.0132	-2.9013	-0.0851			
		H	-0.8058	-4.0427	-0.0781			
		H	1.6494	-3.9070	-0.0073			
		H	2.7923	-1.7020	0.1218			
		H	1.4769	0.3852	0.1809			
		H	-2.9418	2.6633	0.1666			
CS50	-594.396773	C	-13.6494	-0.4958	0.0064	42.3 106.3 135.1 233.4 242.5	1215.887	2
		C	-12.9097	-1.7137	-0.0005	300.6 357.5 378.0 408.0 427.7		
		C	-11.4976	-1.6798	-0.0033	447.7 506.2 531.8 541.5 587.9	4050.084	
		C	-10.7768	-0.4636	0.0007	630.0 645.6 659.5 705.8 710.2		
		C	-11.4709	0.7852	0.0076	742.4 765.6 799.1 813.0 826.5	5265.972	
		C	-12.9524	0.8065	0.0107	869.2 870.4 880.5 888.7 917.9		
		C	-10.7129	1.9665	0.0114	960.0 980.9 989.2 1006.2		
		C	-9.3274	1.9417	0.0085	1047.5 1055.1 1114.7 1126.0		
		C	-8.6439	0.7134	0.0016	1165.0 1170.4 1191.2 1194.7		
		C	-9.3570	-0.4652	-0.0022	1221.3 1262.0 1264.8 1297.2		
		C	-15.0513	-0.5509	0.0091	1346.4 1355.4 1369.2 1419.9		
		C	-15.7162	-1.7664	0.0051	1465.3 1471.8 1494.5 1530.3		
		C	-14.9915	-2.9729	-0.0017	1538.2 1576.4 1579.7 1620.3		
		C	-13.6141	-2.9470	-0.0045	1636.5 3160.0 3161.0 3165.0		
		N	-13.6847	1.8770	0.0168	3167.3 3172.4 3178.5 3185.7		
		H	-10.9473	-2.6150	-0.0086	3191.0 3207.1 3493.5		
		H	-11.2101	2.9298	0.0167			
		H	-8.7715	2.8720	0.0116			
		H	-7.5600	0.6957	-0.0007			
		H	-8.8392	-1.4185	-0.0075			
		H	-15.5969	0.3837	0.0144			
		H	-16.8001	-1.7884	0.0073			
		H	-15.5178	-3.9208	-0.0048			
		H	-13.0468	-3.8717	-0.0097			

		H -13.1189 2.7239 0.0193			
CS51	-744.738552	C -13.7138 -0.5536 0.1597 C -12.9495 -1.7636 -0.0013 C -11.5570 -1.6867 -0.0787 C -10.8768 -0.4661 -0.0275 C -11.6270 0.7588 0.0939 C -13.0367 0.6868 0.2157 C -10.9028 1.9888 0.0878 C -9.5361 2.0054 -0.0021 C -8.7972 0.7952 -0.0964 C -9.4526 -0.4042 -0.1132 C -15.1332 -0.6559 0.2679 C -15.7524 -1.8747 0.2033 C -14.9995 -3.0697 0.0288 C -13.6375 -3.0143 -0.0665 N -13.8289 1.8381 0.4141 H -10.9838 -2.6026 -0.1853 H -11.4350 2.9315 0.1297 H -9.0100 2.9532 -0.0108 H -7.7161 0.8308 -0.1637 H -8.9000 -1.3341 -0.1960 H -15.7055 0.2513 0.4053 H -16.8316 -1.9350 0.2881 H -15.5129 -4.0230 -0.0223 H -13.0540 -3.9200 -0.1930 H -13.3101 2.6084 0.8323 O -14.1426 2.4721 -0.9817 O -14.1933 3.7454 -0.9178	28.0 62.1 77.8 96.2 118.7 192.5 233.9 239.5 277.0 319.3 351.3 394.5 418.1 434.0 468.3 481.3 501.6 553.3 576.9 601.1 619.6 653.9 673.3 722.3 750.1 754.1 770.7 804.1 852.5 860.2 871.8 885.4 913.9 923.5 972.5 981.4 992.9 1003.5 1014.4 1035.1 1051.6 1105.8 1129.0 1172.1 1185.9 1196.5 1211.5 1221.6 1253.3 1284.4 1306.9 1337.6 1363.2 1389.6 1403.9 1415.2 1432.5 1474.9 1483.7 1515.8 1566.6 1588.7 1612.6 1658.1 1665.7 3157.7 3162.6 3163.8 3170.7 3172.8 3182.6 3187.2 3192.4 3212.5 3490.9	2811.627 4141.487 6763.358	2
CS52	-744.751867	C -13.7813 -0.5807 -0.0460 C -12.9617 -1.7592 0.0315 C -11.5581 -1.6621 0.0878 C -10.8923 -0.4222 0.0477 C -11.6483 0.7837 -0.0279 C -13.1204 0.7265 -0.0408 C -10.9538 2.0086 -0.0857 C -9.5725 2.0481 -0.0617 C -8.8226 0.8578 0.0227 C -9.4723 -0.3524 0.0753 C -15.1803 -0.7634 -0.1275 C -15.7481 -2.0271 -0.1233 C -14.9442 -3.1758 -0.0326 C -13.5778 -3.0393 0.0424 N -13.6664 1.9285 -0.0350 H -10.9731 -2.5736 0.1498 H -11.5219 2.9259 -0.1535 H -9.0630 3.0037 -0.1105 H -7.7395 0.8986 0.0422 H -8.9099 -1.2780 0.1357	29.8 86.9 104.5 139.7 147.8 176.9 216.2 237.0 267.6 307.8 335.7 377.2 403.5 414.9 423.2 474.4 514.0 536.0 584.6 622.2 640.0 648.4 669.6 727.7 744.7 745.6 767.0 787.2 833.4 861.6 872.7 875.1 884.4 908.3 931.2 973.5 977.8 994.3 997.0 1011.3 1049.8 1066.3 1120.8 1149.6 1158.6 1176.6 1201.1 1208.0 1226.3 1266.8 1301.0 1330.6 1352.6 1364.3 1399.0 1421.9 1434.14 1469.7 1482.7 1505.2 1536.2 1571.0 1581.0 1621.1 1637.7 3161.0 3162.1 3167.2 3173.3 3175.3 3187.1 3188.7 3214.7 3264.9 3718.0- 90.2474	2878.374 4164.005 7032.642	2

		H -15.8311 0.0909 -0.2026 H -16.8255 -2.1237 -0.1913 H -15.3977 -4.1604 -0.0260 H -12.9409 -3.9151 0.1062 O -15.0353 1.9566 -0.0182 O -15.4283 3.3423 -0.0808 H -15.1575 3.6626 0.7952			
CS53	-744.082227	C -13.7439 -0.5750 0.0912 C -12.9582 -1.7809 0.0237 C -11.5708 -1.6809 -0.0468 C -10.9103 -0.4494 -0.0545 C -11.6666 0.7804 0.0121 C -13.0799 0.6772 0.0838 C -10.9237 2.0040 -0.0000 C -9.5558 2.0014 -0.0718 C -8.8192 0.7901 -0.1369 C -9.4847 -0.4018 -0.1281 C -15.1683 -0.7113 0.1628 C -15.7553 -1.9468 0.1665 C -14.9753 -3.1350 0.0997 C -13.6148 -3.0505 0.0303 N -14.0270 1.7590 0.1571 H -10.9796 -2.5901 -0.0977 H -11.4429 2.9449 0.0478 H -9.0255 2.9471 -0.0789 H -7.7372 0.8174 -0.1930 H -8.9430 -1.3403 -0.1770 H -15.7752 0.1805 0.2140 H -16.8354 -2.0236 0.2213 H -15.4664 -4.1013 0.1043 H -13.0045 -3.9458 -0.0212 O -13.6481 2.9403 -0.5690 O -13.5715 2.9086 0.8900	66.0 81.6 105.1 139.5 205.7 234.3 234.4 273.6 329.3 365.9 402.5 419.9 444.4 479.4 502.7 533.0 561.1 602.9 620.2 646.0 660.6 696.2 704.7 749.8 755.1 771.9 803.6 829.7 861.9 872.2 879.2 883.2 919.3 949.8 977.8 984.0 998.1 1008.4 1032.2 1038.5 1049.8 1127.9 1131.2 1176.4 1182.6 1199.9 1211.0 1258.7 1279.2 1306.5 1341.3 1357.0 1396.9 1416.0 1426.3 1475.7 1481.4 1514.9 1566.1 1588.0 1616.8 1658.8 1667.2 3157.8 3163.2 3164.3 3173.2 3173.5 3188.5 3189.0 3226.7 3277.2	2379.638 4169.833 6427.495	1
TS1	-705.454271	C -2.5986 0.2630 -0.1015 C -2.0307 -0.9746 -0.2259 C -0.6218 -1.1529 -0.0710 C 0.1950 0.0011 0.2208 C -0.4404 1.2748 0.3420 C -1.7930 1.4018 0.1863 C 1.5775 -0.1551 0.3760 C 2.1789 -1.4070 0.2548 C 1.3669 -2.5617 -0.0379 C -0.0125 -2.4069 -0.1928 C 2.0298 -3.8197 -0.1553 C 3.3832 -3.8928 0.0091 C 4.0607 -2.6782 0.2951 N 3.5421 -1.5088 0.4126 H -3.6690 0.3852 -0.2212	-90.2 62.6 102.9 155.4 199.3 238.4 263.1 332.9 364.2 392.7 437.1 456.5 479.9 489.2 531.8 558.1 594.1 633.3 648.5 696.0 755.9 761.6 764.9 775.0 791.3 832.2 852.6 858.5 900.0 912.7 923.6 978.4 983.6 985.1 999.3 1028.6 1110.4 1130.1 1155.1 1173.0 1178.9 1192.1 1218.0 1286.3 1293.9 1303.7 1361.6 1371.1 1410.6 1426.4 1448.1 1490.8 1506.9 1578.6 1591.3 1632.0 1647.3 1669.4 3158.9 3162.3 3167.6 3173.6 3179.4 3187.7 3190.6 3212.0	1042.578 6393.464 7325.542	2

		H -2.6436 -1.8425 -0.4449 H 0.1735 2.1416 0.5614 H H -2.2622 2.3744 0.2813 H 2.2083 0.6984 0.5955 H -0.6241 -3.2766 -0.4123 H 1.4489 -4.7093 -0.3739 H 3.9369 -4.8188 -0.0680 O 5.4778 -2.7574 0.4168 O 5.8459 -2.8902 1.6879			
TS2	-705.388674	C -4.9796 0.5011 0.0990 C -4.3858 -0.6636 -0.3069 C -2.9879 -0.8756 -0.1206 C -2.2034 0.1584 0.5043 C -2.8604 1.3562 0.9124 C -4.2057 1.5217 0.7158 C -0.8244 -0.0334 0.6958 C C -0.2179 -1.2111 0.2865 C C -0.9892 -2.2590 -0.3420 C C -2.3544 -2.0599 -0.5273 C C -0.3040 -3.4544 -0.7433 C C 1.0332 -3.6218 -0.5494 C C 1.7465 -2.5440 0.0806 C N 1.1151 -1.4537 0.4457 N H -6.0428 0.6516 -0.0475 H H -4.9721 -1.4455 -0.7780 H H -2.2731 2.1370 1.3833 H H -4.6901 2.4386 1.0320 H H -0.2237 0.7366 1.1645 H H -2.9427 -2.8413 -0.9985 H H -0.8811 -4.2426 -1.2152 H H 1.5663 -4.5144 -0.8448 H O 2.9931 -2.4864 0.3573 O O 2.7872 -0.8282 1.0640 O	-1447.0 45.7 89.2 136.1 178.9 187.4 248.8 310.6 311.3 385.1 400.1 462.0 462.3 488.0 488.7 543.7 610.8 612.2 637.8 653.7 674.2 711.4 757.7 765.0 768.3 805.0 811.1 851.8 872.5 888.4 894.9 919.8 974.9 977.2 997.4 1031.8 1037.2 1122.5 1161.3 1172.1 1192.4 1219.2 1283.7 1288.6 1297.7 1355.3 1364.4 1380.8 1405.6 1423.1 1462.3 1474.7 1508.3 1556.5 1591.9 1609.3 1653.9 1664.4 3159.3 3162.2 3167.1 3173.4 3179.4 3190.4 3191.8 3221.2	1218.570 5631.554 6850.125	2
TS3	-705.44202866	C -4.3530 0.5762 -0.0725 C -3.7527 -0.6506 -0.2246 C -2.3461 -0.7919 -0.0909 C -1.5571 0.3682 0.2012 C -2.2081 1.6186 0.3510 C -3.5732 1.7202 0.2177 C -0.1508 0.2282 0.3401 C 0.4325 -1.0051 0.2235 C -0.3285 -2.1702 -0.1132 C -1.6982 -2.0389 -0.2581 C 0.3460 -3.4175 -0.4294 C 1.6786 -3.6435 -0.4629 C 2.7209 -2.6993 -0.0818 N 1.8302 -1.1961 0.3655	-549.2 65.6 90.2 166.6 193.7 213.3 267.1 311.7 348.7 361.3 395.1 415.1 467.4 482.0 482.6 514.6 534.7 580.0 589.6 632.6 656.0 738.4 758.5 766.2 775.2 789.2 795.1 822.3 863.2 905.9 911.9 920.6 973.9 984.4 989.1 997.3 1041.4 1086.8 1153.6 1176.8 1185.1 1189.7 1221.1 1255.0 1284.9 1288.1 1344.2 1391.0 1400.0 1429.2 1471.3 1481.2 1526.7 1598.1 1624.6 1642.4 1659.1 1899.8 3156.8 3160.5 3163.2 3168.0 3179.7	1030.733 5867.174 6696.073	2

		H -5.4277 0.6722 -0.1751 H -4.3483 -1.5293 -0.4482 H -1.6116 2.4965 0.5740 H -4.0585 2.6826 0.3340 H 0.4620 1.0923 0.5698 H -2.2923 -2.9054 -0.5322 H -0.2979 -4.2324 -0.7460 H 2.0647 -4.5802 -0.8488 O 3.8755 -2.6317 -0.3084 O 2.1336 -2.0013 1.3989	3184.1 3185.9 3191.4		
TS4	-705.418507	C -4.8074 0.5230 -0.2740 C -4.2718 -0.7447 -0.2715 C -2.9025 -0.9564 0.0220 C -2.0636 0.1817 0.3169 C -2.6562 1.4783 0.3045 C -3.9883 1.6427 0.0166 C -0.7204 -0.0173 0.6689 C -0.1628 -1.3157 0.7112 C -0.9729 -2.4288 0.2287 C -2.3157 -2.2455 -0.0261 C -0.2304 -3.5362 -0.2853 C 1.0712 -3.3022 -0.6398 C 1.5620 -1.9788 -0.4735 H -5.8572 0.6701 -0.4990 H -4.8967 -1.6027 -0.4966 H -2.0331 2.3366 0.5306 H -4.4219 2.6363 0.0115 H -0.1235 0.8138 1.0288 H -2.9151 -3.0817 -0.3760 H -0.7089 -4.4852 -0.4995 H 1.7084 -4.0266 -1.1346 O 2.5286 -1.3255 -0.5959 O 0.8757 -2.5548 2.3332 N 0.7722 -1.4517 1.8492	-243.0 63.6 97.1 130.2 152.2 185.4 222.1 242.2 291.6 304.7 327.3 391.0 398.7 423.0 446.7 468.5 517.0 566.0 595.2 625.0 630.5 721.4 737.8 740.3 755.1 767.7 781.5 809.8 840.1 873.8 891.5 908.7 910.8 954.2 971.2 978.8 992.2 1035.3 1098.9 1148.7 1167.7 1188.5 1227.5 1263.5 1287.0 1319.0 1380.1 1390.1 1404.7 1419.3 1465.6 1498.2 1534.4 1558.5 1576.0 1599.8 1636.1 1942.1 3148.6 3161.6 3166.8 3170.5 3175.3 3179.9 3190.6 3191.4	1464.887 5075.069 5530.091	2
TS5	-705.439431	C -4.8697 0.5956 -0.0029 C -4.2613 -0.5716 -0.4219 C -2.8928 -0.8030 -0.1708 C -2.1345 0.1979 0.5292 C -2.7934 1.3845 0.9540 C -4.1298 1.5786 0.6908 C -0.7735 -0.0288 0.7886 C -0.1287 -1.1921 0.3121 C -0.9101 -2.2305 -0.3306 C -2.2441 -2.0086 -0.5650 C -0.2560 -3.4801 -0.6427 C 1.0133 -3.7290 -0.2664 C 1.8037 -2.7431 0.4762 N 1.2497 -1.3852 0.6622	-543.4 53.6 96.7 111.9 204.8 232.3 240.4 270.3 339.4 376.0 383.2 408.5 471.1 491.4 513.1 530.8 554.9 624.1 629.2 652.2 724.7 733.4 752.1 758.3 774.9 801.4 845.2 857.7 863.8 877.1 883.1 913.3 931.8 971.5 994.1 998.8 1040.9 1099.0 1147.0 1169.6 1184.2 1192.9 1210.6 1254.5 1270.7 1290.2 1326.2 1372.7 1406.5 1418.2 1443.2 1480.5 1513.9 1566.3 1607.9 1625.2 1650.1 1782.3 3160.3 3163.4 3165.8 3171.5 3182.5	1105.664 5419.589 6267.995	2

		H -5.9217 0.7598 -0.2050 H -4.8345 -1.3259 -0.9502 H -2.2214 2.1378 1.4842 H -4.6200 2.4893 1.0146 H -0.1740 0.7014 1.3181 H -2.8351 -2.7836 -1.0432 H -0.8273 -4.2323 -1.1779 H 1.5051 -4.6704 -0.4773 O 2.9000 -2.9585 0.9272 O 1.2597 -0.7358 -0.6355	3193.7 3199.7 3199.9		
TS6	-705.442001	1 C1 -4.8889 0.4848 0.1314 2 C2 -4.2441 -0.6389 - 0.3504 3 C3 -2.8467 -0.7768 - 0.2331 4 C4 -2.0937 0.2738 0.4000 5 C5 -2.7893 1.4187 0.8839 6 C6 -4.1544 1.5193 0.7526 7 C7 -0.7012 0.1600 0.4906 8 C8 -0.0292 -1.0011 0.0149 9 C9 -0.8045 -2.0888 - 0.5722 10 C10 -2.1592 -1.9331 - 0.7085 11 C11 -0.1094 -3.3137 - 0.9144 12 C12 1.0270 -3.6801 - 0.2909 C 1.5393 -2.9341 0.8716 N 1.2940 -1.5224 1.0125 H -5.9645 0.5750 0.0330 H -4.8128 -1.4311 -0.8256 H -2.2216 2.2106 1.3598 H -4.6725 2.3949 1.1261 H -0.0974 0.9570 0.9065 H -2.7411 -2.7298 -1.1615 H -0.5705 -3.9766 -1.6401 H 1.5079 -4.6294 -0.4931 O 2.1271 -3.4688 1.7922 O 1.3089 -0.9034 -0.3183	-478.0 59.4 97.9 126.9 216.8 239.6 253.6 328.9 373.0 375.3 391.4 444.7 463.0 469.9 499.0 534.9 575.1 627.1 637.5 652.3 721.5 723.6 751.9 754.5 771.1 806.3 833.3 838.4 856.4 863.4 873.7 915.3 924.9 969.8 992.1 994.3 1039.9 1104.4 1142.3 1166.7 1176.8 1191.3 1223.0 1241.7 1262.1 1288.6 1318.7 1369.3 1402.9 1412.5 1436.8 1470.1 1508.4 1559.8 1605.0 1619.7 1639.5 1706.9 3159.2 3162.0 3165.6 3171.1 3182.4 3193.7 3196.3 3199.7	1206.387 5361.518 6047.571	2
TS7	-705.355611	C -4.7899 0.5966 -0.2798 C -4.2844 -0.7017 -0.3241 C -2.9291 -0.9669 -0.0299 C -2.0600 0.1348 0.3176 C -2.6076 1.4495 0.3507 C -3.9462 1.6748 0.0577 C -0.7211 -0.1055 0.6577 C -0.1751 -1.4583 0.6823	-678.3 -24.1 93.5 115.0 218.5 245.7 261.3 294.4 340.5 370.6 394.5 405.6 442.8 459.6 497.7 543.8 581.9 612.5 622.0 672.5 690.6 707.2 721.4 749.4 756.2 793.4 803.3 815.9 855.0 874.5 917.6 933.9 941.7 964.0 991.0 1033.6 1040.9 1068.1 1112.2	1311.728 4763.799 5437.172	2

		C -1.0531 -2.5294 0.1481 C -2.3855 -2.2832 -0.1272 C -0.2624 -3.6505 -0.2800 C 1.0571 -3.3459 -0.3765 C 1.3928 -1.9484 0.0797 N 1.7417 -1.9342 1.4906 H -5.8256 0.7758 -0.5049 H -4.9322 -1.5198 -0.5857 H -1.9661 2.2726 0.6107 H -4.3408 2.6742 0.0895 H -0.0976 0.6956 1.0106 H -3.0070 -3.0765 -0.5050 H -0.6826 -4.5970 -0.5658 H 1.8342 -4.0186 -0.6864 O 2.0249 -1.1493 -0.7145 O 0.4702 -1.7504 1.9177	1127.6 1137.3 1151.4 1162.3 1177.2 1215.5 1247.9 1277.6 1279.7 1319.4 1358.8 1374.5 1406.1 1450.5 1484.2 1540.7 1550.1 1579.4 1601.2 3246.8 3250.6 3255.9 3266.0 3271.1 3274.7 3276.9 3298.1		
TS8	-705.422165	C -2.3711 0.4272 -0.2932 C -1.9570 -0.8638 -0.0582 C -0.5872 -1.1615 0.1522 C 0.3652 -0.0868 0.1182 C -0.0964 1.2322 -0.1235 C -1.4332 1.4843 -0.3267 C 1.7372 -0.3702 0.3611 C 2.1281 -1.6605 0.5680 C 1.2082 -2.7460 0.5460 C -0.1325 -2.4909 0.3726 C 1.8698 -4.0431 0.5953 C 3.1997 -3.9930 0.4397 C 3.7887 -2.6462 0.2221 N 3.5697 -1.8038 1.6961 H -3.4223 0.6387 -0.4527 H -2.6785 -1.6736 -0.0332 H 0.6250 2.0419 -0.1449 H -1.7731 2.4970 -0.5109 H 2.4567 0.4403 0.4441 H -0.8513 -3.3046 0.3621 H 1.3208 -4.9686 0.7213 H 3.8731 -4.8396 0.4321 O 4.6435 -2.2669 -0.5159 O 4.1594 -0.7744 1.8564	-548.5 74.6 86.8 137.4 170.8 186.0 227.4 242.7 286.6 309.3 382.1 400.2 404.2 474.0 483.2 503.7 542.6 554.1 564.7 607.8 630.3 675.4 706.8 760.0 768.1 779.8 783.2 803.9 860.9 897.5 902.0 912.4 953.7 971.2 973.4 980.2 996.6 1042.3 1126.1 1149.3 1174.6 1185.1 1225.8 1255.4 1280.2 1330.8 1370.5 1383.7 1424.1 1440.1 1479.4 1532.7 1537.9 1603.1 1616.1 1637.8 1651.1 1816.7 3150.6 3158.6 3162.4 3168.1 3179.3 3189.8 3190.8 3216.8	1443.018 4918.119 5869.464	2
TS9	-705.292128	C -2.3165 0.3892 -0.3983 C -1.8612 -0.9125 -0.3819 C -0.5398 -1.2178 0.0147 C 0.3405 -0.1457 0.4030 C -0.1616 1.1856 0.3679 C -1.4554 1.4448 -0.0195 C 1.6426 -0.4333 0.8542 C 2.1013 -1.7632 0.8833	-578.3 84.0 102.8 164.8 231.6 253.0 297.6 308.5 364.9 397.6 429.9 454.8 469.0 513.9 535.7 580.9 592.9 625.5 637.1 683.2 718.5 733.5 751.4 759.3 763.5 803.5 827.6 839.5 862.4 870.9 895.6 903.9 919.2 929.6 965.3 987.7 989.2 1039.4 1080.5	1339.616 4733.755 5818.372	2

		C 1.2566 -2.8372 0.3442 C -0.0318 -2.5472 -0.0239 C 2.0174 -4.0026 -0.0634 C 3.3623 -3.7956 -0.0155 C 3.6311 -2.5482 0.6530 N 3.1178 -2.2059 1.9560 H -3.3335 0.6065 -0.7031 H -2.5185 -1.7238 -0.6773 H 0.4956 1.9976 0.6600 H -1.8208 2.4654 -0.0344 H 2.2686 0.3578 1.2471 H -0.6549 -3.3317 -0.4436 H 1.5517 -4.9027 -0.4423 H 4.1397 -4.4538 -0.3758 O 4.7506 -1.7452 0.7111 O 4.1741 -1.1802 1.9591	1142.6 1166.2 1178.6 1219.5 1230.6 1252.9 1283.4 1296.0 1342.4 1377.2 1405.2 1417.8 1429.2 1467.8 1503.3 1547.9 1559.2 1613.8 1632.7 3154.5 3159.5 3164.3 3177.5 3190.0 3196.1 3204.4 3225.5		
TS10	-705.340202	C -2.5921 0.1686 0.0322 C -2.0279 -1.0758 -0.1674 C -0.6401 -1.2792 -0.0032 C 0.1752 -0.1628 0.3782 C -0.4318 1.0986 0.5749 C -1.7906 1.2645 0.4053 C 1.5797 -0.3512 0.5567 C 2.1133 -1.5906 0.3460 C 1.3060 -2.7112 -0.0422 C -0.0392 -2.5648 -0.2120 C 2.2116 -3.8570 -0.2075 C 3.4768 -3.4921 0.0838 C 3.4940 -2.0566 0.4730 N 4.5732 -1.1937 0.3138 H -3.6597 0.3043 -0.0990 H -2.6508 -1.9162 -0.4548 H 0.1907 1.9387 0.8636 H -2.2437 2.2368 0.5594 H 2.2048 0.4817 0.8594 H -0.6686 -3.3978 -0.5076 H 1.8991 -4.8431 -0.5249 H 4.3672 -4.1001 0.0533 O 4.4684 -2.3724 2.1046 O 5.3764 -1.6393 1.2722	-503.7 68.2 93.7 136.0 175.7 198.4 276.2 300.7 318.7 356.4 400.7 414.2 475. 486.8 544.3 556.3 583.5 602.4 626.8 711.1 750.6 763.9 771.7 776.7 792.8 811.7 836.2 868.7 908.0 908.9 919.0 942.7 959.1 975.1 998.1 1018.4 1048.6 1088.2 1103.0 1143.9 1169.3 1171.0 1183.9 1219.4 1247.8 1279.8 1321.0 1344.3 1366.9 1370.5 1446.1 1474.1 1486.8 1547.3 1580.3 1634.0 1645.7 1667.4 3162.6 3167.3 3169.1 3179.5 3182.4 3192.1 3207.6 3253.3	1264.459 5522.357 6538.531	2
TS11	-705.331322	C -2.6163 0.3657 -0.5235 C -2.1313 -0.9010 -0.7008 C -0.8183 -1.2350 -0.3154 C -0.0026 -0.2406 0.2602 C -0.5244 1.0555 0.4323 C -1.8032 1.3562 0.0501 C 1.3424 -0.5641 0.6602 C 1.8036 -1.8199 0.4772	-446.4 59.3 88.8 112.5 141.5 173.1 259.9 280.4 302.9 326.6 396.5 414.6 426.9 476.9 532.8 555.9 573.8 626.0 658.1 712.0 716.0 762.3 763.7 772.0 775.8 801.0 834.0 853.4 866.4 906.6 913.0 921.7 934.6 971.6 994.3 1019.1 1049.1 1066.8 1081.7	1251.102 5891.336 7004.204	2

		C 0.9641 -2.8505 -0.1172 C -0.3008 -2.5652 -0.4987 C 1.7501 -4.0740 -0.1727 C 3.0215 -3.8184 0.3624 C 3.0623 -2.4742 0.7533 H -3.6210 0.6052 -0.8229 H -2.7552 -1.6596 -1.1405 H 0.0987 1.8148 0.8719 H -2.1877 2.3509 0.1880 H 1.9578 0.2013 1.0987 H -0.9346 -3.3152 -0.9395 H 1.4075 -5.0139 -0.5605 H 3.8196 -4.5280 0.4551 N 4.7735 -1.4465 1.6647 O 5.3873 -2.3715 2.4018 O 5.8521 -2.0151 1.1272	1140.7 1166.4 1181.0 1210.8 1230.6 1250.2 1280.7 1314.1 1363.3 1366.8 1398.6 1421.7 1474.0 1476.1 1487.9 1550.6 1617.9 1634.0 1638.9 3161.3 3164.9 3167.1 3178.8 3181.1 3191.6 3212.1 3252.3		
TS12	-705.234394	C -2.6163 0.3657 -0.5235 C -2.1313 -0.9010 -0.7008 C -0.8183 -1.2350 -0.3154 C -0.0026 -0.2406 0.2602 C -0.5244 1.0555 0.4323 C -1.8032 1.3562 0.0501 C 1.3424 -0.5641 0.6602 C 1.8036 -1.8199 0.4772 C 0.9641 -2.8505 -0.1172 C -0.3008 -2.5652 -0.4987 C 1.7501 -4.0740 -0.1727 C 3.0215 -3.8184 0.3624 C 3.0623 -2.4742 0.7533 H -3.6210 0.6052 -0.8229 H -2.7552 -1.6596 -1.1405 H 0.0987 1.8148 0.8719 H -2.1877 2.3509 0.1880 H 1.9578 0.2013 1.0987 H -0.9346 -3.3152 -0.9395 H 1.4075 -5.0139 -0.5605 H 3.8196 -4.5280 0.4551 N 4.7735 -1.4465 1.6647 O 5.3873 -2.3715 2.4018 O 5.8521 -2.0151 1.1272	-413.3 -266.9 -172.0 -81.1 60.7 94.8 203.7 221.1 236.1 282.8 327.7 366.6 408.6 454.3 461.8 538.8 552.5 570.2 626.1 651.4 708.6 715.7 724.9 754.8 760.2 801.7 822.3 838.8 844.7 863.4 869.2 879.4 910.1 943.0 966.1 973.8 1015.7 1055.2 1069.7 1140.9 1158.6 1168.4 1172.3 1221.2 1233.1 1273.2 1327.3 1346.3 1374.2 1424.1 1425.8 1458.0 1490.7 1494.9 1571.7 1667.2 1673.1 1682.3 3238.8 3243.3 3246.2 3256.3 3258.5 3268.6 3288.0 3307.0	1370.413 6443.129 7701.155	2
TS13	-667.29342	C -7.8777 0.6401 0.0484 C -7.2569 -0.5266 0.4391 C -5.8426 -0.6183 0.4597 C -5.0735 0.5249 0.0928 C -5.7467 1.7165 -0.3012 C -7.1320 1.7658 -0.3434 C -3.5991 2.8078 -0.5648 C -2.9329 1.6778 -0.2450	-209.4 67.9 116.6 144.7 175.7 217.2 244.1 285.9 421.6 434.0 462.3 477.8 485.9 494.4 520.2 571.3 591.1 638.9 643.9 671.1 759.8 775.1 783.4 796.1 814.6 834.7 849.8 892.1 909.7 959.7 980.6 987.1 1001.7 1056.6 1098.5 1125.6 1144.0 1182.3	1673.900 3268.009 4837.182	2

		C -3.6464 0.4680 0.1022 C -3.0169 -0.7137 0.4662 C -3.7741 -1.8462 0.8237 C -5.1504 -1.8061 0.8209 N -4.9734 2.8237 -0.6785 H -7.6297 2.6710 -0.6645 H -8.9600 0.6951 0.0272 H -7.8445 -1.3916 0.7257 H -5.7257 -2.6869 1.0838 H -3.2622 -2.7613 1.0991 H -3.1171 3.7471 -0.8012 H -1.8497 1.6790 -0.2555 H -1.9336 -0.7625 0.4754 O -5.6171 4.1374 -0.0674 O -4.8837 5.1654 -0.1813	1204.1 1222.5 1228.2 1247.5 1263.0 1339.3 1386.9 1420.6 1426.9 1464.4 1489.2 1534.1 1608.6 1612.3 1622.8 1658.6 3163.0 3167.8 3172.6 3184.3 3185.7 3187.2 3208.1 3212.8		
TS14	-667.240113	C 1.0720 0.1480 -3.6835 C -0.3064 0.0819 -3.7312 C -1.0545 0.0061 -2.5331 C -0.3657 0.0030 -1.2857 C 1.0425 0.1081 -1.2707 C 1.7553 0.1733 -2.4580 C 1.0215 -0.1732 1.1425 C -0.3737 -0.2269 1.1522 C -1.1002 -0.1505 -0.0571 C -2.5017 -0.2406 -0.1056 C -3.1748 -0.1972 -1.3295 C -2.4733 -0.0823 -2.5185 N 1.7155 0.2103 -0.0279 O 2.8182 -0.6590 0.1017 O 2.0686 -1.7675 0.7577 H 2.8351 0.2387 -2.4256 H 1.6421 0.1944 -4.6041 H -0.8266 0.0802 -4.6822 H -3.0062 -0.0610 -3.4629 H -4.2563 -0.2653 -1.3478 H 1.5772 -0.0026 2.0536 H -0.8872 -0.3807 2.0932 H -3.0565 -0.3541 0.8190	-625.2 74.6 122.2 169.0 208.4 250.1 314.1 353.1 405.4 449.2 474.1 477.3 497.6 520.7 546.8 601.7 619.0 640.2 672.5 727.2 759.4 769.8 778.6 800.6 816.6 838.0 842.3 898.7 915.5 933.8 982.3 988.7 998.8 1026.1 1056.6 1103.5 1112.8 1131.9 1176.5 1203.3 1211.6 1238.6 1253.1 1312.8 1359.1 1376.3 1415.7 1418.1 1448.1 1480.3 1485.6 1542.4 1572.0 1598.0 1635.8 3167.2 3170.7 3176.3 3186.2 3190.1 3191.9 3205.4 3215.8	1769.319 2814.045 4325.986	2
TS15	-667.248161	C 0.9020 0.1075 -3.8443 C -0.4761 0.1507 -3.7570 C -1.1235 -0.0463 -2.5150 C -0.3363 -0.2847 -1.3518 C 1.0687 -0.3619 -1.4820 C 1.6810 -0.1652 -2.7120 C 1.2793 -0.5763 0.9752 C -0.1889 -0.6146 1.0727 C -0.9769 -0.4213 -0.0600 C -2.3902 -0.3713 -0.0016	-865.3 89.3 114.5 169.0 226.2 232.5 316.2 352.7 404.8 445.5 457.3 473.1 502.1 528.7 557.9 603.4 626.4 659.5 703.0 723.6 760.2 772.8 785.6 799.7 827.5 852.6 885.9 908.0 914.6 941.6 978.0 986.9 989.0 1053.0 1094.0 1104.5 1127.4 1159.2 1185.3 1204.3 1230.0 1249.0 1271.0 1296.1 1353.2 1369.3	1791.125 2731.911 4320.454	2

		C -3.1504 -0.1640 -1.1516 C -2.5404 0.0057 -2.3849 N 1.8648 -0.7096 -0.3615 O 2.8830 0.1677 -0.0635 O 1.8192 0.7664 1.1676 H 2.7598 -0.2293 -2.7819 H 1.3902 0.2665 -4.7987 H -1.0767 0.3385 -4.6401 H -3.1395 0.1851 -3.2707 H -4.2311 -0.1229 -1.0768 H 1.7817 -1.2620 1.6634 H -0.6359 -0.7638 2.0478 H -2.8769 -0.4834 0.9606	1406.1 1408.6 1446.3 1470.2 1484.7 1528.4 1567.7 1591.0 1630.8 3049.4 3166.3 3169.5 3176.3 3184.7 3188.8 3192.1 3199.3		
TS16	-667.2486629	C 0.9982 0.3735 -3.5680 C -0.3866 0.2977 -3.5537 C -1.0683 -0.1295 -2.3759 C -0.2983 -0.4962 -1.2452 C 1.1443 -0.6368 -1.3525 C 1.7700 -0.0992 -2.5006 C 1.3741 -0.0863 0.7793 C 0.0170 -0.4033 1.1518 C -0.9170 -0.5883 0.0181 C -2.2972 -0.5693 0.1298 C -3.0806 -0.3908 -1.0263 C -2.4802 -0.1268 -2.2423 N 1.7315 -1.8346 -0.7214 O 2.8967 -2.0533 -0.9788 O 0.6433 0.9941 1.0889 H 2.8434 -0.2000 -2.6019 H 1.5021 0.7358 -4.4575 H -0.9626 0.5920 -4.4237 H -3.0886 0.1138 -3.1076 H -4.1613 -0.3851 -0.9449 H 2.3790 -0.2793 1.1364 H -0.2500 -0.6890 2.1624 H -2.7708 -0.6299 1.1036	-348.8 112.5 121.7 154.6 160.9 223.7 262.3 327.4 352.2 362.8 428.7 464.3 477.6 495.9 517.2 529.9 568.1 616.5 642.8 650.2 721.6 748.6 757.6 771.3 802.8 818.1 831.2 869.0 912.6 935.3 971.4 986.6 1001.4 1050.1 1070.9 1089.5 1101.5 1134.5 1167.0 1176.3 1195.9 1235.4 1246.5 1273.8 1347.5 1360.3 1378.8 1421.2 1455.0 1469.6 1508.5 1540.1 1568.1 1595.1 1633.7 3163.7 3164.9 3170.5 3172.4 3182.6 3183.7 3188.7 3196.1	2057.482 2592.393 3877.201	2
TS17	-667.250902	C -7.8081 0.6398 -0.2537 C -7.2380 -0.5005 0.2717 C -5.8258 -0.6316 0.3843 C -5.0037 0.4507 -0.0434 C -5.6235 1.6033 -0.5843 C -7.0127 1.7074 -0.7045 C -3.4606 2.6416 -0.7926 C -2.8392 1.5297 -0.3126 C -3.5891 0.3804 0.0891 C -3.0115 -0.7819 0.6173 C -3.8155 -1.8505 1.0213 C -5.1971 -1.7808 0.9141	-157.9 74.6 113.7 140.8 191.3 206.9 252.3 347.0 365.0 412.7 451.4 481.1 486.3 497.4 528.5 549.5 577.4 639.2 641.0 655.8 747.2 763.0 795.1 807.8 826.0 838.2 891.2 915.7 944.5 984.6 990.8 992.2 1053.8 1099.7 1130.9 1141.1 1178.3 1205.1 1206.8 1241.3 1252.9 1301.6 1321.6 1367.7 1397.5 1431.4 1438.6 1460.9 1493.7 1521.9 1582.0 1595.0 1606.8 1639.8	1815.738 2940.384 4437.229	2

		N -4.8314 2.6918 -0.9532 H -7.4373 2.5809 -1.1742 H -8.8855 0.7175 -0.3351 H -7.8652 -1.3213 0.6023 H -5.8110 -2.6120 1.2428 H -3.3533 -2.7415 1.4302 H -2.9590 3.5517 -1.0872 H -1.7599 1.5332 -0.2219 H -1.9336 -0.8432 0.7173 O -5.3971 3.7570 -1.3501 O -6.7888 3.9791 0.5388	3167.9 3171.1 3176.4 3190.4 3191.8 3192.2 3238.8 3244.4		
TS18	-667.2189805	C -7.2053 0.3225 -1.6031 C -7.3037 -0.0346 -0.1852 C -6.1456 -0.0170 0.6292 C -4.9804 0.6180 0.1456 C -5.0026 1.4167 -1.0960 C -5.9894 1.0374 -2.1305 C -3.1423 1.8011 -1.0767 C -2.6845 1.0925 -0.0282 C -3.7394 0.5046 0.7824 C -3.6622 -0.1582 2.0108 C -4.8273 -0.7187 2.5584 C -6.0408 -0.6666 1.8895 N -4.6178 2.7371 -0.9430 H -6.0862 1.6984 -2.9849 H -8.1284 0.4508 -2.1590 H -8.2452 -0.4127 0.1945 H -6.9124 -1.1601 2.3046 H -4.7688 -1.2332 3.5108 H -2.6204 2.2845 -1.8879 H -1.6283 0.9350 0.1544 H -2.7153 -0.2520 2.5298 O -4.9068 3.5790 -1.8200 O -6.1661 -0.3509 -2.3696	-705.0 117.0 131.4 147.0 225.7 270.4 296.3 310.1 382.9 405.9 426.6 440.5 483.6 521.3 545.9 552.3 572.2 654.4 660.7 675.5 690.9 729.2 752.4 775.7 777.4 807.3 821.3 843.2 880.4 900.0 981.1 1004.8 1013.0 1055.7 1078.5 1100.0 1102.1 1131.5 1186.5 1197.6 1210.6 1231.0 1244.9 1301.6 1341.6 1354.6 1372.4 1377.5 1409.3 1424.0 1462.5 1494.3 1532.1 1584.0 1603.8 3150.5 3167.4 3167.6 3179.4 3185.4 3189.3 3191.0 3249.8	1947.754 2547.160 3863.874	2
TS19	-667.265421	C -7.7603 0.7605 -0.3149 C -7.1859 -0.2963 0.5212 C -5.8330 -0.5467 0.5147 C -4.9842 0.3853 -0.1838 C -5.4009 1.4959 -0.8571 C -6.8262 1.7301 -1.0506 C -4.2065 2.3210 -1.1492 C -3.0519 1.4882 -0.7574 C -3.5304 0.3536 -0.0943 C -2.9345 -0.6967 0.6173 C -3.7645 -1.6488 1.2542 C -5.1486 -1.5862 1.2347 N -3.9948 3.5723 0.0212 H -7.1853 2.7319 -1.2728	-150.9 84.9 114.9 138.0 171.0 208.0 230.7 293.9 373.0 407.7 451.6 467.8 481.6 518.5 546.7 564.3 582.0 644.4 667.4 670.2 710.6 724.8 753.6 765.9 797.2 816.4 851.4 872.4 888.8 971.5 979.1 996.9 1015.9 1048.7 1062.9 1075.6 1101.4 1123.8 1170.1 1189.1 1215.5 1226.5 1235.0 1289.4 1329.9 1351.8 1384.3 1410.7 1441.1 1483.7 1548.1 1567.3 1634.6 1675.1 3123.2 3130.4 3132.2 3162.7 3171.3 3177.7 3186.9 3225.7	2314.687 2371.680 3889.675	2

		H -8.7568 1.1109 -0.0602 H -7.8489 -0.8438 1.1825 H -5.7294 -2.3300 1.7687 H -3.2913 -2.4540 1.8059 H -4.1592 2.9070 -2.0638 H -2.0203 1.7856 -0.8782 H -1.8570 -0.7750 0.7049 O -4.6632 3.4807 0.9845 O -7.5426 0.6959 -1.7368			
TS20	-667.165483	C 1.3173 0.5800 -3.1609 C -0.0156 0.4474 -3.5464 C -1.0016 0.0718 -2.5662 C -0.5521 -0.2555 -1.2935 C 0.8707 -0.3239 -0.9298 C 1.7912 0.2312 -1.8936 C 0.8156 -0.3310 0.6778 C C -0.5828 -0.2260 1.0234 C -1.3904 -0.2764 -0.1561 C -2.7753 -0.1658 -0.3520 C -3.2632 0.0236 -1.6522 C -2.4049 0.1724 -2.7396 N 1.1761 -1.5625 -0.1315 O 2.6398 -1.6874 -0.1165 O 3.0322 -2.4112 0.8838 H 2.8479 0.2912 -1.6722 H 2.0352 0.9471 -3.8864 H -0.3224 0.6970 -4.5551 H -2.8088 0.4125 -3.7172 H -4.3324 0.1124 -1.8071 H 1.6152 0.0189 1.3182 H -0.9350 0.0211 2.0152 H -3.4605 -0.1869 0.4880	-435.5 40.1 112.0 146.7 175.5 199.8 257.6 327.8 357.2 424.0 427.2 479.5 484.3 509.0 517.2 566.9 605.0 622.6 632.8 655.5 693.6 708.5 741.0 751.8 769.0 800.1 807.9 830.0 912.2 953.9 963.9 983.2 996.8 1049.2 1058.6 1082.2 1110.7 1129.5 1171.4 1178.1 1199.4 1230.2 1234.0 1290.0 1327.0 1351.5 1372.6 1402.1 1444.1 1454.0 1501.1 1515.9 1594.7 1611.7 3165.7 3167.2 3176.1 3188.3 3188.6 3189.4 3211.5 3216.4	1573.375 3341.795 4574.952	2
TS21	-667.170771	C 0.8432 0.0361 -3.5198 C -0.4577 -0.4882 -3.5305 C -1.2527 -0.4467 -2.3375 C -0.6114 0.0123 -1.1892 C 0.8186 0.3073 -1.0941 C 1.4681 0.5098 -2.3685 C 0.9309 1.0968 0.1780 C -0.2596 1.0786 0.8194 C -1.2682 0.4014 -0.0175 C -2.6398 0.1906 0.0743 C -3.3054 -0.3751 -1.0341 C -2.6478 -0.6711 -2.2230 N 1.4282 -1.2634 -0.3944 O 2.8279 -1.3340 -0.5720 O 1.9011 -2.1142 -1.3997 H 2.4696 0.9188 -2.4176	-436.7 39.6 94.3 129.8 178.2 225.6 242.7 313.8 333.6 407.2 423.6 472.2 484.6 514.7 545.3 561.7 592.1 630.1 660.1 692.5 700.8 734.1 748.4 765.9 803.5 819.2 842.9 847.6 869.6 911.3 958.0 970.9 982.1 1012.1 1044.5 1068.7 1102.9 1110.6 1161.8 1165.0 1191.0 1194.2 1237.6 1262.9 1320.4 1354.9 1365.7 1400.2 1441.0 1461.7 1495.7 1531.4 1571.1 1624.5 1630.8 3162.8 3164.0 3174.0 3181.8 3186.0 3194.0 3199.9 3222.8	1751.206 2898.572 3706.713	2

		H 1.3836 0.0890 -4.4590 H -0.8882 -0.8465 -4.4587 H -3.2098 -1.0408 -3.0739 H -4.3742 -0.5461 -0.9692 H 1.8555 1.5147 0.5518 H -0.4562 1.5113 1.7918 H -3.2027 0.4728 0.9571			
TS22	-705.447553	C -3.9103 -0.2887 -0.6613 C -2.5457 -0.3420 -0.6006 C -1.7714 0.8562 -0.6578 C -2.4488 2.1251 -0.7810 C -3.8759 2.1341 -0.8405 C -4.5804 0.9637 -0.7823 C -0.3774 0.8689 -0.6012 C -0.4630 3.2836 -0.7850 C 0.3203 2.0770 -0.6617 C 1.7439 2.1597 -0.6057 H 2.3152 1.2423 -0.5131 C 2.3768 3.3701 -0.6667 C 1.6233 4.5708 -0.7883 C 0.2634 4.5153 -0.8426 H 0.1694 -0.0648 -0.5078 H -4.4935 -1.2014 -0.6172 H -2.0312 -1.2927 -0.5080 H -4.3662 3.0957 -0.9315 H -5.6635 0.9811 -0.8279 H 3.4577 3.4281 -0.6240 H 2.1185 5.5327 -0.8415 N -1.7962 3.2948 -0.8411 O -0.4606 5.7106 -1.0217 O -0.7497 6.2978 0.1384	-70.7 77.1 90.3 162.6 187.3 232.9 272.1 317.8 356.3 404.1 436.9 480.7 483.3 500.9 531.1 545.6 583.5 624.6 654.8 666.6 727.7 749.1 771.3 783.8 796.6 828.8 869.5 875.9 914.0 929.4 933.1 979.8 983.1 1001.1 1021.7 1029.0 1073.6 1115.6 1151.6 1162.5 1188.4 1191.4 1222.4 1272.1 1294.5 1329.3 1342.8 1380.0 1412.2 1423.7 1457.9 1497.5 1507.2 1557.1 1586.3 1618.6 1653.5 1671.0 3157.2 3161.6 3167.3 3172.4 3186.8 3187.0 3199.6 3199.8	1636.879 4641.119 6177.084	2
TS23	-705.390684	C -3.9020 -0.1743 -0.6444 C -2.5333 -0.2456 -0.5159 C -1.7304 0.9267 -0.4587 C -2.4242 2.1881 -0.5159 C -3.8232 2.2445 -0.6189 C -4.5541 1.0755 -0.7025 C -0.3212 0.8753 -0.3297 C -0.3156 3.2601 -0.4765 C 0.4288 2.0728 -0.3942 C 1.8418 2.2344 -0.4873 H 2.4832 1.3653 -0.3998 C 2.3881 3.4758 -0.7517 C 1.5948 4.6302 -0.9875 C 0.2351 4.4803 -0.8511 H 0.1748 -0.0852 -0.2566 H -4.4857 -1.0859 -0.6993 H -2.0382 -1.2096 -0.4716	-634.3 86.4 111.6 -634.3 86.4 111.6 180.4 207.7 244.1 252.8 308.2 373.7 407.4 438.3 483.9 503.3 520.0 561.5 574.9 585.4 610.4 638.8 681.1 704.4 728.2 740.4 755.0 769.9 804.4 810.4 845.5 864.1 870.2 883.4 933.0 960.2 964.6 985.4 1040.5 1052.5 1072.5 1135.6 1167.5 1186.3 1189.9 1212.6 1245.5 1279.8 1298.4 1323.9 1342.3 1392.7 1420.4 1456.0 1472.8 1490.3 1521.3 1564.4 1590.8 1620.2 1648.8 3164.6 3172.7 3177.9 3185.0 3188.3 3188.8 3199.8 3211.2	1501.558 4078.074 5522.497	2

		H -4.3049 3.2142 -0.6482 H -5.6320 1.1190 -0.8019 H 3.4641 3.5696 -0.8418 H 2.0379 5.5676 -1.2956 N -1.6803 3.3394 -0.3574 O -0.7537 5.4076 -1.0981 O -1.9677 4.6332 -1.3298			
TS24	-705.380404	C -3.7372 0.0019 -0.9086 C -2.5272 -0.2513 -0.3472 C -1.5976 0.8277 -0.1334 C -2.1215 2.2117 -0.2905 C -3.3643 2.4305 -0.9859 C -4.1347 1.3491 -1.2666 C -0.2434 0.7539 0.0195 C -0.5240 3.1278 -0.3336 C 0.4119 2.0212 -0.2253 C 1.7178 2.2269 -0.5655 H 2.4353 1.4173 -0.4859 C 2.1400 3.4898 -1.1205 C 1.2611 4.4933 -1.3660 C -0.1722 4.3784 -1.0330 H 0.3023 -0.1679 0.1760 H -4.4184 -0.8127 -1.1233 H -2.2097 -1.2653 -0.1310 H -3.6874 3.4466 -1.1713 H -5.1002 1.4928 -1.7388 H 3.1817 3.6043 -1.3998 H 1.5572 5.4046 -1.8720 N -1.6239 3.1503 0.6508 O -0.9844 5.2585 -1.2963 O -2.2144 4.1877 1.0428	-605.8 75.6 98.9 154.1 183.5 191.3 215.0 285.5 304.4 358.3 411.9 440.3 479.5 485.0 504.8 534.4 546.7 564.0 616.3 643.6 655.5 697.7 730.9 743.8 769.4 807.9 822.9 836.5 861.3 876.0 915.9 974.4 982.0 993.6 996.7 999.5 1045.9 1057.7 1110.5 1163.3 1174.5 1186.4 1199.6 1230.5 1238.9 1299.0 1374.0 1381.6 1388.1 1402.5 1429.4 1456.0 1523.1 1557.1 1577.8 1637.02 1647.4 1665.3 3165.2 3169.0 3175.9 3178.6 3192.8 3196.1 3200.9 3210.2	1757.378 3701.458 4703.068	2
TS25	-705.322066	C -3.9220 -0.1894 -0.5927 C -2.5532 -0.2702 -0.5575 C -1.7503 0.9045 -0.5522 C -2.4282 2.1656 -0.5846 C -3.8370 2.2400 -0.6376 C -4.5636 1.0729 -0.6360 C -0.3442 0.8746 -0.5883 C -0.3020 3.3008 -0.5177 C 0.4047 2.0490 -0.5833 C 1.8226 2.1332 -0.7321 H 2.3989 1.2176 -0.7914 C 2.4326 3.3604 -0.8110 C 1.7022 4.5797 -0.6472 C 0.3483 4.5381 -0.4553 H 0.1587 -0.0836 -0.6699 H -4.5199 -1.0929 -0.5925 H -2.0565 -1.2336 -0.5337	-399.3 83.8 104.8 146.3 178.0 234.5 247.5 283.6 390.6 408.4 425.5 442.6 462.4 491.2 512.4 536.5 567.7 589.9 641.7 655.8 710.2 723.7 735.5 747.0 768.1 824.6 850.4 860.5 869.2 885.3 912.1 957.2 973.7 975.4 989.6 997.8 1036.6 1043.4 1127.1 1168.3 1179.1 1195.1 1224.4 1276.3 1298.6 1315.9 1348.5 1367.6 1388.5 1405.4 1436.1 1468.1 1501.5 1524.9 1585.9 1594.7 1611.6 1652.6 3149.5 3162.0 3167.7 3172.9 3183.1 3186.0 3195.8 3224.9	1612.754 4009.856 5589.654	2

		H -4.3154 3.2085 -0.6714 H -5.6457 1.1206 -0.6688 H 3.5109 3.4106 -0.9271 H 2.2509 5.5138 -0.5811 N -1.6519 3.2845 -0.5742 O -1.3607 5.4733 -1.1488 O -2.2776 4.5260 -0.6101			
TS26	-705.184637	C -3.8097 0.3304 -0.8256 C -2.6332 0.0077 -0.2204 C -1.5440 0.9335 -0.2685 C -1.8039 2.3773 -0.6653 C -2.9781 2.5191 -1.5911 C -3.9479 1.5656 -1.5603 C -0.2048 0.7257 -0.1468 C -0.4203 2.9216 -0.9100 C 0.5219 1.9239 -0.5371 C 1.8901 2.1922 -0.5967 H 2.6120 1.4379 -0.3050 C 2.3224 3.4481 -1.0290 C 1.4020 4.4426 -1.3968 C 0.0596 4.1324 -1.3028 H 0.2621 -0.2015 0.1618 H -4.6349 -0.3711 -0.8308 H -2.4849 -0.9718 0.2210 H -3.0977 3.4469 -2.1357 H -4.8490 1.7158 -2.1456 H 3.3840 3.6639 -1.0833 H 1.7449 5.4117 -1.7407 N -2.5055 3.1005 0.4766 O -1.8820 4.5509 1.5916 O -2.4480 4.4201 0.2887	-497.7 62.3 84.3 88.0 135.6 165.4 204.5 240.6 296.9 354.5 402.0 425.6 433.3 478.3 507.1 527.1 554.7 565.1 597.7 626.6 643.5 708.2 727.9 741.8 762.6 811.2 825.9 851.6 865.4 873.9 881.9 907.8 969.7 975.1 986.9 996.4 1007.1 1065.5 1069.3 1114.9 1145.7 1166.2 1174.7 1182.7 1206.3 1239.8 1268.3 1338.1 1351.5 1393.5 1436.4 1444.0 1461.0 1509.5 1557.2 1594.1 1628.7 1644.9 3164.2 3166.4 3172.7 3177.6 3186.8 3194.6 3198.0 3203.5	1956.712 3626.695 4596.265	2
TS27	-705.209146	C -3.8341 0.3980 -0.9362 C -2.6114 -0.0124 -0.4838 C -1.5216 0.9096 -0.5041 C -1.7884 2.3191 -0.8309 C -3.0276 2.6523 -1.4670 C -4.0278 1.7217 -1.4655 C -0.1669 0.7413 -0.3057 C -0.4739 2.9691 -0.9306 C 0.5156 1.9990 -0.5728 C 1.8624 2.3494 -0.5378 H 2.6154 1.6176 -0.2672 C 2.2421 3.6607 -0.8528 C 1.2861 4.6262 -1.1969 C -0.0390 4.2292 -1.2145 H 0.3240 -0.1787 -0.0157 H -4.6696 -0.2923 -0.9449 H -2.4517 -1.0342 -0.1577	-543.1 27.2 76.8 98.7 113.6 160.4 206.5 235.5 277.1 300.3 338.2 412.7 428.6 473.9 506.7 527.0 545.8 554.0 621.2 641.2 679.3 696.9 718.2 734.5 737.2 756.0 806.9 833.6 846.5 853.1 869.5 893.1 967.4 970.1 990.4 993.5 1003.6 1063.1 1097.2 1133.9 1160.9 1172.6 1179.5 1196.7 1211.1 1264.3 1283.6 1344.5 1358.8 1382.7 1440.1 1445.7 1470.4 1490.0 1550.4 1569.2 1622.0 1636.6 3161.9 3164.4 3171.5 3175.6 3184.9 3185.2 3191.9 3203.3	1820.882 3852.731 4201.253	2

		H -3.1778 3.6431 -1.8791 H -4.9942 1.9719 -1.8894 H 3.2907 3.9374 -0.8320 H 1.5860 5.6387 -1.4416 N -2.3402 2.8828 1.1066 O -1.7237 4.0757 1.4792 O -1.2549 2.7546 1.9524			
TS28	-897.22336	C -3.6146 0.2704 0.9276 C -3.0037 -0.8832 0.4789 C -1.6263 -0.8836 0.1694 C -0.8800 0.3164 0.3322 C -1.5366 1.4884 0.7838 C -2.8924 1.4651 1.0731 C 0.6087 2.7170 0.6935 C 1.2587 1.5412 0.2422 C 0.5199 0.3339 0.0485 C 2.6581 1.5700 -0.0108 C 3.3717 2.7678 0.2108 C 2.7144 3.8948 0.6613 C 1.3305 3.8835 0.8955 C 1.1682 -0.8309 -0.3984 C 0.3983 -2.0224 -0.5700 C -0.9386 -2.0484 -0.2979 C 2.5717 -0.7778 -0.6614 C 3.2852 0.3705 -0.4755 N -0.7947 2.6896 0.8648 H -4.6720 0.2656 1.1657 H -3.5738 -1.7979 0.3615 H -3.3887 2.3628 1.4169 H 0.8996 -2.9178 -0.9225 H -1.5067 -2.9622 -0.4347 H 4.4395 2.7910 0.0244 H 3.2666 4.8118 0.8317 H 0.8292 4.7783 1.2395 H 3.0680 -1.6761 -1.0136 H 4.3500 0.3917 -0.6810 O -1.2294 3.5339 2.0237 O -0.8953 3.0344 3.1722	-52.6 63.4 93.3 95.4 171.0 210.0 234.2 254.2 265.9 305.8 318.1 321.7 399.3 419.4 447.7 451.1 481.5 513.1 521.0 533.4 540. 558.9 599.6 609.9 644.8 650.5 682.6 698.6 727.9 747.6 761.6 768.6 771.3 801.2 809.1 826.4 835.4 849.9 898.4 901.1 954.2 958.4 972.6 977.4 981.2 984.1 1054.8 1070.4 1096.6 1120.4 1131.5 1167.8 1173.3 1195.9 1200.0 1226.9 1240.0 1254.1 1264.1 1309.9 1312.3 1362.1 1374.9 1397.8 1422.4 1438.7 1448.3 1458.6 1480.4 1522.9 1527.1 1553.3 1612.5 1632.3 1636.1 1641.7 1665.1 3158.7 3160.8 3168.2 3168.3 3177.1 3178.6 3184.5 3184.7 3205.6 3205.9	3898.711 4843.867 8404.827	2
TS29	-897.185607	C -3.4926 0.3547 1.0823 C -2.9644 -0.7497 0.4655 C -1.5552 -0.9123 0.2454 C -0.7092 0.1582 0.6262 C -1.2524 1.2569 1.2919 C -2.6532 1.4122 1.5899 C 0.7717 2.5543 1.0019 C 1.4040 1.3919 0.4670 C 0.6619 0.1939 0.2559 C 2.7598 1.4667 0.0485	-306.9 81.7 91.4 120.4 197.8 215.9 252.4 279.6 287.0 303.5 354.3 384.1 402.0 440.0 458.3 465.5 493.4 511.4 531.8 544.1 547.9 572.2 593.0 603.2 622.3 661.7 679.4 697.4 727.2 740.0 759.0 766.0 773.9 797.6 801.1 824.7 851.1 857.5 895.1 913.7 950.8 962.4 974.3 978.5 983.9 990.9 1003.4 1068.8 1084.1	3693.626 4865.397 8410.854	2

		C 3.4445 2.6921 0.1814 C 2.7953 3.8096 0.6829 C 1.4580 3.7590 1.0962 C 1.2408 -0.9248 -0.3826 C 0.4050 -2.0391 -0.6677 C -0.9493 -2.0214 -0.3894 C 2.6242 -0.8471 -0.7399 C 3.3482 0.2919 -0.5283 N -0.5366 2.3970 1.4386 H -4.5590 0.4120 1.2633 H -3.6282 -1.5483 0.1504 H -2.9327 1.8720 2.5325 H 0.8406 -2.9066 -1.1517 H -1.5663 -2.8662 -0.6774 H 4.4805 2.7582 -0.1311 H 3.3305 4.7489 0.7614 H 0.9574 4.6350 1.4859 H 3.0927 -1.7089 -1.2034 H 4.3917 0.3329 -0.8215 O -1.4200 3.5106 1.5450 O -2.6105 3.1070 0.8194	1121.5 1136.4 1168.0 1170.2 1199.8 1209.3 1227.7 1237.8 1250.6 1274.3 1311.2 1357.3 1363.1 1404.1 1412.3 1415.0 1435.2 1441.1 1453.6 1469.6 1509.5 1532.0 1538.4 1581.1 1610.0 1619.6 1628.4 1650.7 3137.2 3160.3 3161.6 3163.8 3169.6 3177.5 3179.0 3185.7 3189.9 3212.3		
TS30	-897.192761	C -3.5240 0.4553 0.8988 C -3.0008 -0.6867 0.3944 C -1.5751 -0.9408 0.2911 C -0.7084 0.0938 0.7338 C -1.2281 1.1679 1.4294 C -2.6713 1.4809 1.5845 C 0.7540 2.5105 1.0245 C 1.3776 1.3495 0.4798 C 0.6561 0.1276 0.3309 C 2.7068 1.4436 -0.0137 C 3.3709 2.6871 0.0492 C 2.7291 3.8010 0.5618 C 1.4194 3.7252 1.0601 C 1.2156 -0.9842 -0.3312 C 0.3725 -2.0949 -0.6127 C -0.9909 -2.0476 -0.3485 C 2.5832 -0.8897 -0.7468 C 3.2923 0.2672 -0.5911 N -0.5160 2.3306 1.6026 H -4.5958 0.6124 0.9097 H -3.6757 -1.4402 -0.0008 H -2.9723 1.6010 2.6356 H 0.7945 -2.9626 -1.1073 H -1.6245 -2.8667 -0.6736 H 4.3863 2.7654 -0.3230 H 3.2460 4.7532 0.5912 H 0.9289 4.5963 1.4745	-575.5 77.6 98.0 124.9 195.6 220.3 256.9 272.1 291.4 297.2 369.2 398.1 406.8 416.6 460.8 470.5 482.2 501.6 519.5 545.7 550.5 558.7 591.1 612.6 642.5 665.1 679.2 695.6 714.2 749.8 759.3 765.6 789.0 796.3 814.9 845.3 853.6 896.5 899.9 917.6 945.8 951.7 977.3 983.0 986.4 993.5 1017.8 1067.6 1097.3 1122.1 1155.7 1168.1 1195.7 1196.6 1212.9 1231.2 1244.0 1261.2 1297.3 1301.9 1338.3 1359.0 1381.6 1385.7 1400.8 1416.3 1426.6 1447.5 1455.8 1511.0 1530.0 1546.3 1565.3 1599.8 1627.9 1632.3 1651.5 2967.2 3155.3 3159.2 3160.2 3168.3 3176.8 3179.4 3184.7 3188.6 3205.0	3637.984 4859.662 8331.557	2

		H 3.0460 -1.7496 -1.2195 H 4.3202 0.3226 -0.9335 O -1.4304 3.3803 1.7019 O -2.7113 2.8235 0.9942			
TS31	-897.141003	C -3.5258 0.9417 0.7608 C -3.0233 -0.4000 0.4152 C -1.7202 -0.5682 -0.0741 C -0.9132 0.5685 -0.3096 C -1.4040 1.9572 -0.2141 C -2.7027 2.1502 0.5165 C 0.3819 2.7730 -0.1286 C 1.1738 1.6276 -0.2465 C 0.4690 0.4171 -0.4146 C 2.5674 1.6568 -0.0865 C 3.1411 2.9148 0.2299 C 2.3343 4.0340 0.3711 C 0.9314 3.9967 0.1649 C 1.1246 -0.8233 -0.4463 C 0.2809 -1.9772 -0.4121 C -1.0743 -1.8509 -0.2221 C 2.5544 -0.7881 -0.3862 C 3.2432 0.3920 -0.2086 N -1.0847 2.8491 -1.2474 H -4.2692 0.9872 1.5519 H -3.6454 -1.2597 0.6345 H -2.8032 3.0324 1.1412 H 0.7236 -2.9660 -0.4702 H -1.6846 -2.7420 -0.1225 H 4.2123 3.0011 0.3744 H 2.7878 4.9848 0.6283 H 0.3345 4.9006 0.1796 H 3.1056 -1.7213 -0.4372 H 4.3246 0.3685 -0.1253 O -1.7247 3.9085 -1.3171 O -3.8245 1.8696 -0.3278	-626.0 81.9 89.3 130.4 142.7 178.0 199.6 220.2 280.1 298.7 325.9 376.2 391.0 393.5 430.1 450.3 470.9 479.0 501.4 527.0 539.1 558.4 576.9 616.6 625.2 645.6 666.0 693.5 706.0 727.0 736.9 757.5 764.2 781.0 795.1 812.6 834.5 843.7 867.6 901.6 931.5 947.6 969.0 976.2 980.5 1002.5 1040.4 1057.9 1092.0 1113.5 1134.8 1158.3 1162.5 1191.9 1200.3 1210.0 1230.7 1246.3 1259.5 1284.6 1339.0 1351.0 1368.9 1392.1 1405.2 1416.8 1431.2 1438.1 1452.5 1455.2 1466.6 1497.4 1516.0 1556.8 1599.1 1626.8 1648.4 3131.4 3145.9 3160.9 3162.8 3166.9 3177.6 3179.4 3182.5 3183.8 3195.1	3599.374 5038.233 8106.134	2
TS32		C -3.6146 0.2704 0.9276 C -3.0037 -0.8832 0.4789 C -1.6263 -0.8836 0.1694 C -0.8800 0.3164 0.3322 C -1.5366 1.4884 0.7838 C -2.8924 1.4651 1.0731 C 0.6087 2.7170 0.6935 C 1.2587 1.5412 0.2422 C 0.5199 0.3339 0.0485 C 2.6581 1.5700 -0.0108 C 3.3717 2.7678 0.2108 C 2.7144 3.8948 0.6613 C 1.3305 3.8835 0.8955			

		C 1.1682 -0.8309 -0.3984 C 0.3983 -2.0224 -0.5700 C -0.9386 -2.0484 -0.2979 C 2.5717 -0.7778 -0.6614 C 3.2852 0.3705 -0.4755 N -0.7947 2.6896 0.8648 H -4.6720 0.2656 1.1657 H -3.5738 -1.7979 0.3615 H -3.3887 2.3628 1.4169 H 0.8996 -2.9178 -0.9225 H -1.5067 -2.9622 -0.4347 H 4.4395 2.7910 0.0244 H 3.2666 4.8118 0.8317 H 0.8292 4.7783 1.2395 H 3.0680 -1.6761 -1.0136 H 4.3500 0.3917 -0.6810 O -1.2294 3.5339 2.0237 O -0.8953 3.0344 3.1722			
TS33	-897.051136	C -3.6200 0.2714 0.0809 C -3.0067 -0.9623 -0.0434 C -1.5972 -1.0787 0.0349 C -0.8660 0.1091 0.2727 C -1.5157 1.3378 0.3486 C -2.8729 1.4646 0.2944 C 0.3388 2.4763 0.8965 C 1.1560 1.3623 0.4465 C 0.5533 0.0965 0.3045 C 2.4534 1.5541 -0.0669 C 2.8740 2.8836 -0.3270 C 2.0033 3.9488 -0.1070 C 0.7732 3.7735 0.5296 C 1.2770 -1.0492 -0.0521 C 0.5344 -2.2624 -0.2286 C -0.8369 -2.2792 -0.1695 C 2.6672 -0.8749 -0.3367 C 3.2144 0.3825 -0.3962 N -0.2913 2.2729 2.2158 H -4.6997 0.3429 0.0020 H -3.6079 -1.8481 -0.2182 H -3.3814 2.4173 0.3873 H 1.0727 -3.1779 -0.4512 H -1.3689 -3.2107 -0.3334 H 3.8612 3.0639 -0.7380 H 2.3230 4.9544 -0.3563 H 0.2010 4.6325 0.8543 H 3.2695 -1.7393 -0.5957 H 4.2399 0.5095 -0.7267 O 0.1853 3.2736 3.1642	-367.5 70.7 87.4 92.1 136.6 164.4 193.7 231.6 255.0 286.5 306.6 363.5 373.5 417.1 437.2 455.5 468.9 498.0 506.4 521.2 524.7 544.4 581.5 594.7 627.6 639.3 666.8 679.2 687.4 730.4 749.0 757.4 762.2 787.2 811.7 817.3 842.8 851.2 856.5 890.4 899.4 932.5 959.9 968.9 973.6 978.9 982.8 1027.2 1051.5 1083.9 1127.9 1133.4 1149.4 1163.8 1168.3 1190.1 1200.3 1219.8 1237.0 1248.8 1296.3 1339.2 1347.3 1389.4 1415.9 1425.8 1437.7 1444.6 1447.6 1483.4 1501.2 1522.3 1539.9 1573.8 1614.5 1627.7 1648.5 3157.4 3158.4 3161.3 3167.5 3173.1 3175.3 3178.4 3182.2 3183.1 3206.9	4003.730 4980.690 7908.431	2

		O -1.1358 3.3614 2.5489			
TS34	-897.092028	C -3.5022 0.4612 -0.0105 C -3.0138 -0.8340 -0.1377 C -1.6168 -1.0682 -0.0585 C -0.8515 0.0703 0.1788 C -1.3082 1.4036 0.2742 C -2.6710 1.5996 0.1905 C -0.0588 2.2633 0.4852 C 1.0480 1.3094 0.3091 C 0.5527 0.0201 0.2027 C 2.3787 1.5892 0.0344 C 2.6749 2.9710 -0.1677 C 1.6190 3.9026 -0.2057 C 0.2791 3.5858 0.0181 C 1.3072 -1.1107 -0.0807 C 0.5254 -2.3067 -0.2758 C -0.8571 -2.2842 -0.2560 C 2.7108 -0.8555 -0.2284 C 3.2147 0.4363 -0.1865 N -0.1883 2.3309 2.3302 H -4.5724 0.6201 -0.0837 H -3.7044 -1.6517 -0.3153 H -3.1230 2.5829 0.2559 H 1.0286 -3.2479 -0.4719 H -1.3937 -3.2113 -0.4304 H 3.6868 3.2996 -0.3767 H 1.8615 4.9307 -0.4533 H -0.4781 4.3557 -0.0626 H 3.3915 -1.6762 -0.4296 H 4.2735 0.5878 -0.3698 O 0.5878 3.3727 2.8466 O -0.8664 3.5090 2.6969	-468.9 31.4 71.2 86.5 120.4 144.3 200.7 244.7 249.1 270.4 291.5 331.1 351.9 416.1 441.4 451.9 456.3 465.3 515.4 538.9 545.6 574.4 592.7 593.4 627.5 643.9 662.9 672.0 708.6 722.7 755.8 765.4 771.4 776.8 806.8 825.6 837.1 840.0 859.2 871.9 926.6 935.8 968.2 972.8 975.6 977.1 985.4 1042.8 1056.1 1060.8 1127.3 1148.4 1157.7 1172.5 1187.3 1201.7 1209.7 1229.0 1244.4 1256.1 1290.4 1333.5 1361.2 1388.0 1405.2 1431.7 1435.5 1452.5 1470.8 1477.5 1497.0 1522.5 1537.9 1621.6 1633.7 1659.4 1671.4 3157.3 3158.5 3161.7 3162.6 3173.8 3174.4 3175.4 3181.1 3185.5 3193.3	3854.956 4887.222 7526.738	2
TS35	-744.782436	C -5.2027 0.6108 -0.0038 C -4.5054 -0.5820 0.0538 C -3.0892 -0.5942 0.1014 C -2.3438 0.6441 0.1260 C -3.1132 1.8514 0.1855 C -4.5140 1.8167 0.0576 C -0.9162 0.5848 -0.0557 C -0.2447 -0.7091 -0.0402 C -1.0177 -1.9084 0.0163 C -2.4212 -1.8257 0.0631 C -0.3543 -3.1646 0.0100 C 1.0176 -3.2413 -0.0324 C 1.7834 -2.0591 -0.0676 C 1.1612 -0.8260 -0.0754 N -0.2331 1.7061 -0.3030	-393.7 60.7 81.9 136.5 151.7 218.9 237.6 286.8 309.9 336.3 360.3 400.4 431.0 473.9 493.9 519.3 540.7 562.8 598.3 623.7 636.2 653.4 654.5 674.5 731.3 748.4 774.7 782.8 806.6 837.7 858.2 871.3 884.4 899.7 917.0 960.6 979.4 985.6 993.0 1048.7 1063.6 1102.3 1135.9 1173.6 1175.5 1189.8 1202.8 1209.3 1246.3 1274.6 1307.9 1330.3 1371.9 1393.6 1404.9 1422.1 1450.7 1469.7 1498.3 1535.5 1558.6 1576.1 1584.9 1636.1 1644.1 1966.0 3165.2	1966.650 4806.353 6659.686	2

		H -6.2847 0.6124 -0.0645 H -5.0312 -1.5296 0.0381 H -5.0350 2.7658 0.0739 H -3.0056 -2.7389 0.0529 H -0.9547 -4.0673 0.0431 H 1.5117 -4.2060 -0.0330 H 2.8654 -2.1156 -0.0840 H 1.7885 0.0572 -0.0899 H 0.7698 1.6168 -0.3801 O -2.6622 3.1044 0.3468 O -1.4889 3.2658 1.1125 H -0.6262 2.5847 0.2456	3170.8 3172.2 3175.2 3182.7 3188.3 3194.3 3202.5 3610.1		
TS36	-744.764901	C -5.1929 0.2555 0.4039 C -4.4463 -0.8698 0.0809 C -3.0222 -0.8324 0.0321 C -2.3399 0.3938 0.2798 C -3.1233 1.5444 0.7202 C -4.5528 1.4442 0.7156 C -0.8881 0.4551 0.0764 C -0.1545 -0.8300 0.0097 C -0.8777 -2.0390 -0.1992 C -2.2915 -2.0082 -0.2405 C -0.1634 -3.2547 -0.3471 C 1.2122 -3.2822 -0.2554 C 1.9206 -2.0943 -0.0097 C 1.2422 -0.8909 0.1143 N -0.3203 1.6102 -0.1123 H -6.2752 0.1969 0.4262 H -4.9434 -1.8082 -0.1388 H -5.0974 2.3343 1.0044 H -2.8319 -2.9291 -0.4311 H -0.7199 -4.1691 -0.5227 H 1.7467 -4.2191 -0.3617 H 2.9995 -2.1168 0.0885 H 1.8115 0.0088 0.3193 H 0.6790 1.5092 -0.2881 O -2.5902 2.5973 1.1899 O -2.0789 3.8439 -0.3443 H -1.2840 3.2633 -0.3556	-245.4 58.0 64.7 103.3 129.8 157.0 202.8 225.4 263.5 292.3 329.9 365.5 405.6 431.5 476.4 489.9 514.4 532.1 572.6 586.2 594.1 618.9 639.2 654.5 678.3 708.8 753.5 765.6 802.9 810.3 815.1 836.9 848.6 874.5 881.9 899.1 909.9 967.4 983.8 994.9 1051.9 1076.2 1085.8 1127.2 1148.5 1175.9 1186.6 1197.6 1226.9 1258.9 1281.4 1314.2 1328.6 1350.1 1363.1 1390.6 1431.4 1446.7 1487.8 1497.5 1520.5 1536.4 1559.3 1583.4 1627.9 3164.2 3167.0 3168.5 3171.7 3181.4 3183.6 3193.8 3206.2 3480.4 3489.5	2044.985 5039.276 6878.932	2
TS37	-668.860979	C -5.1738 0.6448 0.0347 C -4.5763 -0.6087 0.0766 C -3.1650 -0.7434 0.1679 C -2.3996 0.4585 0.3102 C -3.0345 1.6988 0.1428 C -4.4119 1.8267 0.0277 C -1.0165 0.4436 0.4587 C -0.2781 -0.7464 0.2281 C -1.0349 -1.9641 0.0183	-833.2 85.7 100.1 172.7 212.2 234.4 260.7 304.5 357.6 375.9 418.6 439.4 497.3 498.5 511.6 549.7 576.1 591.8 611.1 616.5 665.1 710.5 724.7 750.3 759.7 781.0 797.1 830.6 868.6 874.9 880.8 921.6 963.1 965.6 986.2 987.3 1037.3 1053.0 1072.2 1137.0 1161.5 1180.6 1191.8	1561.215 4321.310 5840.767	3

		C -2.4501 -1.9488 0.0548 C -0.3104 -3.1708 -0.1859 C 1.0659 -3.1884 -0.1730 C 1.7959 -2.0024 0.0597 C 1.1322 -0.8110 0.2697 N -0.8820 2.3696 0.0649 H -6.2515 0.7182 -0.0518 H -5.1884 -1.4997 -0.0115 H -4.8694 2.7978 -0.1111 H -2.9883 -2.8850 -0.0480 H -0.8653 -4.0858 -0.3667 H 1.5954 -4.1200 -0.3387 H 2.8793 -2.0319 0.0784 H 1.6849 0.1027 0.4564 H -0.3544 3.0602 -0.4871 O -2.1980 2.7479 -0.0786	1212.7 1231.1 1266.1 1299.3 1329.4 1351.0 1368.9 1393.6 1427.7 1448.7 1470.4 1489.7 1519.3 1558.4 1562.8 1599.2 1629.9 3155.4 3165.6 3167.4 3168.9 3177.9 3184.1 3189.7 3203.5 3320.8		
TS38	-668.894639	C -5.1375 0.6540 -0.0147 C -4.5065 -0.5595 -0.0001 C -3.0787 -0.6683 -0.0008 C -2.2818 0.5468 -0.0174 C -3.0410 1.7257 -0.0314 C -4.3741 1.8696 -0.0313 C -0.8872 0.4717 -0.0185 C -0.2338 -0.7650 -0.0037 C -1.0145 -1.9786 0.0130 C -2.4117 -1.8961 0.0139 C -0.3290 -3.2321 0.0280 C 1.0373 -3.2859 0.0266 C 1.8078 -2.0878 0.0102 C 1.1915 -0.8674 -0.0045 N -2.6252 4.5076 -0.0672 H -6.2201 0.7132 -0.0139 H -5.0900 -1.4736 0.0124 H -4.8555 2.8425 -0.0430 H -2.9949 -2.8119 0.0265 H -0.9158 -4.1446 0.0405 H 1.5441 -4.2442 0.0381 H 2.8900 -2.1510 0.0094 H 1.7768 0.0458 -0.0170 H -0.3085 1.3874 -0.0310 O -1.9930 3.5046 -0.0554	-254.8 49.4 71.1 82.1 93.2 142.4 234.4 234.8 268.0 316.5 391.1 394.1 425.6 475.4 486.4 518.9 524.7 571.3 606.9 632.8 654.0 725.8 753.6 759.3 768.1 777.6 821.6 852.1 873.8 889.6 902.5 905.4 924.8 970.7 978.6 996.2 1025.6 1031.9 1105.5 1162.9 1171.0 1176.9 1193.6 1241.8 1285.6 1292.6 1323.1 1359.2 1382.3 1400.0 1423.9 1451.7 1478.1 1498.9 1534.5 1551.8 1584.9 1621.8 1664.5 1677.6 3156.0 3158.3 3160.5 3165.5 3167.8 3177.8 3184.5 3189.0 3190.6	1706.916 5195.233 6902.149	3
TS40	-668.846953	C -5.3931 0.4027 0.1052 C -4.6654 -0.7532 0.1647 C -3.2359 -0.7397 0.1105 C -2.5601 0.5528 0.1439 C -3.3674 1.6794 -0.0177 C -4.7166 1.6456 -0.1283 C -1.1345 0.5192 0.2199	-293.3 79.0 109.4 113.8 209.0 224.1 233.8 270.6 358.9 394.3 402.6 432.0 471.2 490.0 515.6 546.3 562.3 587.7 647.2 673.4 693.3 743.1 748.6 761.5 798.2 804.4 834.6 862.0 870.6 893.3 910.4 942.8 965.7 978.4 998.1	1840.767 4025.300 5786.366	1

		C -0.3855 -0.6567 0.0439 C -1.0889 -1.9082 -0.0430 C -2.4869 -1.9136 0.0439 C -0.3351 -3.1138 -0.1645 C 1.0317 -3.0853 -0.2106 C 1.7240 -1.8461 -0.1186 C 1.0406 -0.6682 0.0197 N -0.5135 1.7664 0.4158 H -6.4772 0.3769 0.1470 H -5.1661 -1.7146 0.2048 H -5.2936 2.5157 -0.4295 H -3.0052 -2.8676 0.0806 H -0.8707 -4.0552 -0.2231 H 1.5945 -4.0061 -0.3108 H 2.8074 -1.8382 -0.1548 H 1.5736 0.2711 0.0958 H -0.8625 2.2871 1.2260 O -0.1709 2.5070 -0.5539	1035.4 1040.5 1059.7 1106.2 1163.7 1177.8 1197.4 1203.8 1247.3 1268.1 1295.7 1324.5 1353.2 1365.4 1383.5 1414.6 1441.3 1459.2 1475.2 1505.5 1540.4 1565.3 1605.1 1625.1 1661.2 3135.5 3151.9 3159.5 3164.1 3173.9 3178.1 3188.0 3199.8 3374.7		
TS41	-668.899747	C -5.4561 0.3804 -0.0024 C -4.7213 -0.7780 -0.0345 C -3.2965 -0.7537 0.0036 C -2.6514 0.5407 0.0776 C -3.4387 1.7184 0.1092 C -4.8115 1.6393 0.0701 C -1.2362 0.5312 0.1140 C -0.5070 -0.6823 0.0794 C -1.1427 -1.9467 0.0070 C -2.5504 -1.9518 -0.0300 C -0.2789 -3.0836 -0.0207 C 1.0876 -2.9317 0.0216 C 1.7096 -1.6416 0.0948 C 0.8851 -0.5606 0.1211 N -0.3454 1.5666 0.1829 H -6.5388 0.3350 -0.0325 H -5.2196 -1.7399 -0.0901 H -5.4053 2.5455 0.0947 H -3.0833 -2.8953 -0.0856 H -0.7117 -4.0765 -0.0758 H 1.7244 -3.8097 -0.0005 H 2.7903 -1.5637 0.1265 H 0.7240 0.9640 0.1842 O -0.5167 2.7966 0.2328 H -2.9400 2.6776 0.1646	-1876.7 83.4 115.7 132.7 205.0 231.8 257.3 287.6 303.3 376.3 407.0 427.8 477.3 479.3 499.0 542.3 561.8 593.3 620.2 645.0 673.2 713.3 720.5 751.2 761.2 771.1 842.8 872.4 875.7 888.7 893.2 958.4 968.3 974.5 978.9 997.8 1024.8 1044.1 1058.9 1128.5 1169.1 1181.8 1191.7 1218.3 1230.2 1289.4 1315.9 1356.6 1375.2 1381.3 1427.2 1440.9 1472.0 1489.0 1514.1 1541.1 1564.7 1592.9 1627.2 1645.4 1853.7 3160.0 3161.9 3166.7 3175.0 3175.6 3183.9 3187.1 3203.1	1818.211 3999.836 5818.048	3
TS42	-744.734603	C 0.0000 0.0000 0.0000 C 0.0000 0.0000 1.4402 C 1.2183 0.0000 2.1233 C 2.4453 -0.0227 1.4531 C 2.4652 -0.0626 0.0122	-450.6 47.6 72.4 91.4 118.2 186.6 226.9 241.4 248.7 319.5 344.2 373.7 398.0 423.9 433.4 476.2 501.2 538.9 567.6 578.6 620.4 649.4 660.8 704.7 749.1	2990.004 4187.683 6911.861	2

		C 1.2349 -0.0200 -0.6891 C 3.7344 -0.1406 -0.6360 C 4.8987 -0.1489 0.0854 C 4.8770 -0.0840 1.5049 C 3.6822 -0.0276 2.1666 C -1.2547 0.0313 -0.6795 C -2.4291 0.0442 0.0231 C -2.4312 0.0287 1.4461 C -1.2503 0.0112 2.1334 N 1.1800 0.0211 -2.0989 H 1.2136 0.0149 3.2089 H 3.7880 -0.2199 -1.7152 H 5.8499 -0.2148 -0.4306 H 5.8100 -0.0889 2.0563 H 3.6527 0.0112 3.2504 H -1.2540 0.0479 -1.7606 H -3.3739 0.0685 -0.5086 H -3.3746 0.0364 1.9799 H -1.2410 0.0060 3.2181 H 2.0297 0.3954 -2.5174 O 1.2707 -1.7585 -2.7586 O 1.9079 -1.8176 -3.8624	752.0 771.0 800.6 833.8 861.9 873.9 879.8 889.6 908.5 937.8 974.2 982.8 994.5 1007.8 1019.9 1034.7 1039.9 1122.5 1132.8 1168.8 1179.4 1186.8 1192.6 1213.0 1250.6 1258.6 1298.8 1334.7 1382.8 1399.4 1413.7 1416.0 1472.0 1481.6 1507.3 1565.8 1570.3 1612.6 1657.2 1662.6 3158.4 3162.4 3163.7 3171.0 3172.6 3183.6 3187.3 3192.7 3216.1 3506.4		
TS43	-744.699898	C -13.7724 -0.5603 -0.0513 C -12.9662 -1.7494 -0.0023 C -11.5661 -1.6600 0.0561 C -10.8995 -0.4234 0.0509 C -11.6515 0.7921 -0.0004 C -13.1019 0.7184 -0.0174 C -10.9465 2.0179 -0.0286 C -9.5689 2.0482 0.0066 C -8.8249 0.8498 0.0703 C -9.4782 -0.3567 0.0896 C -15.1791 -0.7090 -0.1236 C -15.7625 -1.9608 -0.1381 C -14.9728 -3.1267 -0.0815 C -13.6052 -3.0198 -0.0162 N -13.7286 1.8981 -0.0091 H -10.9824 -2.5733 0.0972 H -11.4862 2.9532 -0.0896 H -9.0540 3.0014 -0.0184 H -7.7421 0.8867 0.0986 H -8.9196 -1.2854 0.1321 H -15.8125 0.1621 -0.1727 H -16.8416 -2.0424 -0.1953 H -15.4450 -4.1022 -0.0927 H -12.9846 -3.9083 0.0239 H -13.6777 3.0584 0.2373 O -15.0697 2.0895 0.0381	-1673.8 27.5 74.9 104.9 130.0 153.7 177.6 234.7 246.3 301.1 349.8 380.9 407.7 415.0 438.4 473.4 506.1 538.8 590.3 619.2 634.0 653.5 686.4 739.8 745.3 767.5 773.3 798.0 826.6 842.9 869.3 878.0 885.0 919.8 942.9 966.5 974.7 983.5 995.0 1000.4 1050.9 1056.9 1116.5 1128.6 1167.3 1177.2 1181.2 1211.1 1214.8 1249.5 1271.2 1309.9 1348.2 1366.3 1378.8 1423.7 1439.4 1477.4 1483.8 1510.7 1549.6 1569.1 1583.4 1628.8 1644.8 2278.8 3165.0 3166.4 3170.9 3178.1 3179.1 3190.8 3191.6 3207.4 3250.2	2857.91 4110.771 6954.934	2

		O -15.0064 3.5045 0.3445			
TS44	-744.740579	C -13.8737 -0.7402 -0.1303 C -12.9966 -1.8677 -0.0320 C -11.6175 -1.6561 0.0924 C -11.0557 -0.3702 0.1065 C -11.8962 0.7934 -0.0076 C -13.3236 0.5970 -0.0972 C -11.2599 2.0613 -0.0288 C -9.8903 2.1771 0.0846 C -9.0720 1.0355 0.2213 C -9.6462 -0.2097 0.2263 C -15.2667 -0.9802 -0.2372 C -15.7626 -2.2633 -0.2483 C -14.8960 -3.3793 -0.1542 C -13.5443 -3.1839 -0.0478 N -14.2749 1.5617 -0.2170 H -10.9585 -2.5144 0.1782 H -11.8544 2.9542 -0.1325 H -9.4381 3.1621 0.0639 H -7.9975 1.1453 0.3119 H -9.0330 -1.0998 0.3177 H -15.9332 -0.1322 -0.3111 H -16.8318 -2.4226 -0.3303 H -15.3054 -4.3829 -0.1663 H -12.8668 -4.0276 0.0274 O -13.9313 2.7794 -0.0922 O -15.1542 3.5810 0.7815 H -15.2919 4.2919 0.1367	-595.0 47.1 76.5 93.6 107.4 131.1 170.2 224.7 237.9 250.6 308.6 364.5 381.4 402.4 425.0 432.3 478.2 508.2 544.6 574.6 615.2 634.1 655.1 675.0 728.8 748.9 751.9 771.0 794.3 862.1 873.0 874.8 891.7 899.7 954.7 977.6 982.4 998.4 1005.9 1038.3 1043.2 1054.5 1087.1 1115.0 1128.9 1175.2 1184.6 1197.0 1208.4 1243.0 1266.6 1308.7 1335.7 1351.1 1381.4 1407.8 1419.0 1468.9 1478.6 1504.8 1548.0 1568.7 1590.0 1634.9 1649.6 3160.7 3163.7 3165.7 3174.4 3175.5 3188.5 3189.6 3216.1 3248.7 3772.9	2939.715 4155.348 7017.567	2
TS45	-744.578605	C -13.7527 -0.5604 0.0647 C -12.9684 -1.7668 0.0953 C -11.5752 -1.6766 0.0515 C -10.9153 -0.4502 -0.0441 C -11.6779 0.7776 -0.0739 C -13.0783 0.6745 0.0178 C -10.9608 2.0059 -0.2362 C -9.5963 2.0163 -0.3286 C -8.8455 0.8101 -0.2645 C -9.4901 -0.3856 -0.1300 C -15.1770 -0.6732 0.0941 C -15.7778 -1.9016 0.1542 C -15.0037 -3.0936 0.1989 C -13.6389 -3.0252 0.1701 N -13.9378 1.8362 -0.0701 H -10.9870 -2.5884 0.0795 H -11.4974 2.9414 -0.2957 H -9.0778 2.9597 -0.4558 H -7.7645 0.8464 -0.3336	-849.6 65.3 79.0 103.4 117.1 181.7 225.7 234.0 251.8 332.0 353.7 371.5 400.1 403.9 425.4 442.1 478.9 498.5 520.4 573.2 577.4 618.3 651.2 665.0 670.6 716.8 746.7 749.9 767.9 801.0 832.9 855.9 865.9 877.0 884.2 908.8 949.2 974.1 979.1 992.9 998.1 1030.5 1039.3 1044.0 1117.2 1130.8 1174.8 1183.2 1203.8 1210.1 1258.0 1290.4 1307.2 1348.5 1361.7 1401.2 1418.2 1426.5 1480.3 1483.3 1518.7 1568.8 1589.1 1616.6 1660.3 1667.1 3160.5 3164.0 3165.5 3174.7 3175.2 3188.5 3189.3 3206.7 3219.6	2397.210 4151.334 6373.133	2

		H -8.9316 -1.3149 -0.0956 H -15.7847 0.2212 0.0613 H -16.8596 -1.9691 0.1697 H -15.5026 -4.0542 0.2531 H -13.0390 -3.9284 0.2010 O -13.4896 2.9144 0.7202 O -14.5641 2.1147 1.2794 H -13.7684 2.4774 -1.7299			
O ₂	-150.370414	O -2.0403 1.9378 0.7143 O -2.6754 2.9322 0.9626	1632.9589	0 41.521 41.521	3
NO	-129.931655	N -3.9616 1.0039 0.0000 O -2.8137 0.9912 0.0000	1980.0513	0 35.141 35.141	2
NO ₂	-205.140695	N -4.0717 1.3066 0.0000 O -2.9742 0.8380 0.0000 O -5.1741 0.8497 0.0000	764.711 1391.122 1701.569	7.4458 138.219 145.665	2
OH	-75.762412	H -5.4728 0.4245 0.1201 O -5.0760 1.3025 -0.0351	3707.8141	0 3.224 3.224	2
H	-0.502257	H 0.0000 0.0000 0.0000	0	0	2