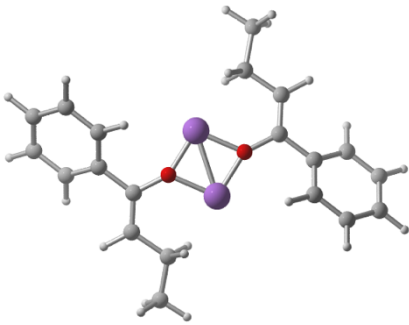
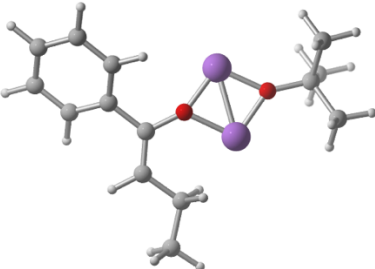


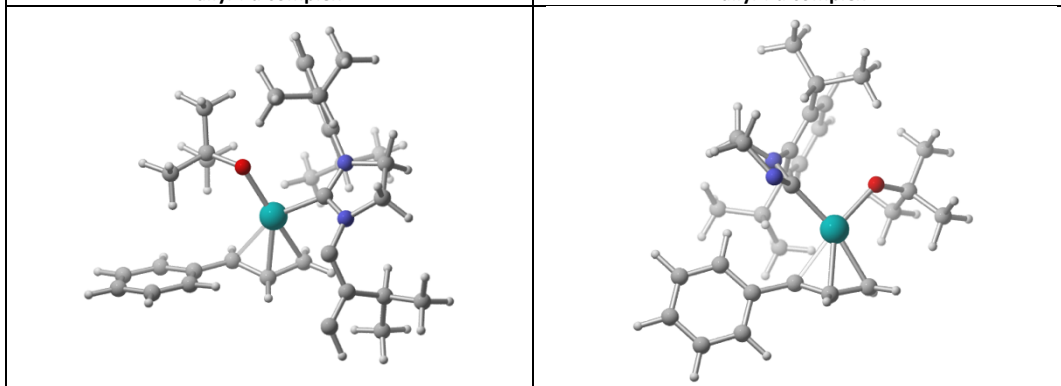
## Energies and coordinates of calculated structures

Energies are in hartree; cartesian coordinates are in angstrom. Pictures are generated by CYLview [Legault, C. Y.mCYLview, 1.0b. Université de Sherbrooke. <http://www.cylview.org> (2009)]. Carbon and hydrogen atoms are in grey, oxygen in red, nitrogen in blue, palladium in turquoise. Some atoms of the bulky substituent on NHC are omitted for clarity.

lithium enolate				<sup>t</sup> BuOLi			
							
Gas phase energy= -159.313305075				Gas phase energy= -124.107569174			
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C	2.4985070000	1.0051220000	0.0252230000	C	-1.3198400000	0.6631750000	-0.0831700000
O	1.3012720000	0.3909920000	0.1745420000	O	-0.0965060000	0.0859000000	-0.1166550000
C	3.6936090000	0.1160610000	0.0529590000	C	-2.4818890000	-0.2678960000	-0.0263240000
C	3.6708040000	-1.0603170000	0.8178220000	C	-2.3941370000	-1.5296930000	-0.6335550000
C	4.8485960000	0.4120960000	-0.6872360000	C	-3.6696690000	0.0765620000	0.6370650000
C	4.7755640000	-1.9116670000	0.8539940000	C	-3.4691750000	-2.4180230000	-0.5942070000
H	2.7901560000	-1.2872180000	1.4120250000	H	-1.4847380000	-1.7963450000	-1.1632900000
C	5.9539250000	-0.4382120000	-0.6510850000	C	-4.7449090000	-0.8116240000	0.6774620000
H	4.8690400000	1.3002390000	-1.3102220000	H	-3.7403020000	1.0353060000	1.1402330000
C	5.9223800000	-1.6036320000	0.1185570000	C	-4.6496490000	-2.0622110000	0.0622710000
H	4.7454160000	-2.8112960000	1.4604850000	H	-3.3884280000	-3.3850820000	-1.0803210000
H	6.8372400000	-0.1966790000	-1.2330150000	H	-5.6542040000	-0.5321370000	1.1993850000
H	6.7809140000	-2.2662630000	0.1421890000	H	-5.4849460000	-2.7535140000	0.0970350000
H	3.5263470000	2.8494930000	-0.1942170000	H	-2.4258890000	2.4740400000	-0.1524320000
C	1.3185830000	3.1906420000	-0.1584510000	C	-0.2334580000	2.9033620000	-0.1672040000
C	1.5968610000	4.6843840000	-0.3615650000	C	-0.5759370000	4.3974970000	-0.1464480000
H	0.6508730000	2.8481960000	-0.9745180000	H	0.4290980000	2.6852720000	0.6940290000
H	0.7529280000	3.0671220000	0.7874480000	H	0.3570600000	2.6960590000	-1.0833770000
H	0.6709400000	5.2685020000	-0.3695420000	H	0.3258250000	5.0176020000	-0.1803110000
H	2.1133130000	4.8519130000	-1.3125170000	H	-1.1290470000	4.6504520000	0.7642060000
H	2.2354460000	5.0675870000	0.4412520000	H	-1.2024070000	4.6599120000	-1.0055040000
C	-2.5663930000	-2.3464890000	-0.1247390000	O	2.5891180000	-0.5011570000	0.0630090000
C	-2.4984680000	-1.0051040000	0.0250780000	Li	1.5270390000	0.8928360000	-0.2327880000
O	-1.3011980000	-0.3909570000	0.1739570000	Li	1.0022900000	-1.2605180000	0.2045630000
C	-3.6935680000	-0.1160400000	0.0529200000	C	3.9857190000	-0.7700500000	0.1010680000
C	-3.6708160000	1.0602100000	0.8179810000	C	4.4434010000	-0.8441160000	1.5678600000
C	-4.8484740000	-0.4119370000	-0.6874440000	C	4.2571960000	-2.1084840000	-0.6072140000
C	-4.7755800000	1.9115450000	0.8542250000	C	4.7266050000	0.3665710000	-0.6254110000
H	-2.7902190000	1.2870280000	1.4123000000	H	4.2219750000	0.1025060000	2.0727300000
C	-5.9538120000	0.4383650000	-0.6512340000	H	3.8988720000	-1.6417420000	2.0859430000
H	-4.8688340000	-1.2999710000	-1.3105920000	H	5.5182140000	-1.0441950000	1.6523240000
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H	-4.7454900000	2.8110560000	1.4608920000	H	5.3247160000	-2.3577320000	-0.6180450000

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H	-6.7808680000	2.2662680000	0.1423030000	H	5.8117360000	0.2121110000	-0.6352030000
H	-3.5264370000	-2.8494590000	-0.1937290000	H	4.3756920000	0.4326120000	-1.6619480000
C	-1.3186720000	-3.1907050000	-0.1585220000	H	4.5232960000	1.3215190000	-0.1238080000
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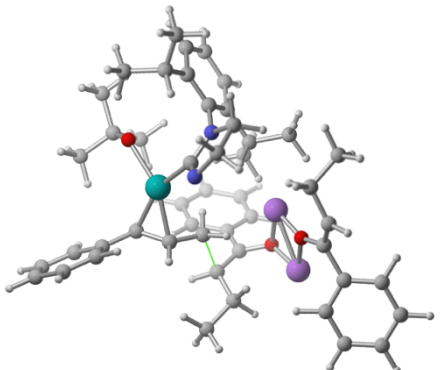
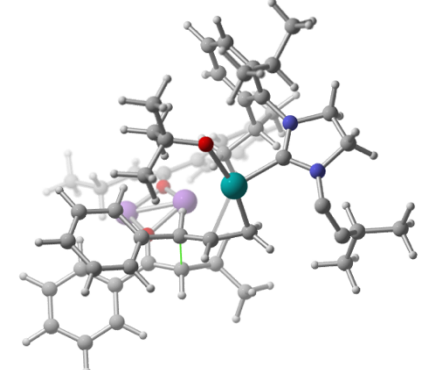
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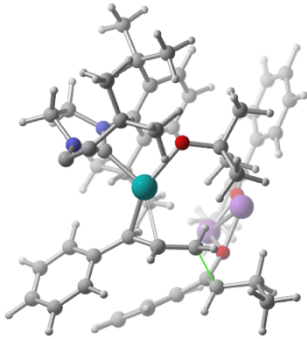
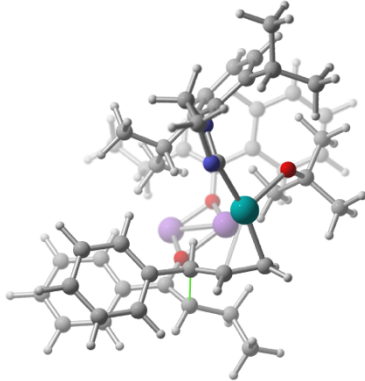
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C	2.1800210000	0.1023910000	-1.8540370000	C	1.5496130000	0.6663860000	-2.7397280000
C	1.0406050000	0.7492740000	-2.3928470000	C	1.5242730000	1.6056100000	-1.6862280000
H	2.9100740000	0.6897360000	-1.3027330000	H	2.3615310000	-0.0551180000	-2.7904100000
H	0.4991830000	0.2932320000	-3.2206920000	H	0.8198150000	2.4350960000	-1.8033470000
Pd	0.4078250000	-0.4102760000	-0.7143090000	Pd	-0.1080930000	0.1490350000	-1.4089440000
C	3.2595940000	-2.0524320000	-1.0709300000	C	0.7338750000	-1.0021430000	2.6885980000
C	3.5882220000	-3.3592560000	-1.4635220000	C	-0.1463010000	0.2286820000	2.9381530000
C	3.9183350000	-1.5042550000	0.0443840000	H	0.2656920000	-1.9362320000	3.0163670000
C	4.5402550000	-4.0996180000	-0.7622460000	H	-0.9440670000	0.0518380000	3.6593630000
H	3.0807400000	-3.8009730000	-2.3165950000	C	-0.0094270000	-0.1408410000	0.6154530000
C	4.8726390000	-2.2419820000	0.7402360000	N	0.8631760000	-0.9931260000	1.2128570000
H	3.6505920000	-0.5124190000	0.3976930000	N	-0.6936820000	0.5019210000	1.5913280000
C	5.1871260000	-3.5450800000	0.3433650000	C	-1.9602040000	1.1676030000	1.4286300000
H	4.7714670000	-5.1123520000	-1.0753900000	C	-2.0204440000	2.4949820000	0.9686870000
H	5.3583640000	-1.8065720000	1.6074490000	C	-3.1225490000	0.4496580000	1.7718840000
H	5.9205320000	-4.1230890000	0.8953440000	C	-3.2757190000	3.1030490000	0.8650380000
H	0.9740520000	1.8287980000	-2.3458190000	C	-4.3563960000	1.0977980000	1.6534050000
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H	-1.4734450000	3.2442520000	1.8731710000	H	-5.2665780000	0.5627580000	1.9064780000
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C	-0.8448280000	1.0666230000	-0.0763110000	C	0.8441220000	-3.0593590000	-0.1266750000
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C	-3.0742120000	0.0111800000	-0.2158780000	C	3.6560840000	-3.0847070000	-0.1204210000
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C	-4.5304530000	-1.5862620000	0.8325860000	C	-0.6719080000	-3.1870490000	-0.0304030000
C	-4.8162150000	-2.1324020000	-0.4172290000	H	-1.1187910000	-2.2002590000	0.1120250000

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H	-4.9765990000	-2.0202780000	1.7217430000	H	3.1567120000	-0.2018780000	1.5925170000
C	1.0072860000	2.5030440000	0.6627240000	C	-3.0844230000	-0.9846010000	2.2890980000
C	1.5954670000	1.7745940000	1.7218150000	H	-2.0485050000	-1.3382270000	2.2601050000
C	1.7467230000	3.4348320000	-0.0942270000	C	-0.7561720000	3.2573180000	0.6129440000
C	2.9590120000	1.9701720000	1.9706300000	H	-0.0156630000	2.5137820000	0.3183490000
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C	3.7102840000	2.8668140000	1.2154770000	H	3.4865310000	-4.8477290000	-1.3393060000
H	3.4373510000	1.4160600000	2.7703770000	C	-0.9299430000	4.2012930000	-0.5849560000
H	3.6958750000	4.3089270000	-0.3716500000	H	0.0468570000	4.5957490000	-0.8884490000
C	0.7894860000	0.8524710000	2.6306380000	H	-1.5659430000	5.0607890000	-0.3445320000
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H	-2.0026510000	0.8164600000	-2.4608010000	H	5.7354560000	-1.2587210000	0.3266760000
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H	-1.5166760000	-0.5463900000	-4.4448780000	H	3.5137460000	-2.1230190000	3.2453570000
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H	1.2230190000	1.9371640000	4.4781030000	H	-4.9249820000	-1.6271520000	1.2863500000
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H	-1.2465810000	-2.1352200000	2.4639220000	H	1.4299250000	-0.8529990000	0.0832190000
C	-0.0002260000	-0.3898680000	2.0463150000	C	-0.2121540000	-1.9022810000	0.9977950000
C	0.9489910000	-1.0880800000	1.2207720000	C	-0.8883670000	-0.8589570000	1.7561800000
H	0.3364310000	0.5137220000	2.5502280000	H	-0.6052100000	-2.9118240000	1.1196930000
H	0.5197970000	-1.8903090000	0.6272780000	H	-0.3446650000	0.0284170000	2.0851270000
Pd	-1.4988600000	-0.1797500000	0.5496290000	Pd	-1.7124570000	-0.6631250000	-0.0937880000
C	-1.9846040000	-0.4581490000	3.6142580000	C	1.5283500000	-2.9106410000	-0.5122320000
C	-2.6951770000	-1.2798440000	4.5064370000	C	2.1478860000	-2.5724580000	-1.7201010000
C	-2.0356860000	0.9334560000	3.8218180000	C	1.3033750000	-4.2638570000	-0.2318560000
C	-3.4339200000	-0.7356840000	5.5575390000	C	2.5154080000	-3.5563870000	-2.6376370000
H	-2.6737450000	-2.3575920000	4.3644370000	H	2.3208630000	-1.5277430000	-1.9554460000
C	-2.7665720000	1.4768420000	4.8755200000	C	1.6814440000	-5.2515520000	-1.1401420000
H	-1.5300280000	1.5970160000	3.1277100000	H	0.8255600000	-4.5490430000	0.7003310000
C	-3.4729260000	0.6470760000	5.7512580000	C	2.2866160000	-4.9014750000	-2.3492530000
H	-3.9821280000	-1.3930400000	6.2254370000	H	2.9678880000	-3.2702210000	-3.5817400000
H	-2.7948490000	2.5550670000	5.0026900000	H	1.4956880000	-6.2950060000	-0.9092430000
H	-4.0490260000	1.0714370000	6.5673240000	H	2.5672090000	-5.6695560000	-3.0617980000
H	1.6570520000	-0.4502840000	0.6844400000	H	-1.6077070000	-1.1943870000	2.5048210000
C	-0.5950290000	3.1505440000	-2.0861600000	C	-4.7882980000	2.1123950000	1.2067970000
C	-0.6013990000	2.0393430000	-3.1443830000	C	-3.9626880000	3.0302450000	0.2975570000
H	-1.4316160000	3.8505160000	-2.1964610000	H	-5.7711630000	1.8727800000	0.7822480000
H	-1.2899890000	2.2372130000	-3.9683900000	H	-4.5648730000	3.5593580000	-0.4441780000
C	-1.0680130000	1.0765320000	-1.0224420000	C	-3.0027940000	0.8612260000	0.2654900000
N	-0.7457090000	2.3830700000	-0.8333490000	N	-3.9489250000	0.8967060000	1.2453840000
N	-1.0414500000	0.8623380000	-2.3633950000	N	-3.0502850000	2.0690240000	-0.3516640000
C	-1.6276960000	-0.2585180000	-3.0342440000	C	-2.3856190000	2.3925670000	-1.5749290000
C	-0.9072600000	-1.4538580000	-3.1829690000	C	-1.0404810000	2.7909230000	-1.5577940000
C	-2.9227510000	-0.1020380000	-3.5630310000	C	-3.1258400000	2.3097290000	-2.7680250000
C	-1.4985810000	-2.4984320000	-3.9027880000	C	-0.4268350000	3.1031000000	-2.7757310000
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C	-2.7714930000	-2.3558150000	-4.4487850000	C	-1.1381320000	3.0162520000	-3.9703680000
H	-0.9707950000	-3.4370170000	-4.0353000000	H	0.6161390000	3.4092350000	-2.7935520000
H	-4.4793940000	-1.0756780000	-4.6804610000	H	-3.0162430000	2.5463940000	-4.9027670000
C	-0.8490810000	3.0617870000	0.4244380000	C	-4.3327970000	-0.2372340000	2.0285330000
C	-2.1263630000	3.3517300000	0.9480390000	C	-4.9646810000	-1.3297480000	1.3992040000
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C	-2.1918790000	4.0713800000	2.1472490000	C	-5.3386680000	-2.4155760000	2.2002110000
C	0.2158820000	4.1655710000	2.2833440000	C	-4.4818120000	-1.3238270000	4.1753490000
C	-1.0360670000	4.4766560000	2.8091410000	C	-5.1036290000	-2.4150520000	3.5729990000
H	-3.1620530000	4.3016840000	2.5749020000	H	-5.8208150000	-3.2723230000	1.7411640000
H	1.1118400000	4.4783910000	2.8108370000	H	-4.3010910000	-1.3328250000	5.2463600000

C	-3.4149200000	2.9279670000	0.2545160000	C	-5.2792500000	-1.3461320000	-0.0923050000
H	-3.1677390000	2.2212900000	-0.5414760000	H	-4.7078300000	-0.5551100000	-0.5833830000
C	1.7043420000	3.1348140000	0.5122140000	C	-3.4009620000	0.9639510000	4.0893390000
H	1.5665520000	2.4114050000	-0.2999450000	H	3.0275830000	1.6224590000	3.2964420000
C	-3.7354180000	1.1705640000	-3.3568530000	C	-4.5908100000	1.8917140000	-2.7692350000
H	-3.1143620000	1.8905940000	-2.8146440000	H	-4.8997670000	1.7536030000	-1.7279270000
C	0.4929000000	-1.6159220000	-2.6007510000	C	-0.2688450000	2.9013170000	-0.2510880000
H	0.5883360000	-0.8459310000	-1.8176180000	H	-0.9396690000	2.5836430000	0.5537280000
H	-3.2196210000	-3.1779860000	-4.9964220000	H	-0.6467250000	3.2462510000	-4.9099420000
H	-1.1106620000	5.0273040000	3.7410890000	H	-5.4051840000	-3.2669170000	4.1740610000
C	0.6844400000	-2.9977020000	-1.9552170000	C	0.9326940000	1.9389630000	-0.2184270000
H	1.6720010000	-3.1174060000	-1.4901950000	H	1.4199090000	2.0360520000	0.7669230000
H	0.6186570000	-3.7996730000	-2.6969260000	H	1.6594070000	2.1711240000	-1.0090270000
H	-0.0733530000	-3.1832490000	-1.1884260000	H	0.5635340000	0.9163450000	-0.3530440000
C	1.5570400000	-1.3592200000	-3.6874530000	C	0.1596360000	4.3510980000	0.0269440000
H	1.4176010000	-0.3780680000	-4.1473640000	H	-0.7079500000	5.0190660000	0.0242010000
H	1.4818700000	-2.1185340000	-4.4745180000	H	0.8604470000	4.7113280000	-0.7360870000
H	2.5871460000	-1.3971220000	-3.2978070000	H	0.6495990000	4.4240740000	1.0052090000
C	2.6287350000	2.4802600000	1.5503910000	C	-2.1884380000	0.5482530000	4.9417050000
H	2.8906050000	3.1753340000	2.3562730000	H	-2.4879510000	-0.0905860000	5.7803620000
H	3.5568630000	2.1658420000	1.0612310000	H	-1.7025450000	1.4376070000	5.3599040000
H	2.1499680000	1.6066490000	2.0019350000	H	-1.4547200000	0.0029640000	4.3422140000
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H	1.7441000000	4.8768620000	-0.8219390000	H	-5.2898140000	2.0484520000	4.3724350000
H	3.3352240000	4.1374850000	-0.5242150000	H	-3.9434750000	2.6546870000	5.3634780000
H	2.5563130000	5.1319840000	0.7263800000	H	-4.7576400000	1.1373810000	5.7893830000
C	-4.1073950000	4.1468970000	-0.3851990000	C	-6.7769340000	-1.0687450000	-0.3277250000
H	-3.4415760000	4.6671710000	-1.0839660000	H	-7.0838310000	-0.1178120000	0.1237130000
H	-4.4184140000	4.8675310000	0.3807680000	H	-7.3973890000	-1.8621110000	0.1070300000
H	-5.0008320000	3.8266980000	-0.9325730000	H	-6.9830430000	-1.0227510000	-1.4029420000
C	-4.3676270000	2.1767790000	1.1982620000	C	-4.8416410000	-2.6514610000	-0.7738230000
H	-5.2416620000	1.8351390000	0.6346920000	H	-4.9666030000	-2.5536710000	-1.8563140000
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C	-4.1354450000	1.8147120000	-4.6965750000	C	-5.4866280000	2.9842790000	-3.3810480000
H	-3.2618960000	2.0129430000	-5.3294000000	H	-5.3468910000	3.9498100000	-2.8800470000
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C	-4.9558810000	0.9093410000	-2.4593900000	C	-4.7959910000	0.5309140000	-3.4519430000
H	-4.6178670000	0.4645980000	-1.5137020000	H	-4.1177750000	-0.2047150000	-2.9969450000
H	-5.6596590000	0.2178330000	-2.9387940000	H	-4.5763910000	0.5909460000	-4.5252730000
H	-5.4853100000	1.8512200000	-2.2679960000	H	-5.8403410000	0.2121350000	-3.3397800000
O	-3.3746020000	-0.7046160000	-0.2576550000	O	-2.3448910000	-0.8992920000	-2.1171500000
H	0.3915380000	1.8574120000	-3.5654230000	H	-3.3827270000	3.7693780000	0.8648080000
H	0.3352970000	3.7221060000	-2.0818590000	H	-4.9335430000	2.5247930000	2.2065600000
C	-3.9499770000	-1.9947620000	-0.0081560000	C	-1.4861600000	-1.4745720000	-3.1038700000
C	-2.9105420000	-3.1111220000	-0.2475810000	C	-0.1736900000	-0.6680920000	-3.1685740000
C	-4.4946690000	-2.0741790000	1.4274140000	C	-1.2169200000	-2.9545330000	-2.7706340000
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H	-2.5225300000	-3.0258110000	-1.2688310000	H	-0.4067080000	0.3662660000	-3.4405990000
H	-2.0739400000	-2.9978870000	0.4527110000	H	0.2863270000	-0.6583590000	-2.1751580000
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H	-5.2129430000	-1.2635140000	1.5890180000	H	-2.1648710000	-3.5040110000	-2.7981910000
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H	-3.6814420000	-1.9454230000	2.1438080000	H	-0.8080030000	-3.0347740000	-1.7592080000
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H	-4.7384160000	-2.0943550000	-2.0270240000	H	-2.3488170000	-0.3400440000	-4.7438760000
C	4.2850550000	1.9574710000	-2.0604570000	C	6.9243280000	2.5846890000	-0.4730460000
C	4.6966800000	1.0019520000	-1.2061910000	C	5.6799320000	2.7225410000	0.0377420000
O	3.9727560000	-0.0928250000	-0.8438540000	O	4.8193700000	1.6697150000	0.0661810000
C	6.0406920000	1.0628150000	-0.5484600000	C	5.1912000000	4.0107080000	0.6031550000
C	6.1692100000	0.7949480000	0.8276320000	C	3.8639100000	4.4199570000	0.4097170000
C	7.2029390000	1.3286100000	-1.2862490000	C	6.0508760000	4.8377880000	1.3432050000
C	7.4220410000	0.7912920000	1.4457740000	C	3.4170430000	5.6400200000	0.9183520000
H	5.2752980000	0.6793780000	1.4393880000	H	3.1913130000	3.7933800000	-0.1671720000

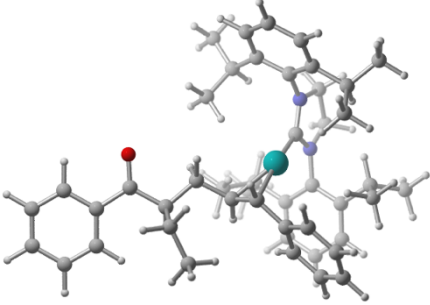
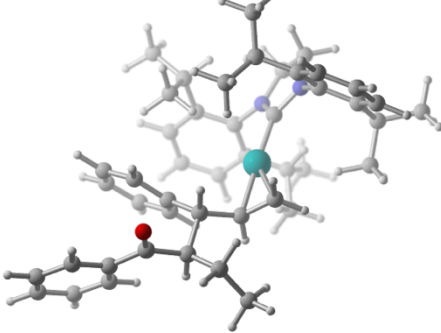
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H	7.1178100000	1.5190710000	-2.3508250000	H	7.0700990000	4.5149170000	1.5287820000
C	8.5709320000	1.0521310000	0.6965970000	C	4.2826170000	6.4604560000	1.6449440000
H	7.4980400000	0.6055910000	2.5120920000	H	2.3950180000	5.9560780000	0.7423200000
H	9.3430010000	1.5323630000	-1.2549300000	H	6.2758420000	6.6776280000	2.4344010000
H	9.5451990000	1.0477090000	1.1721190000	H	3.9307900000	7.4060980000	2.0430460000
H	4.9528060000	2.7965100000	-2.2476880000	H	7.5863740000	3.4435980000	-0.5283620000
C	2.9838160000	1.9474380000	-2.8078140000	C	7.4372560000	1.2747570000	-1.0136170000
C	3.1913850000	1.7738360000	-4.3226960000	C	8.8179050000	1.3905160000	-1.6707770000
H	2.3363660000	1.1495590000	-2.4201560000	H	7.5181410000	0.5203930000	-0.2010740000
H	2.4502870000	2.8922160000	-2.6275630000	H	6.7323940000	0.8719520000	-1.7700270000
H	2.2426340000	1.8082780000	-4.8713500000	H	9.1634110000	0.4267350000	-2.0578350000
H	3.6764520000	0.8153120000	-4.5364430000	H	9.5560800000	1.7524290000	-0.9477750000
H	3.8335660000	2.5690050000	-4.7173940000	H	8.7828960000	2.1013640000	-2.5022710000
C	2.2582720000	-2.0744120000	2.2359170000	C	2.3689080000	-1.9136620000	1.7743020000
C	2.6037580000	-2.9857640000	1.2151360000	C	3.6125440000	-1.9887250000	1.0499450000
O	3.4565390000	-2.5941400000	0.2871000000	O	4.0254690000	-0.8982670000	0.4760760000
C	1.8885080000	-4.2553610000	0.9949200000	C	4.3538150000	-3.2364950000	0.8160730000
C	2.4381870000	-5.2061160000	0.1186010000	C	5.1241170000	-3.3842480000	-0.3493240000
C	0.6352620000	-4.5077480000	1.5800060000	C	4.3107510000	-4.2907730000	1.7437830000
C	1.7530880000	-6.3851780000	-0.1607800000	C	5.8231240000	-4.5626510000	-0.5899450000
H	3.3993950000	-5.0029440000	-0.3385030000	H	5.1136650000	-2.5993850000	-1.0979100000
C	-0.0569870000	-5.6791400000	1.2813870000	C	5.0224670000	-5.4641270000	1.5077460000
H	0.1787680000	-3.7794640000	2.2404030000	H	3.7344520000	-4.1883420000	2.6559550000
C	0.5000670000	-6.6202110000	0.4132980000	C	5.7752120000	-5.6044660000	0.3397710000
H	2.1878130000	-7.1167080000	-0.8329870000	H	6.3864760000	-4.6791370000	-1.5087950000
H	-1.0362630000	-5.8466470000	1.7141560000	H	4.9874010000	-6.2698650000	2.2319120000
H	-0.0414700000	-7.5300680000	0.1809430000	H	6.3157480000	-6.5248280000	0.1510170000
H	1.6619700000	-2.4701010000	3.0547440000	H	2.1160780000	-2.8297190000	2.3083280000
C	3.2968850000	-1.0452040000	2.6658840000	C	2.2410160000	-0.6623920000	2.6627830000
C	2.9883290000	-0.4228420000	4.0308800000	C	1.5698990000	-0.9636790000	4.0055400000
H	4.2918520000	-1.5240200000	2.7145250000	H	3.2400280000	-0.2397660000	2.8511650000
H	3.3602770000	-0.2396090000	1.9193200000	H	1.6573730000	0.1125650000	2.1449600000
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H	3.0182690000	-1.1829570000	4.8182450000	H	2.1957080000	-1.6323320000	4.6073280000
H	1.9909480000	0.0262900000	4.0394050000	H	0.6009650000	-1.4443150000	3.8459220000
Li	2.7218280000	-1.3108300000	-1.0508390000	Li	5.4068750000	-0.0050880000	-0.2466510000
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TS-outer-linear-2				TS-outer-branched-2			
							
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Gas phase free energy correction=		1.174114		Gas phase free energy correction=		1.169966	
SMD energy=		-2811.86963039		SMD energy=		-2811.86429685	
C	0.2285990000	1.6731940000	2.6466320000	C	0.9234430000	0.5059570000	-2.8417600000
H	1.0217570000	1.0945920000	2.1880360000	H	-0.0371800000	0.2316150000	-3.2643720000
C	-0.9918420000	1.8209160000	1.9125790000	C	1.0650950000	1.6726370000	-2.0015550000
C	-1.0921400000	1.8903820000	0.4672530000	C	-0.0322960000	2.2809350000	-1.2416910000
H	-1.8650140000	2.0950150000	2.5027450000	H	1.9542900000	2.2912170000	-2.1198920000
H	-0.1230680000	1.9142270000	-0.0421580000	H	-0.6815410000	1.5389670000	-0.7706680000

Pd	-1.2152740000	-0.1512500000	0.8814810000	Pd	1.3397880000	-0.2993380000	-0.9883730000
C	-3.4798650000	-2.0363220000	-2.3191680000	C	3.9581520000	-1.0047090000	2.4231920000
C	-2.0757720000	-2.0509570000	-2.9269370000	C	2.6456440000	-1.3906620000	3.1091840000
H	-3.8379030000	-3.0360960000	-2.0474120000	H	4.6054870000	-1.8672240000	2.2227570000
H	-1.7782540000	-3.0284730000	-3.3079080000	H	2.6716900000	-2.3792450000	3.5690000000
C	-1.9593770000	-1.0774960000	-0.7744100000	C	2.1589810000	-0.6926660000	0.8903160000
N	-3.2739740000	-1.2276440000	-1.0949910000	N	3.4707020000	-0.4340860000	1.1520560000
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C	0.1245190000	-2.0794030000	-1.6755010000	C	0.5003110000	-2.1660700000	2.0389370000
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C	0.3664690000	-3.4307600000	-1.3635680000	C	0.6684630000	-3.5618560000	1.9844370000
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C	1.6954740000	-3.8595700000	-1.2908360000	C	-0.4613580000	-4.3713980000	2.1407960000
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H	3.3214790000	-0.9751610000	-2.0194020000	H	-2.8791890000	-2.0085300000	2.3688920000
H	1.9109140000	-4.8950280000	-1.0446550000	H	-0.3534950000	-5.4508460000	2.0966990000
C	-4.3763550000	-0.9646600000	-0.2105700000	C	4.4081410000	0.0392840000	0.1777980000
C	-4.4992880000	-1.7037870000	0.9886650000	C	4.8081230000	-0.8156150000	-0.8719620000
C	-5.3549750000	-0.0262560000	-0.5965120000	C	4.9473820000	1.3283350000	0.3294360000
C	-5.5932100000	-1.4277250000	1.8178840000	C	5.7541520000	-0.3310790000	-1.7823640000
C	-6.4416830000	0.1959460000	0.2571320000	C	5.8980220000	1.7673370000	-0.5988360000
C	-6.5537110000	-0.4857730000	1.4634280000	C	6.2950910000	0.9460750000	-1.6504750000
H	-5.7004080000	-1.9705640000	2.7500810000	H	6.0753710000	-0.9649600000	-2.6024510000
H	-7.2034360000	0.9157170000	-0.0238490000	H	6.3275930000	2.7599270000	-0.4989700000
C	-3.5619240000	-2.8469140000	1.3612030000	C	4.2913490000	-2.2434370000	-1.0089990000
H	-2.5915290000	-2.7051180000	0.8800130000	H	3.3985510000	-2.3559420000	-0.3889540000
C	-5.2951240000	0.7200530000	-1.9219290000	C	4.5212460000	2.2388980000	1.4706060000
H	-4.2801180000	0.6117190000	-2.3231120000	H	3.6987240000	1.7434650000	1.9984830000
C	-0.7598860000	-4.4352140000	-1.1488420000	C	2.0164230000	-4.2134020000	1.6994510000
H	-1.7135070000	-3.9004030000	-1.1999430000	H	2.7739770000	-3.4264530000	1.6318720000
C	0.8741300000	0.2664760000	-2.2968080000	C	-0.9227670000	-0.0698050000	2.1826210000
H	-0.1286130000	0.4910940000	-1.9244300000	H	-0.2250340000	0.3162800000	1.4279950000
H	3.7710450000	-3.3292630000	-1.4594270000	H	-2.5934950000	-4.4557260000	2.3887630000
H	-7.3943490000	-0.2928800000	2.1220160000	H	7.0296630000	1.2990730000	-2.3671820000
C	1.8340680000	1.2662780000	-1.6362580000	C	-2.3342860000	0.3930180000	1.8043800000
H	1.5000920000	2.2952860000	-1.8180820000	H	-2.3357590000	1.4765990000	1.6444950000
H	2.8492960000	1.1498820000	-2.0404730000	H	-3.0576800000	0.1708600000	2.5984210000
H	1.8524900000	1.0885990000	-0.5540010000	H	-2.6941960000	-0.0950790000	0.8935130000
C	0.8725210000	0.4467990000	-3.8257570000	C	-0.5363270000	0.5212040000	3.5520070000
H	0.1567580000	-0.2344590000	-4.2973020000	H	0.5073970000	0.3092190000	3.7947790000
H	1.8641890000	0.2322860000	-4.2421680000	H	-1.1681320000	0.0961800000	4.3409390000
H	0.6000760000	1.4747830000	-4.0941310000	H	-0.6696260000	1.6102360000	3.5594310000
C	-5.5558980000	2.2230560000	-1.7491950000	C	3.9739670000	3.5737880000	0.9462320000
H	-6.6010010000	2.4222370000	-1.4851090000	H	4.7509620000	4.1565090000	0.4371590000
H	-5.3439870000	2.7543100000	-2.6824160000	H	3.5847490000	4.1801270000	1.7710510000
H	-4.9176750000	2.6384460000	-0.9676810000	H	3.1584840000	3.3978970000	0.2402380000
C	-6.3072370000	0.1320280000	-2.9284970000	C	5.6752550000	2.4665390000	2.4649010000
H	-6.1890650000	-0.9487460000	-3.0576430000	H	6.0659250000	1.5189190000	2.8523390000
H	-6.1991850000	0.6136640000	-3.9071380000	H	5.3377770000	3.0746180000	3.3120380000
H	-7.3308370000	0.3062880000	-2.5762030000	H	6.5063190000	2.9931900000	1.9807720000
C	-4.1684510000	-4.1804530000	0.8783800000	C	5.3545880000	-3.2430130000	-0.5118020000
H	-4.3085570000	-4.1912320000	-0.2088020000	H	5.6354640000	-3.0472700000	0.5294970000
H	-5.1471450000	-4.3523440000	1.3434020000	H	6.2645880000	-3.1813560000	-1.1211160000
H	-3.5095360000	-5.0122180000	1.1474630000	H	4.9679230000	-4.2658810000	-0.5775840000
C	-3.2521370000	-2.9096590000	2.8635390000	C	3.8475860000	-2.5823750000	-2.4402400000
H	-2.4533670000	-3.6381590000	3.0290270000	H	3.3671000000	-3.5655740000	-2.4465920000
H	-4.1240280000	-3.2104730000	3.4587260000	H	4.6935300000	-2.6062220000	-3.1389760000
H	-2.8825760000	-1.9432470000	3.2160920000	H	3.1046130000	-1.8602040000	-2.7889790000
C	-0.7518660000	-5.5086920000	-2.2552290000	C	2.4388250000	-5.1838360000	2.8168880000
H	-0.7850100000	-5.0637620000	-3.2565720000	H	2.4471730000	-4.6960010000	3.7988150000
H	-1.6138090000	-6.1761340000	-2.1436080000	H	3.4422140000	-5.5763390000	2.6170610000
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C	-0.7142010000	-5.0761140000	0.2444590000	C	2.0023770000	-4.9016310000	0.3235710000
H	-0.8209790000	-4.2939610000	1.0018300000	H	1.7397830000	-4.1621210000	-0.4436070000
H	0.2306650000	-5.6057060000	0.4135270000	H	1.2645320000	-5.7128890000	0.2960870000
H	-1.5256870000	-5.8060690000	0.3456020000	H	2.9877060000	-5.3345660000	0.1111150000

O	-0.5058180000	-2.0616860000	1.6562190000	O	0.7483210000	-2.3520920000	-1.1707260000
H	-1.9692910000	-1.3160630000	-3.7334260000	H	2.3562790000	-0.6655780000	3.8780240000
H	-4.2125790000	-1.5735000000	-2.9777340000	H	4.5315750000	-0.2663840000	2.9876970000
C	0.6161480000	-2.1321530000	2.5324480000	C	-0.3909520000	-2.7087200000	-1.9493530000
C	1.8401430000	-1.4269840000	1.8791980000	C	-1.5521160000	-1.7060590000	-1.6997150000
C	0.2617340000	-1.5219310000	3.9044880000	C	-0.0371030000	-2.7610950000	-3.4487780000
C	1.0182400000	-3.6043370000	2.7589100000	C	-0.8824090000	-4.0989060000	-1.5026050000
H	2.2271230000	-2.0319160000	1.0539590000	H	-1.8402790000	-1.7714510000	-0.6419440000
H	1.4974910000	-0.4805210000	1.4427570000	H	-1.1516240000	-0.7043130000	-1.9139500000
H	2.6484130000	-1.2737340000	2.6192560000	H	-2.4248720000	-1.9362990000	-2.3279740000
H	-0.4457190000	-2.1842760000	4.4143100000	H	0.7563930000	-3.5019070000	-3.5922980000
H	1.1396080000	-1.3877720000	4.5524130000	H	-0.9003120000	-3.0481990000	-4.0654400000
H	-0.2384670000	-0.5630130000	3.7624660000	H	0.3434720000	-1.7966950000	-3.7922680000
H	1.8325840000	-3.6830110000	3.4924340000	H	-1.8019410000	-4.3870420000	-2.0276280000
H	0.1580710000	-4.1677180000	3.1341860000	H	-0.1123260000	-4.8485750000	-1.7077130000
H	1.3495280000	-4.0574010000	1.8206080000	H	-1.0795440000	-4.0894610000	-0.4275590000
C	-2.0203600000	2.8194800000	-0.2341880000	C	0.3768570000	3.3892310000	-0.3081430000
C	-1.9506150000	2.9265500000	-1.6365520000	C	0.0913690000	3.3293850000	1.0580320000
C	-2.8434760000	3.7359610000	0.4434800000	C	1.0021850000	4.5401350000	-0.8100760000
C	-2.6211740000	3.9357730000	-2.3241660000	C	0.3938020000	4.3992800000	1.9019550000
H	-1.3316660000	2.2230210000	-2.1863450000	H	-0.3712180000	2.4379630000	1.4617060000
C	-3.5206360000	4.7468120000	-0.2442830000	C	1.3041320000	5.6128460000	0.0277440000
H	-2.9273310000	3.6854160000	1.5239870000	H	1.2470450000	4.5974430000	-1.8672980000
C	-3.4007640000	4.8661810000	-1.6302160000	C	0.9919820000	5.5500130000	1.3877510000
H	-2.5291040000	4.0024910000	-3.4039420000	H	0.1595860000	4.3310810000	2.9592550000
H	-4.1379670000	5.4469980000	0.3097080000	H	1.7861960000	6.4953170000	-0.3798220000
H	-3.9190870000	5.6576020000	-2.1616210000	H	1.2224200000	6.3851780000	2.0405910000
H	0.0762930000	1.3956130000	3.6850490000	H	1.7354190000	0.3206630000	-3.5472580000
C	6.1011690000	0.6389530000	-1.5135110000	C	-5.8297410000	-0.9293730000	1.1277410000
C	5.4784240000	-0.0915130000	-0.5585380000	C	-5.1580530000	-1.2268810000	-0.0081080000
O	4.5673820000	0.4904000000	0.2560170000	O	-4.6180880000	-0.2347640000	-0.7631810000
C	5.7283300000	-1.5457210000	-0.3395980000	C	-4.9638330000	-2.6129710000	-0.5110640000
C	5.3426490000	-2.1448000000	0.8663380000	C	-4.9490160000	-2.8547830000	-1.8922330000
C	6.3085480000	-2.3575440000	-1.3285610000	C	-4.7765800000	-3.6906410000	0.3652240000
C	5.5240560000	-3.5101380000	1.0846690000	C	-4.7657670000	-4.1457120000	-2.3852500000
H	4.8892220000	-1.5356220000	1.6384670000	H	-5.0885950000	-2.0218530000	-2.5732800000
C	6.5013430000	-3.7210880000	-1.1098310000	C	-4.5865020000	-4.9815710000	-0.1277810000
H	6.5839490000	-1.9305000000	-2.2865780000	H	-4.7550390000	-3.5103840000	1.4351850000
C	6.1060860000	-4.3055220000	0.0965540000	C	-4.5821950000	-5.2139530000	-1.5039390000
H	5.2040530000	-3.9523620000	2.0221120000	H	-4.7583940000	-4.3187210000	-3.4563810000
H	6.9452360000	-4.3318540000	-1.8888110000	H	-4.4252670000	-5.8030130000	0.5623920000
H	6.2452590000	-5.3684150000	0.2608100000	H	-4.4236940000	-6.2157040000	-1.8879290000
H	6.8603000000	0.1910630000	-2.1468290000	H	-6.3048240000	-1.7156420000	1.7070360000
C	5.8351450000	2.1120510000	-1.6964180000	C	-6.0080100000	0.4944640000	1.5877500000
C	6.8159260000	2.7859760000	-2.6635460000	C	-6.7363050000	0.6156660000	2.9309380000
H	4.8115940000	2.2883290000	-2.0861620000	H	-5.0212850000	0.9880170000	1.6930090000
H	5.9013770000	2.6266390000	-0.7177500000	H	-6.5792430000	1.0729680000	0.8312350000
H	6.6046770000	3.8547900000	-2.7719680000	H	-6.8594630000	1.6616300000	3.2303080000
H	6.7549270000	2.3248140000	-3.6549590000	H	-6.1756570000	0.0981370000	3.7164730000
H	7.8430390000	2.6751880000	-2.3013390000	H	-7.7296690000	0.1595350000	2.8698500000
C	1.3768820000	3.1442590000	3.0194170000	C	-1.3786730000	3.1115240000	-2.2738980000
C	2.0923590000	3.2440320000	1.8055040000	C	-2.4517750000	3.1329310000	-1.3314810000
O	3.0047490000	2.3485430000	1.5174340000	O	-3.1655810000	2.0514390000	-1.1859200000
C	1.7769190000	4.2174090000	0.7413560000	C	-2.7045610000	4.2466320000	-0.3949140000
C	2.7719800000	4.5744540000	-0.1899880000	C	-3.4113570000	4.0082440000	0.7979430000
C	0.4864820000	4.7410400000	0.5909640000	C	-2.2393260000	5.5469200000	-0.6492930000
C	2.4682110000	5.4011960000	-1.2682070000	C	-3.6313460000	5.0291940000	1.7163920000
H	3.8056270000	4.2718220000	-0.0254700000	H	-3.7355190000	3.0020240000	1.0438020000
C	0.1774530000	5.5464750000	-0.5047970000	C	-2.4570540000	6.5688850000	0.2712480000
H	-0.2940540000	4.4722750000	1.2912240000	H	-1.7034520000	5.7633030000	-1.5644090000
C	1.1620130000	5.8721740000	-1.4384460000	C	-3.1496630000	6.3144520000	1.4559230000
H	3.2453760000	5.6842080000	-1.9700150000	H	-4.1592470000	4.8216590000	2.6406240000
H	-0.8405080000	5.8948150000	-0.6366840000	H	-2.0790630000	7.5635250000	0.0660740000
H	0.9162410000	6.4963190000	-2.2899440000	H	-3.3097890000	7.1102280000	2.1742140000
H	0.7228870000	3.9845980000	3.2481540000	H	-0.9322890000	4.0834020000	-2.4749390000
C	2.1499160000	2.6061890000	4.2272040000	C	-1.6640910000	2.3311390000	-3.5581430000



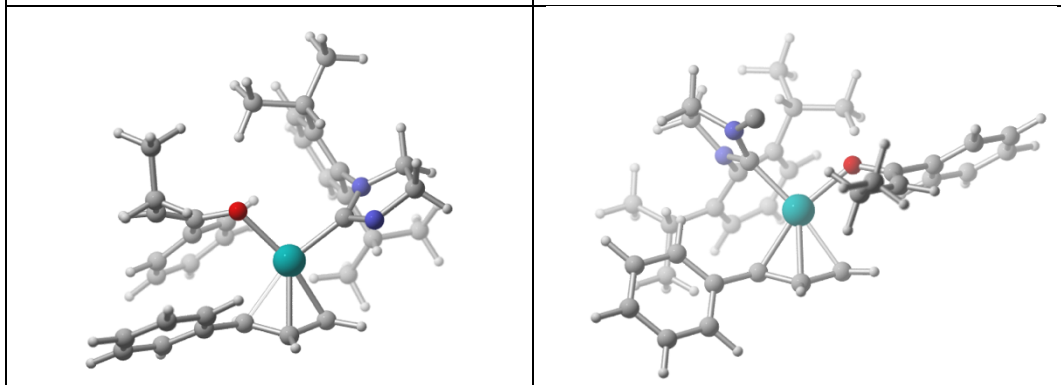
C	1.4279130000	2.8769790000	5.5506640000	C	-0.7247330000	2.7266750000	-4.6993140000
H	2.3153590000	1.5237690000	4.1143840000	H	-1.6021290000	1.2521650000	-3.3819630000
H	3.1482400000	3.0616740000	4.2558650000	H	-2.7030210000	2.5235090000	-3.8618580000
H	1.9933410000	2.4681790000	6.3937340000	H	-0.9224960000	2.1258970000	-5.5927020000
H	0.4310730000	2.4222150000	5.5684090000	H	0.3204380000	2.5761840000	-4.4169940000
H	1.3067040000	3.9533940000	5.7139930000	H	-0.8664420000	3.7817750000	-4.9626790000
Li	3.8079800000	2.0748630000	-0.1310600000	Li	-4.7245600000	1.5013290000	-0.4267700000
Li	3.4314700000	0.5168410000	1.6123860000	Li	-2.9947150000	0.1425710000	-1.4542440000
<b>P-linear</b>				<b>P-branched</b>			
							
Gas phase energy= -459.582373061				Gas phase energy= -459.578045666			
Gas phase free energy correction= 0.865819				Gas phase free energy correction= 0.866005			
SMD energy= -2100.68731150				SMD energy= -2100.67986638			
Pd	-0.6054740000	-0.0937510000	-0.5620920000	Pd	0.6727000000	-0.4335530000	-0.5337820000
C	-3.6044590000	0.8896470000	2.4379220000	C	3.9675340000	2.1548650000	0.7378080000
C	-3.6676360000	2.1857120000	1.6029750000	C	4.4834320000	0.7842300000	1.2099370000
H	-4.5441180000	0.3282100000	2.4235500000	H	4.5465370000	2.5566230000	-0.1027630000
H	-4.6293900000	2.3196150000	1.0965130000	H	5.4754830000	0.5418130000	0.8216970000
C	-1.9827360000	0.7724840000	0.6995910000	C	2.3581550000	0.4975800000	0.1910870000
N	-2.5444930000	0.1271950000	1.7506880000	N	2.5984200000	1.8269580000	0.2919140000
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C	-1.8045410000	4.8127220000	-2.3890670000	C	3.7644490000	-4.3084750000	1.0147420000
H	-0.4504710000	5.7084000000	-0.9849400000	H	2.6349800000	-4.0964060000	2.8288590000
H	-3.1748320000	3.7001470000	-3.6116500000	H	4.8511950000	-4.2440960000	-0.8354910000
C	-2.2024700000	-1.2127930000	2.1199620000	C	1.6646830000	2.8390430000	-0.0941360000
C	-2.8796460000	-2.2798060000	1.5032500000	C	1.5630390000	3.2083430000	-1.4459110000
C	-1.1731760000	-1.4206090000	3.0549490000	C	0.8641550000	3.4239420000	0.9064160000
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C	-0.8174100000	-2.7393340000	3.3582860000	C	-0.0457300000	4.4128400000	0.5241920000
C	-1.4740870000	-3.8114210000	2.7556140000	C	-0.1570700000	4.7995700000	-0.8111080000
H	-2.9932820000	-4.4249130000	1.3660130000	H	0.5285670000	4.5010940000	-2.8246270000
H	-0.0174690000	-2.9311680000	4.0668650000	H	-0.6870850000	4.8729760000	1.2678010000
C	-3.9793620000	-2.0446330000	0.4773370000	C	2.4073580000	2.5459080000	-2.5256300000
H	-4.1175050000	-0.9619180000	0.3769850000	H	3.0888110000	1.8410730000	-2.0366050000
C	-0.4240400000	-0.2515740000	3.6798190000	C	0.9403440000	2.9273170000	2.3441500000
H	-0.9822800000	0.6630930000	3.4488380000	H	1.9352450000	2.4915480000	2.4952040000
C	-3.9042560000	1.6490110000	-1.9610730000	C	4.8068770000	-1.5607960000	-1.4382030000
H	-4.0989650000	1.1182330000	-1.0220010000	H	4.9597930000	-0.5075590000	-1.1738770000
C	-0.6391310000	4.0058100000	1.1654220000	C	2.2076240000	-1.4112180000	2.9557610000
H	-1.2103970000	3.4303520000	1.9039880000	H	2.2485080000	-0.3470570000	2.6972450000
H	-1.1844990000	-4.8285290000	2.9993020000	C	-0.8706420000	5.5675820000	-1.0919480000
C	0.7155280000	3.2915810000	0.9893150000	C	0.7218290000	-1.8126450000	2.9634540000
H	1.2494690000	3.2355600000	1.9451240000	H	0.1700890000	-1.2194190000	3.7010540000
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H	0.5624680000	2.2745430000	0.6117050000	H	0.2772320000	-1.6344420000	1.9774590000
C	-0.4557870000	5.4245640000	1.7261130000	C	2.8398030000	-1.5790090000	4.3494760000
H	-1.4147660000	5.9460480000	1.8161710000	H	3.8948260000	-1.2833650000	4.3447670000
H	0.2032550000	6.0279370000	1.0923630000	H	2.7836140000	-2.6197810000	4.6885220000
H	0.0055990000	5.3746970000	2.7183900000	H	2.3093090000	-0.9600920000	5.0817390000
C	0.9685360000	-0.0959800000	3.0411990000	C	-0.0879880000	1.8025190000	2.5698990000
H	1.5779660000	-0.9914160000	3.2155500000	H	-1.1064200000	2.1861970000	2.4533990000
H	1.4933170000	0.7656880000	3.4692680000	H	0.0139110000	1.3874830000	3.5797870000
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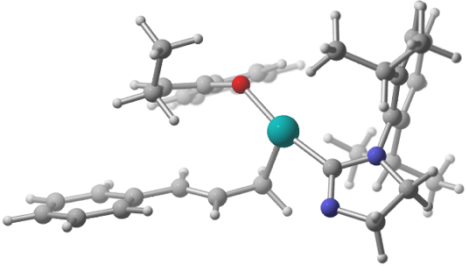
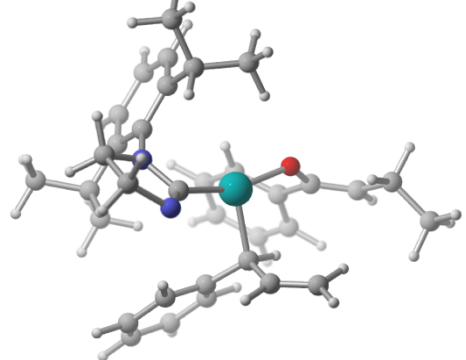
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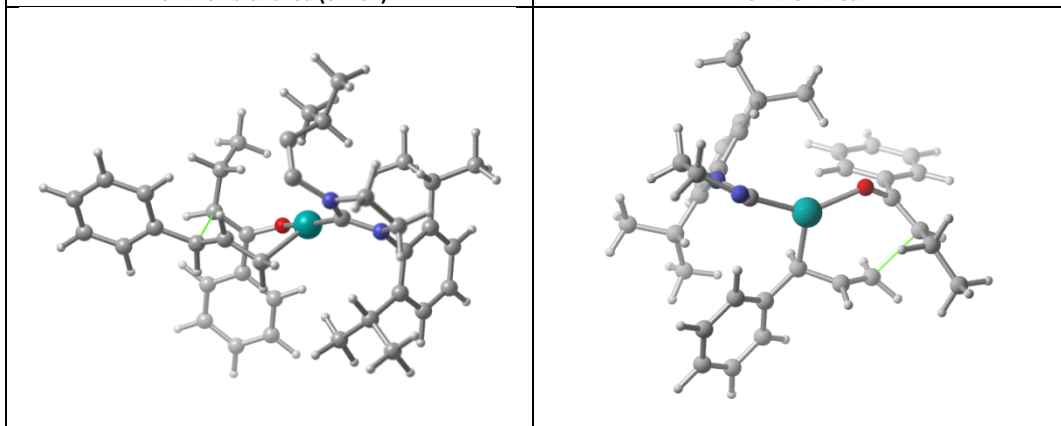
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C	2.9534780000	-1.7732960000	-2.6766400000	C	-5.0389930000	1.6625850000	-2.8375690000
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H	2.3638130000	-2.1604460000	-4.7527860000	C	-5.6472930000	1.6420000000	-1.5810800000

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H	-4.0285900000	2.3689800000	0.0509280000	H	-6.6154350000	2.1083790000	-1.4341450000
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C	1.6730810000	2.5337560000	-1.1955150000	C	-2.7065100000	-2.5437840000	0.1968740000
C	3.1150310000	0.5946160000	0.8661650000	C	1.0506190000	-3.1864560000	-1.8012460000
H	3.0450720000	1.6427910000	1.1493720000	H	0.2093510000	-3.7973810000	-1.4817530000
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H	2.0685740000	-1.2341670000	0.7252740000	H	1.8046890000	-1.2717220000	-2.2152810000
H	0.7061110000	1.3938720000	1.6413090000	H	-1.1607970000	-1.7999820000	-1.5997960000
Pd	-0.4346480000	0.3973110000	-0.4158360000	Pd	-0.3018940000	-0.6152120000	0.4014230000
C	4.4448160000	0.1393310000	0.4352240000	C	3.0886660000	2.0132570000	1.0648940000
C	5.5559720000	0.9738590000	0.6470920000	C	1.8797640000	2.8433330000	1.5232720000
C	4.6533460000	-1.0926700000	-0.2114580000	H	3.6768480000	1.6192780000	1.9014630000
C	6.8336020000	0.5890650000	0.2421950000	H	1.9093020000	3.0943930000	2.5865210000
H	5.4079930000	1.9340340000	1.1339280000	C	1.1098080000	0.8269180000	0.5364390000
C	5.9308230000	-1.4788490000	-0.6127050000	N	2.4539850000	0.8827480000	0.3436660000
H	3.8079060000	-1.7391450000	-0.4239100000	C	0.7609300000	1.9277000000	1.2455380000
C	7.0281080000	-0.6424380000	-0.3873170000	C	-0.5417680000	2.1218650000	1.8188720000
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C	-1.6616620000	-1.0125560000	0.2666080000	C	3.4026600000	-1.3834270000	0.5291890000
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C	-3.7567680000	1.4162750000	1.0197510000	C	4.9185970000	-2.1805530000	-1.1972970000
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H	-5.2415910000	1.9199150000	-2.5496250000	H	3.1285670000	1.9811860000	-1.7104620000
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H	2.0489230000	-4.0964100000	-1.7851870000	C	-2.2674950000	3.3528210000	-1.2346710000
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H	1.8792950000	-2.8965760000	4.2685230000	H	1.3716460000	-3.0624730000	2.8083470000
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TS-inner-branched (or TS2)	TS-inner-linear
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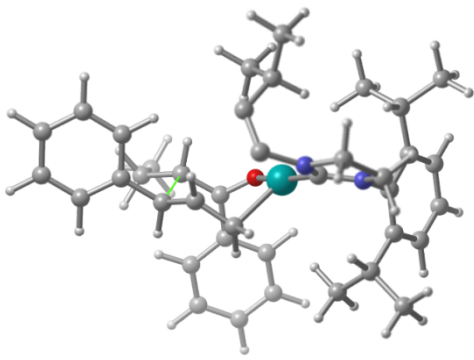
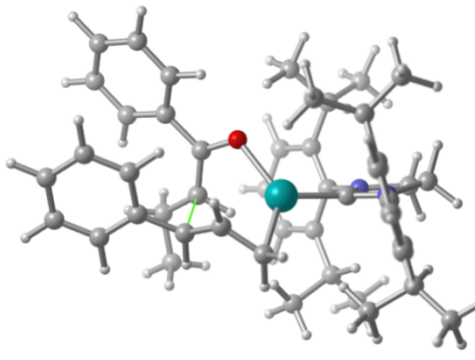
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C	0.855215	0.302560	1.347197	C	-0.3966200000	0.3728100000	-2.1052450000
H	2.075261	-1.344365	0.748484	H	-0.0630260000	-1.3710500000	-3.3311470000
H	0.891173	1.348168	1.663324	H	-1.2025860000	1.0756160000	-1.8460340000
Pd	-0.443214	0.472884	-0.400432	Pd	-0.2433180000	-0.5987930000	-0.2438770000
C	4.525052	-0.189071	0.397138	C	2.9839740000	0.7810870000	2.2625180000
C	5.686064	0.566824	0.629243	C	2.0096420000	1.9668060000	2.3850490000
C	4.670374	-1.545769	0.063064	H	3.1353080000	0.2494730000	3.2056690000
C	6.951954	-0.011770	0.537861	H	1.5893730000	2.0706200000	3.3907930000
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C	5.936251	-2.124347	-0.028046	N	2.3043030000	-0.0965380000	1.2843610000
H	3.792351	-2.151952	-0.134860	N	0.9415890000	1.6103670000	1.4298580000
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H	6.028227	-3.174482	-0.286774	C	-1.3207450000	1.9056500000	2.3156280000
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H	0.223620	-0.320654	1.975178	C	-2.5342830000	2.6020320000	2.3045120000
C	-2.933354	-2.764355	1.035236	C	-2.7278520000	3.6887500000	1.4562840000
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H	-3.255548	-3.440852	0.233923	H	-3.3352220000	2.2872970000	2.9663380000
H	-4.852926	-1.712967	0.731908	C	2.7860490000	-1.4302600000	1.0445540000
C	-1.838931	-0.785115	0.311738	C	2.0933440000	-2.5321120000	1.6029470000
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H	-5.582580	2.458752	-1.949338	H	4.1160980000	0.4481490000	-0.2388300000
C	-0.496738	-2.854739	0.338034	C	-1.1276200000	0.7633610000	3.3049900000
C	-0.195459	-3.134999	-1.010513	H	-0.1380590000	0.3275140000	3.1362580000
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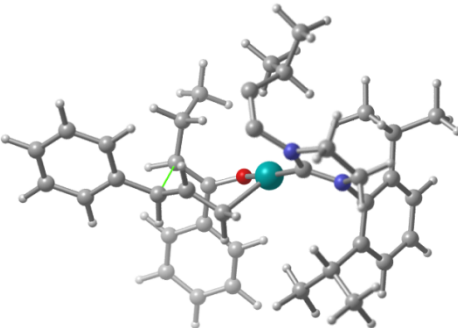
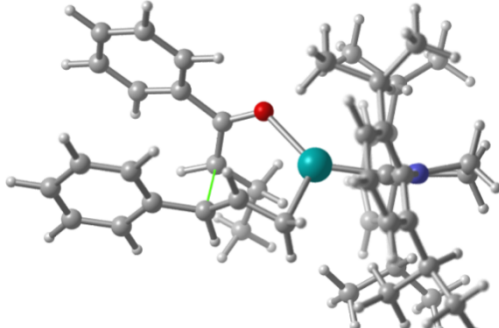
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H	2.137457	-4.375670	1.853265	H	1.0342370000	4.4617230000	-2.3691510000
C	-1.132253	-2.764368	-2.154675	H	-0.3794550000	5.2831970000	-1.6875560000
H	-1.949572	-2.158537	-1.750835	H	-0.4705240000	3.5669590000	-2.1312120000
C	-0.025454	-3.060534	2.849481	C	1.3738750000	5.1327950000	0.3706040000
H	-0.805853	-2.289448	2.873311	H	1.7436010000	4.8780550000	1.3696240000
C	-4.491902	-0.059384	-1.911570	H	0.6883290000	5.9819360000	0.4779520000
H	-4.245857	-1.018735	-1.440622	C	2.2237480000	5.4543150000	-0.2418180000
C	-2.776597	1.592040	2.603287	C	4.9439630000	-0.7020900000	-1.8405440000
H	-2.307043	0.604509	2.536344	H	5.5973440000	-1.5643680000	-2.0127630000
H	-5.404121	4.226088	-0.236547	H	5.4167910000	0.1694700000	-2.3055430000
H	2.727219	-4.816980	-0.502339	H	3.9924000000	-0.8832560000	-2.3486250000
C	-1.641083	2.625466	2.709451	C	6.0738580000	-0.1998260000	0.3700440000
H	-0.982002	2.382211	3.550222	H	5.9396580000	-0.0294660000	1.4437790000
H	-2.034727	3.635743	2.871074	H	6.5721900000	0.6757250000	-0.0610010000
H	-1.043902	2.631494	1.792137	H	6.7427480000	-1.0602470000	0.2529330000
C	-3.669302	1.610198	3.857615	C	1.1410970000	-2.1349280000	3.9069270000
H	-4.461265	0.855974	3.790904	H	1.7821760000	-1.2580670000	4.0486460000
H	-4.147754	2.588263	3.984852	H	1.6592260000	-3.0047390000	4.3275010000
H	-3.073179	1.407225	4.754313	H	0.2178590000	-1.9762310000	4.4758690000
C	1.166460	-2.545129	3.676303	C	-0.1762180000	-3.5256910000	2.2476620000
H	1.935531	-3.317103	3.792139	H	-1.1247640000	-3.2657540000	2.7272560000
H	0.828888	-2.266788	4.680798	H	0.1880880000	-4.4512610000	2.7085630000
H	1.633578	-1.670854	3.214580	H	-0.3871420000	-3.7044800000	1.1896780000
C	-0.589593	-4.345731	3.490889	C	-1.1507520000	1.2911240000	4.7532140000
H	-1.434780	-4.749341	2.923527	H	-0.4132570000	2.0882960000	4.9002950000
H	-0.920544	-4.150532	4.517036	H	-0.9273200000	0.4789630000	5.4541770000
H	0.183422	-5.122242	3.525396	H	-2.1365580000	1.6959390000	5.0086250000
C	-1.754313	-4.035353	-2.766485	C	-2.1598880000	-0.3602320000	3.1130190000
H	-2.262734	-4.635243	-2.003436	H	-2.0906170000	-0.8089220000	2.1171920000
H	-0.986908	-4.664582	-3.231795	H	-3.1831400000	0.0100940000	3.2449130000
H	-2.483908	-3.764797	-3.538064	H	-1.9948160000	-1.1482230000	3.8574820000
C	-0.440753	-1.914300	-3.231138	O	-1.9239410000	-1.8520230000	-0.0881260000
H	-1.142598	-1.686439	-4.040652	C	-4.1848320000	-1.1899440000	-0.5248150000
H	0.419247	-2.433063	-3.669598	C	-4.0130350000	0.0912600000	0.0230380000
H	-0.090513	-0.967233	-2.807948	C	-5.4853670000	-1.6428140000	-0.7927050000
C	-5.882492	-0.204050	-2.550482	C	-5.1163970000	0.9017540000	0.2859800000
H	-6.655554	-0.359034	-1.790439	H	-3.0105000000	0.4475770000	0.2370930000
H	-5.892482	-1.059974	-3.234131	C	-6.5894540000	-0.8331330000	-0.5230170000
H	-6.153225	0.682499	-3.134401	H	-5.6328960000	-2.6409270000	-1.1933200000
C	-3.414483	0.209384	-2.979602	C	-6.4082940000	0.4431810000	0.0151710000
H	-2.418938	0.271920	-2.525011	H	-4.9636540000	1.8930180000	0.6998790000
H	-3.608135	1.157911	-3.493713	H	-7.5902370000	-1.2008190000	-0.7251750000
H	-3.405801	-0.592862	-3.726601	H	-7.2667250000	1.0730560000	0.2246760000
O	0.737487	1.797726	-1.403311	H	-3.8109730000	-2.9792480000	-2.5477590000
C	2.253231	3.459825	-0.631771	C	-1.7914910000	-3.8207220000	-2.1195980000
C	1.167902	4.184133	-0.110566	H	-0.8350730000	-3.3269500000	-1.9032930000
C	3.544307	4.000752	-0.504720	C	-1.7485120000	-4.4834110000	-3.5003490000
C	1.367300	5.406862	0.526950	H	-1.5365660000	-3.7527280000	-4.2891950000
H	0.173955	3.766131	-0.219403	H	-0.9662330000	-5.2483210000	-3.5416960000
C	3.741977	5.226087	0.132111	H	-2.7036550000	-4.9667180000	-3.7379920000
H	4.401142	3.476286	-0.914179	H	2.4705670000	2.9168310000	2.1051540000
C	2.655523	5.932809	0.653363	H	3.9625500000	1.0904560000	1.8865210000
H	0.516652	5.949442	0.926381	H	-1.8997030000	-4.5955070000	-1.3459240000
H	4.744643	5.632080	0.218390	C	0.7779330000	1.1096380000	-2.7212420000
H	2.811662	6.884995	1.149239	C	0.5609530000	1.6981000000	-3.9825720000
H	4.024569	1.547665	-1.507331	C	2.0347950000	1.2689420000	-2.1371580000
C	2.720533	-0.057176	-2.271294	C	1.5534570000	2.4446820000	-4.6137080000
C	2.397721	0.267568	-3.737692	H	-0.4047050000	1.5660080000	-4.4614880000
H	3.591991	-0.720693	-2.227602	C	3.0310970000	2.0274340000	-2.7594930000
H	1.880558	-0.604979	-1.825012	H	2.2303160000	0.7885020000	-1.1898790000
H	2.221052	-0.651322	-4.308567	C	2.7957260000	2.6231610000	-3.9971090000
H	3.224355	0.807990	-4.212642	H	1.3583610000	2.8909800000	-5.5834390000
H	1.499145	0.889461	-3.799565	H	3.9958350000	2.1431960000	-2.2747150000
H	-4.063120	-1.337053	2.276857	H	3.5696720000	3.2090830000	-4.4819160000



H	-2.804078	-3.346749	1.948455	H	-2.3784950000	-1.7069340000	-4.0162310000
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TS1				TS3			
							
Gas phase energy= -459.529216242				Gas phase energy= -459.533926723			
Gas phase free energy correction= 0.866850				Gas phase free energy correction= 0.870864			
SMD energy= -2100.62027722				SMD energy= -2100.62448381			
C	2.982461	1.629145	-1.263027	C	-2.327892	0.854122	-0.814631
C	1.834150	2.380200	-0.935965	C	-2.451183	0.184860	0.416570
C	3.191997	0.422252	0.435940	C	-1.896686	-1.043051	-2.128761
H	3.421678	1.294957	1.048077	H	-1.746546	-0.327345	-2.931042
C	2.014864	-0.288543	0.762159	C	-0.750041	-1.767731	-1.706127
C	0.853547	0.262116	1.340612	C	0.605131	-1.467172	-2.114867
H	1.997755	-1.350804	0.531925	H	-0.921414	-2.717973	-1.205152
H	0.908356	1.287363	1.715425	H	0.755934	-0.769312	-2.940226
Pd	-0.450129	0.435846	-0.389313	Pd	0.385458	-0.517558	-0.281759
C	4.380288	-0.387748	0.046141	C	-3.256265	-1.600922	-2.024749
C	5.639741	-0.132505	0.606769	C	-4.243783	-1.209294	-2.945058
C	4.263313	-1.420973	-0.898565	C	-3.611246	-2.503370	-1.005558
C	6.751610	-0.894886	0.243532	C	-5.547635	-1.696943	-2.845908
H	5.744063	0.664224	1.338059	H	-3.982740	-0.521520	-3.744727
C	5.372814	-2.182748	-1.261363	C	-4.914956	-2.978606	-0.900625
H	3.297226	-1.617627	-1.354720	H	-2.874559	-2.797163	-0.266102
C	6.623194	-1.923466	-0.692068	C	-5.889387	-2.578333	-1.819289
H	7.717448	-0.686699	0.692316	H	-6.295483	-1.383890	-3.567044
H	5.265292	-2.973305	-1.997492	H	-5.176408	-3.647507	-0.088093
H	7.487789	-2.513281	-0.978220	H	-6.905152	-2.948519	-1.731754
H	0.231309	-0.388970	1.947426	H	1.329952	-2.280414	-2.103125
C	-2.871598	-2.961357	0.816878	C	3.381645	2.149122	1.277173
C	-3.923363	-1.841043	0.779666	C	4.117863	0.805166	1.415728
H	-3.003863	-3.692905	0.010348	H	3.268259	2.672586	2.228586
H	-4.770271	-2.066725	0.126570	H	4.157685	0.455122	2.454903
C	-1.805858	-0.930313	0.205357	C	2.041473	0.431231	0.337179
N	-1.610370	-2.217264	0.607580	N	2.069358	1.722219	0.757521
N	-3.141874	-0.710922	0.247868	N	3.261643	-0.094216	0.617834
C	-3.767489	0.520436	-0.126517	C	3.623663	-1.451460	0.347365
C	-3.862259	1.563857	0.809562	C	3.173878	-2.471335	1.202354
C	-4.265069	0.644295	-1.437735	C	4.408872	-1.718266	-0.791546
C	-4.498228	2.745898	0.412443	C	3.511634	-3.792177	0.881602
C	-4.890907	1.842591	-1.794256	C	4.721844	-3.050820	-1.075538
C	-5.012435	2.882956	-0.874159	C	4.272148	-4.079918	-0.247630
H	-4.581258	3.570078	1.114418	H	3.171756	-4.601465	1.520621
H	-5.275601	1.972434	-2.800575	H	5.316184	-3.293990	-1.949476

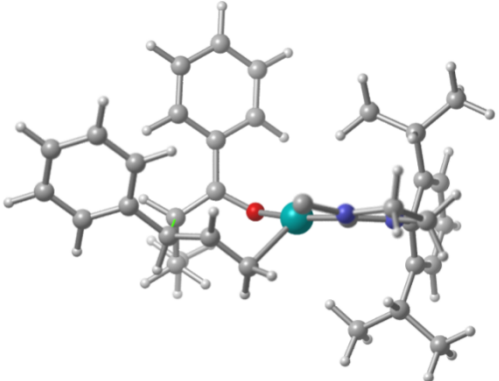
C	-0.356015	-2.908757	0.549871	C	0.975367	2.629515	0.589775
C	0.198776	-3.235031	-0.704677	C	0.809029	3.268754	-0.652259
C	0.290121	-3.258583	1.753428	C	0.086846	2.837838	1.661481
C	1.428536	-3.903501	-0.728229	C	-0.279364	4.133337	-0.808652
C	1.512225	-3.935559	1.679872	C	-0.998224	3.696526	1.455694
C	2.083358	-4.249173	0.450038	C	-1.181004	4.338549	0.232934
H	1.882314	-4.152313	-1.682668	H	-0.428055	4.642600	-1.756427
H	2.033325	-4.201272	2.593469	H	-1.709769	3.861531	2.258006
C	-0.485758	-2.900199	-2.023683	C	2.351853	-2.177452	2.450117
H	-1.393297	-2.327538	-1.808360	H	2.156521	-1.100248	2.483955
C	-0.307640	-2.926502	3.114131	C	4.854110	-0.584343	-1.709417
H	-1.111392	-2.197382	2.950625	H	4.960227	0.317888	-1.094914
C	-4.049348	-0.459336	-2.464896	C	0.317927	2.194830	3.021577
H	-3.796788	-1.378556	-1.922888	H	1.085739	1.422862	2.892547
C	-3.257775	1.452839	2.201332	C	1.763018	3.022578	-1.812955
H	-2.810532	0.456914	2.296471	H	2.529192	2.316606	-1.475408
H	-5.499055	3.807489	-1.166106	H	4.518086	-5.109642	-0.484947
H	3.043564	-4.750983	0.409326	H	-2.028670	5.000932	0.091685
C	-2.122926	2.477439	2.385143	C	3.135047	-2.552738	3.722688
H	-1.637293	2.339942	3.357844	H	4.100967	-2.036877	3.760738
H	-2.504356	3.504443	2.339815	H	3.328375	-3.631009	3.763225
H	-1.366901	2.358403	1.601745	H	2.561137	-2.279954	4.615390
C	-4.327920	1.596882	3.298484	C	0.982359	-2.877263	2.412499
H	-5.121216	0.850748	3.178520	H	1.092251	-3.968460	2.410628
H	-4.792656	2.589113	3.271144	H	0.420804	-2.578603	1.520723
H	-3.876276	1.465809	4.288095	H	0.391689	-2.595704	3.291131
C	0.716270	-2.286411	4.070366	C	0.851524	3.245235	4.017880
H	1.471640	-3.013129	4.389450	H	1.092925	2.773537	4.976946
H	0.209626	-1.923044	4.971228	H	0.095935	4.018471	4.200603
H	1.235286	-1.445951	3.600722	H	1.751111	3.743549	3.639052
C	-0.914903	-4.185949	3.765980	C	-0.932090	1.497862	3.581713
H	-1.640451	-4.677132	3.109267	H	-1.278658	0.725389	2.890609
H	-1.415283	-3.930172	4.706608	H	-1.747669	2.208835	3.758193
H	-0.127287	-4.915497	3.987961	H	-0.693789	1.028515	4.543442
C	-0.911455	-4.181993	-2.764499	C	3.773041	-0.278745	-2.763216
H	-1.559774	-4.804889	-2.138233	H	3.607456	-1.150331	-3.407321
H	-0.039950	-4.783576	-3.047677	H	4.081823	0.562731	-3.395050
H	-1.456213	-3.926167	-3.680370	H	2.823002	-0.029219	-2.282239
C	0.405098	-2.014726	-2.911784	C	6.212972	-0.843181	-2.378512
H	-0.132202	-1.727081	-3.821961	H	6.148292	-1.641038	-3.126731
H	1.317791	-2.542190	-3.214386	H	6.975502	-1.123335	-1.644299
H	0.690046	-1.099230	-2.380538	H	6.549124	0.060897	-2.897531
C	-5.302291	-0.751843	-3.306110	C	1.036355	2.364388	-2.998079
H	-6.166038	-0.971240	-2.669536	H	1.752765	2.089479	-3.780346
H	-5.123168	-1.615725	-3.955597	H	0.298318	3.045161	-3.438250
H	-5.562712	0.093850	-3.951987	H	0.518402	1.458208	-2.668528
C	-2.843237	-0.117129	-3.360934	C	2.476565	4.316666	-2.243390
H	-1.940856	0.048791	-2.759888	H	3.007228	4.773420	-1.400935
H	-3.034955	0.796944	-3.934690	H	1.762328	5.053349	-2.628836
H	-2.643910	-0.932498	-4.066439	H	3.202147	4.105171	-3.036842
O	0.673580	1.872386	-1.270826	H	-1.304910	1.174184	-1.018562
C	1.781086	3.577298	-0.053949	C	-3.376242	1.660418	-1.542857
C	0.535070	4.205825	0.130747	C	-2.836419	2.297699	-2.829056
C	2.885492	4.075247	0.658565	H	-3.742278	2.471286	-0.894358
C	0.400413	5.292626	0.989596	H	-4.250290	1.041339	-1.788147
H	-0.320720	3.813211	-0.404587	H	-3.603585	2.912107	-3.311982
C	2.748736	5.163760	1.522208	H	-1.975034	2.935490	-2.607052
H	3.859317	3.616587	0.552105	H	-2.511922	1.543156	-3.553843
C	1.507769	5.778231	1.691481	C	-3.726198	-0.142910	1.127518
H	-0.570849	5.760127	1.115230	C	-3.664288	-1.130692	2.127485
H	3.615061	5.528617	2.064451	C	-4.974196	0.433945	0.846575
H	1.403538	6.623217	2.363958	C	-4.807714	-1.547978	2.800876
H	2.723913	0.818316	-1.943535	H	-2.697363	-1.565564	2.347089
C	4.380020	2.186966	-1.497922	C	-6.122543	0.014589	1.521489
C	4.395640	3.402278	-2.438712	H	-5.073132	1.212035	0.106275
H	4.888743	2.439740	-0.559196	C	-6.047807	-0.981136	2.494270

H 4.986090 1.386417 -1.935794	H -4.733810 -2.317340 3.562717
H 5.423791 3.720191 -2.644819	H -7.077653 0.470962 1.283155
H 3.856316 4.250053 -2.003447	H -6.943461 -1.308109 3.012117
H 3.915558 3.156726 -3.391864	O -1.381946 -0.340566 0.956474
H -4.311333 -1.592829 1.774796	H 3.868291 2.824981 0.562681
H -2.858085 -3.495910 1.767562	H 5.136446 0.829955 1.022752
<b>TS2 (or TS-inner-branched)</b>	
<b>TS4</b>	
	
Gas phase energy= -459.539803013	Gas phase energy= -459.537279738
Gas phase free energy correction= 0.869345	Gas phase free energy correction= 0.868156
SMD energy= -2100.63186908	SMD energy= -2100.62852628
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C 1.987788 2.134230 -1.252318	C -2.690233 0.748114 0.755797
C 3.195684 0.478187 0.501530	C -2.480071 -0.205234 -1.828722
H 3.263117 1.479711 0.924458	H -2.121881 0.522174 -2.555343
C 2.053566 -0.264947 0.871096	C -1.528494 -1.142780 -1.377017
C 0.855215 0.302560 1.347197	C -0.144979 -1.149873 -1.742844
H 2.075261 -1.344365 0.748484	H -1.881237 -1.988404 -0.791438
H 0.891173 1.348168 1.663324	H 0.159718 -0.521594 -2.581273
Pd -0.443214 0.472884 -0.400432	Pd 0.196979 -0.164272 0.055594
C 4.525052 -0.189071 0.397138	C -3.925237 -0.515010 -1.941460
C 5.686064 0.566824 0.629243	C -4.744535 0.327909 -2.713065
C 4.670374 -1.545769 0.063064	C -4.523168 -1.610927 -1.298304
C 6.951954 -0.011770 0.537861	C -6.112743 0.092711 -2.830602
H 5.587553 1.618101 0.888138	H -4.298227 1.183072 -3.214985
C 5.936251 -2.124347 -0.028046	C -5.893098 -1.843063 -1.409791
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H 8.066100 -1.815977 0.135542	H -7.761509 -1.176906 -2.257974
H 0.223620 -0.320654 1.975178	H 0.379568 -2.104707 -1.708864
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C -3.592969 1.806436 1.337729	C 2.090338 -3.130435 1.075513
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C -5.038601 2.261570 -1.031578	C 2.914501 -4.294827 -1.350694
C -4.933082 3.263558 -0.068010	C 2.188134 -5.040177 -0.421514
H -4.129095 3.830466 1.840706	H 1.227355 -5.057857 1.497530
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H	2.137457	-4.375670	1.853265	H	0.653024	4.700792	2.427865
C	-1.132253	-2.764368	-2.154675	C	1.661339	-2.532498	2.408253
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C	-0.025454	-3.060534	2.849481	C	4.006114	-2.122013	-2.118935
H	-0.805853	-2.289448	2.873311	H	4.620381	-1.402611	-1.564208
C	-4.491902	-0.059384	-1.911570	C	1.698414	2.238918	2.945807
H	-4.245857	-1.018735	-1.440622	H	2.108668	1.240329	2.756216
C	-2.776597	1.592040	2.603287	C	2.784218	2.511723	-2.043944
H	-2.307043	0.604509	2.536344	H	3.237566	1.550893	-1.776786
H	-5.404121	4.226088	-0.236547	H	1.940352	-6.074319	-0.636169
H	2.727219	-4.816980	-0.502339	H	0.599502	5.933591	0.287603
C	-1.641083	2.625466	2.709451	C	2.451516	-3.169065	3.567923
H	-0.982002	2.382211	3.550222	H	3.531420	-3.054205	3.421637
H	-2.034727	3.635743	2.871074	H	2.236130	-4.240921	3.649037
H	-1.043902	2.631494	1.792137	H	2.178226	-2.696075	4.517722
C	-3.669302	1.610198	3.857615	C	0.144666	-2.653291	2.635930
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H	-3.073179	1.407225	4.754313	H	-0.138956	-2.134588	3.557952
C	1.166460	-2.545129	3.676303	C	2.620624	2.944902	3.958637
H	1.935531	-3.317103	3.792139	H	2.678328	2.368251	4.888489
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H	1.633578	-1.670854	3.214580	H	3.634769	3.064565	3.560326
C	-0.589593	-4.345731	3.490889	C	0.283199	2.046624	3.517404
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H	-0.920544	-4.150532	4.517036	H	-0.178526	3.009201	3.768453
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H	-2.483908	-3.764797	-3.538064	H	2.416388	-0.647334	-2.392095
C	-0.440753	-1.914300	-3.231138	C	4.960438	-2.953758	-2.990148
H	-1.142598	-1.686439	-4.040652	H	4.411362	-3.596237	-3.687495
H	0.419247	-2.433063	-3.669598	H	5.612506	-3.587531	-2.380169
H	-0.090513	-0.967233	-2.807948	H	5.589910	-2.288232	-3.590380
C	-5.882492	-0.204050	-2.550482	C	1.671965	2.217267	-3.065043
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H	-6.153225	0.682499	-3.134401	H	0.910956	1.568137	-2.621683
C	-3.414483	0.209384	-2.979602	C	3.886613	3.393852	-2.656298
H	-2.418938	0.271920	-2.525011	H	4.680002	3.595121	-1.928417
H	-3.608135	1.157911	-3.493713	H	3.485618	4.357054	-2.991831
H	-3.405801	-0.592862	-3.726601	H	4.331812	2.896837	-3.525481
O	0.737487	1.797726	-1.403311	H	-3.666238	1.887725	-0.762281
C	2.253231	3.459825	-0.631771	C	-1.520276	2.408214	-0.777295
C	1.167902	4.184133	-0.110566	C	-1.829374	3.356526	-1.938181
C	3.544307	4.000752	-0.504720	H	-0.658931	1.772437	-1.036742
C	1.367300	5.406862	0.526950	H	-1.175119	2.984810	0.093555
H	0.173955	3.766131	-0.219403	H	-0.952266	3.962970	-2.186426
C	3.741977	5.226087	0.132111	H	-2.120486	2.803535	-2.840255
H	4.401142	3.476286	-0.914179	H	-2.651359	4.036142	-1.684276
C	2.655523	5.932809	0.653363	C	-3.947496	0.179381	1.317999
H	0.516652	5.949442	0.926381	C	-3.872664	-1.008957	2.059800
H	4.744643	5.632080	0.218390	C	-5.205786	0.756512	1.091829
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C	2.720533	-0.057176	-2.271294	C	-6.362706	0.144303	1.570502
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H	3.591991	-0.720693	-2.227602	C	-6.279986	-1.050552	2.288887

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H 2.221052 -0.651322 -4.308567	H -7.329334 0.598181 1.379618
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Pd 0.244486 -0.320254 -0.458809	Pd -0.552591 -0.441063 -0.708938
C -4.720425 1.051619 -0.957795	C 4.124366 0.840772 -1.130913
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C 3.160588 -2.888752 -3.587240	C 2.063813 3.594484 1.776558
H 2.624628 -1.391641 -5.030379	H 2.391359 1.950736 3.115378
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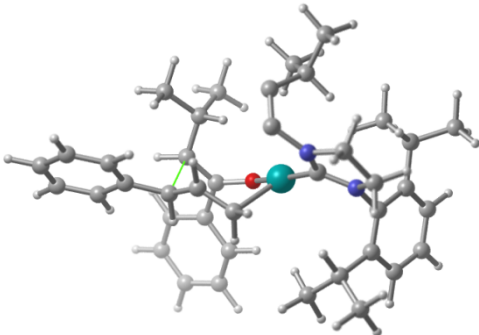
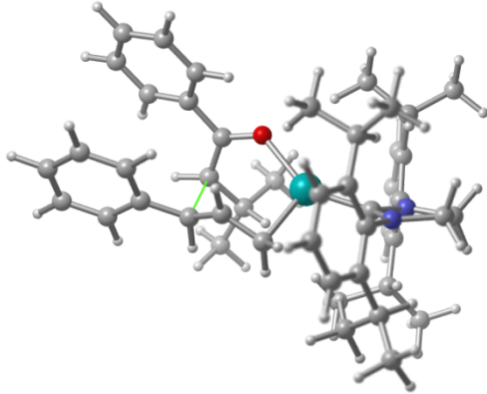
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H	3.857056	-1.507923	0.696072	H	-3.099139	-1.064338	2.331130
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H	-3.080774	-2.274497	4.370999	H	4.571955	-2.955646	2.403015
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H -5.051295 -1.671287 0.796012	H 5.358384 -3.656045 -3.094951
H -6.066022 -3.751164 -0.171544	H 3.731041 -3.555212 -3.797463
H -4.909110 -3.694925 -1.516454	H 3.934631 -4.034033 -2.104951
H -4.333530 -3.990635 0.132391	O 0.607749 -1.882012 -1.593750
H 4.054934 2.898403 0.657758	H -3.093209 3.328390 1.614323
H 4.609516 1.614695 -1.285891	H -4.693605 1.876911 0.584424
<b>TS6</b> <span style="margin-left: 200px;"><b>TS8</b></span>	
Optimization leads to TS2.	
	Gas phase energy= -459.530193342 Gas phase free energy correction= 0.869264 SMD energy= -2100.62263465
	C 2.823580 -1.788182 -2.008590 C 1.846080 -2.216346 -1.085916 C 2.993130 0.264163 -1.765912 H 3.077939 0.313169 -2.848910 C 1.863358 0.943716 -1.233279 C 0.600340 1.012163 -1.832473 H 1.968703 1.422591 -0.262992 H 0.483390 0.633635 -2.849388 Pd -0.506092 -0.481138 -0.646363 C 4.303701 0.416838 -1.072283 C 5.494415 0.354531 -1.814643 C 4.397015 0.593940 0.318381 C 6.737601 0.474258 -1.193277 H 5.439544 0.210692 -2.890675 C 5.639316 0.716929 0.940249 H 3.495505 0.614238 0.921391 C 6.816094 0.658368 0.189252 H 7.644424 0.426196 -1.787340 H 5.688471 0.850899 2.016310 H 7.781547 0.752754 0.675036 H -0.040297 1.852576 -1.594505 C -2.792830 2.549358 1.498968 C -3.903842 1.617678 0.994069 H -2.647450 2.483672 2.584223 H -4.540729 1.231802 1.794058 C -1.805390 0.803020 0.226293 N -1.596376 2.018116 0.808327 N -3.125142 0.530027 0.376770 C -0.315245 2.617455 1.044843 C 0.526286 2.080170 2.039251 C 0.057266 3.757162 0.302153 C 1.763435 2.697338 2.262350 C 1.302569 4.339342 0.558942 C 2.153062 3.812604 1.527291 H 2.431975 2.295017 3.017293 H 1.615408 5.208560 -0.010136

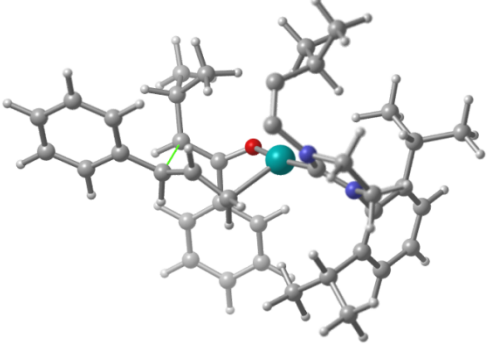
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	C	-4.203289	-0.799787	-1.377367
	C	-3.889037	-1.727852	0.881024
	C	-4.823552	-1.996005	-1.756254
	C	-4.511516	-2.906841	0.460730
	C	-4.979481	-3.037964	-0.846119
	H	-5.174561	-2.118241	-2.776333
	H	-4.622970	-3.734450	1.153597
	C	-3.304503	-1.607975	2.282719
	H	-3.143247	-0.542901	2.488811
	C	-3.985955	0.308243	-2.396840
	H	-3.506369	1.148563	-1.882121
	C	0.144681	0.863093	2.870350
	H	-0.804515	0.470174	2.492798
	C	-0.866181	4.374291	-0.740503
	H	-1.661447	3.647218	-0.947584
	C	-0.149612	4.676082	-2.069574
	H	0.580810	5.484691	-1.954393
	H	-0.878816	4.996936	-2.821580
	H	0.379238	3.798633	-2.451972
	C	-1.513659	5.663846	-0.193936
	H	-2.243409	6.060625	-0.908583
	H	-0.748871	6.431497	-0.027413
	H	-2.020551	5.493567	0.761459
	C	-5.315435	0.812529	-2.985694
	H	-5.992297	1.159798	-2.197350
	H	-5.828239	0.020896	-3.543930
	H	-5.133506	1.643166	-3.676682
	C	-3.019592	-0.155081	-3.502668
	H	-2.804163	0.669743	-4.191651
	H	-3.451368	-0.979002	-4.083080
	H	-2.076151	-0.501458	-3.065270
	C	-1.924948	-2.290876	2.342675
	H	-1.240621	-1.858722	1.601629
	H	-2.015440	-3.363609	2.133970
	H	-1.473387	-2.168511	3.334166
	C	-4.242162	-2.152007	3.372479
	H	-5.231009	-1.685057	3.314694
	H	-3.820662	-1.950311	4.363297
	H	-4.373525	-3.236333	3.287811
	C	-0.060533	1.239859	4.349141
	H	-0.822495	2.019547	4.460183
	H	0.868933	1.613504	4.794178
	H	-0.378509	0.360648	4.920983
	C	1.184185	-0.257839	2.717602
	H	0.859650	-1.163525	3.239278
	H	2.156961	0.032122	3.131968
	H	1.319908	-0.513126	1.661913
	H	3.121259	4.267793	1.703750
	H	-5.457065	-3.960664	-1.157997
	H	3.851206	-2.069949	-1.783149
	C	2.176404	-2.736148	0.266113
	C	1.180383	-3.427565	0.976569
	C	3.435783	-2.570470	0.863015
	C	1.430124	-3.927352	2.250912
	H	0.211251	-3.558759	0.509782
	C	3.679687	-3.056830	2.148252
	H	4.224174	-2.041628	0.340857
	C	2.680278	-3.736157	2.847670
	H	0.648921	-4.462393	2.781783
	H	4.653824	-2.904047	2.601260
	H	2.873951	-4.117681	3.844809
	C	2.475696	-1.871989	-3.486958
	C	2.350063	-3.324462	-3.970321
	H	1.531278	-1.348406	-3.670784
	H	3.254221	-1.362259	-4.070399



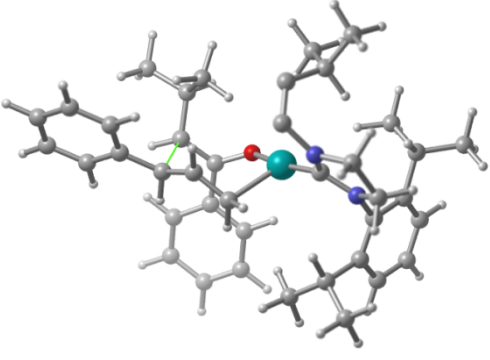
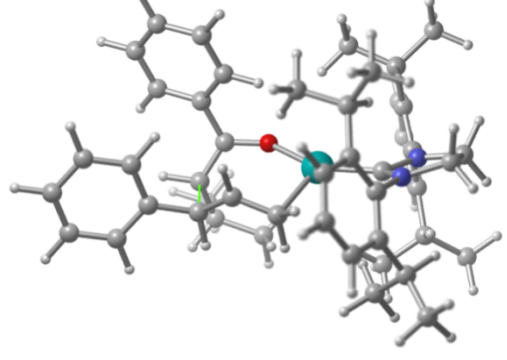
	H	2.156153	-3.363027	-5.048162
	H	1.524276	-3.824810	-3.455276
	H	3.270090	-3.885388	-3.769581
	O	0.584951	-2.068883	-1.390110
	H	-2.963033	3.594392	1.236389
	H	-4.545282	2.092497	0.241897

TS2a-Me				TS4a-Me			
							
Gas phase energy= -466.414582932				Gas phase energy= -466.417272253			
Gas phase free energy correction= 0.897058				Gas phase free energy correction= 0.895080			
SMD energy= -2139.94608978				SMD energy= -2139.94723377			
C	2.946574	0.842850	-1.378103	C	2.689579	-1.585619	-0.882171
C	2.116724	1.965280	-1.166847	C	2.658876	-1.145799	0.453879
C	3.071768	0.243562	0.631086	C	2.638928	0.401403	-1.774258
H	3.078612	1.261526	1.018446	H	2.304439	-0.065861	-2.697783
C	1.910383	-0.495424	0.936678	C	1.692603	1.247457	-1.154097
C	0.726781	0.083243	1.436168	C	0.317070	1.310266	-1.484436
H	1.893813	-1.560713	0.719412	H	2.037939	1.930292	-0.381657
H	0.810609	1.086737	1.860987	H	-0.005258	0.822695	-2.406295
Pd	-0.499258	0.543788	-0.299082	Pd	-0.241894	0.019540	0.116715
C	4.433304	-0.373822	0.698880	C	4.095830	0.702439	-1.751672
C	5.563065	0.449944	0.560630	C	4.936828	0.071592	-2.684128
C	4.638885	-1.739702	0.949634	C	4.680362	1.569421	-0.815219
C	6.852529	-0.074936	0.637810	C	6.314019	0.287722	-2.674911
H	5.422610	1.515690	0.398779	H	4.502331	-0.605698	-3.415617
C	5.928158	-2.267367	1.021484	C	6.057823	1.783088	-0.801649
H	3.788985	-2.397452	1.099425	H	4.066689	2.063903	-0.071856
C	7.041872	-1.440425	0.860908	C	6.882592	1.143144	-1.728127
H	7.708506	0.583142	0.529348	H	6.943053	-0.212251	-3.404429
H	6.063613	-3.327175	1.212016	H	6.486824	2.441310	-0.053832
H	8.043412	-1.852895	0.921744	H	7.954795	1.307892	-1.712625
H	0.052837	-0.565291	1.989314	H	-0.213214	2.235956	-1.270862
C	-3.260133	-2.550574	0.933233	C	-4.465772	-0.344780	0.807409
C	-4.099858	-1.296196	1.215611	C	-4.275167	1.165635	1.019477
H	-3.651779	-3.138373	0.093415	H	-4.818023	-0.861617	1.703411
H	-5.086164	-1.322038	0.746157	H	-4.273499	1.442041	2.081201
C	-2.008591	-0.629726	0.310498	C	-2.229815	0.238759	0.245042
N	-1.951784	-1.970653	0.566220	N	-3.097456	-0.780759	0.468540
N	-3.267109	-0.233749	0.621351	N	-2.933007	1.387543	0.446217
C	-3.770186	1.099053	0.481638	C	-2.388282	2.700068	0.283894
C	-3.548531	2.039253	1.501363	C	-1.556685	3.240339	1.279744
C	-4.499167	1.416928	-0.680615	C	-2.689128	3.399748	-0.902811
C	-4.096820	3.318270	1.347394	C	-0.993680	4.502277	1.050191
C	-5.022946	2.707526	-0.798515	C	-2.108100	4.657630	-1.089075
C	-4.829207	3.649314	0.210906	C	-1.259945	5.200306	-0.123604
H	-3.940469	4.064731	2.120169	H	-0.337554	4.939057	1.796617

H	-5.578609	2.985380	-1.687946	H	-2.307259	5.218409	-1.995282
C	-0.851297	-2.804794	0.181893	C	-2.788441	-2.171088	0.331552
C	-0.604147	-3.017668	-1.190130	C	-2.952195	-2.784031	-0.924437
C	-0.048303	-3.398012	1.176376	C	-2.367763	-2.892408	1.463005
C	0.516852	-3.773728	-1.548769	C	-2.713839	-4.158536	-1.023336
C	1.047933	-4.168365	0.769995	C	-2.137817	-4.265440	1.319717
C	1.343315	-4.336342	-0.580150	C	-2.318266	-4.895309	0.091345
H	0.740540	-3.932474	-2.598770	H	-2.828470	-4.656180	-1.981499
H	1.684706	-4.629904	1.517981	H	-1.807923	-4.844960	2.176427
C	-1.552034	-2.522938	-2.276794	C	-1.275646	2.510126	2.585767
H	-2.304221	-1.875671	-1.814771	H	-1.716367	1.510008	2.515499
C	-0.363545	-3.255784	2.659730	C	-3.578683	2.771518	-1.972667
H	-1.078912	-2.430904	2.767979	H	-4.311753	2.133620	-1.464633
C	-4.644776	0.408455	-1.812026	C	-2.153236	-2.217501	2.809569
H	-4.457600	-0.589556	-1.397575	H	-2.355361	-1.147844	2.682353
C	-2.717210	1.709775	2.731986	C	-3.324083	-1.976041	-2.159614
H	-2.313877	0.699222	2.605313	H	-3.609001	-0.969526	-1.832487
H	-5.243510	4.646278	0.105148	H	-0.807453	6.172263	-0.288620
H	2.211350	-4.914343	-0.878377	H	-2.134756	-5.960264	-0.002715
C	-1.514997	2.662940	2.853001	C	-1.943410	3.240762	3.766890
H	-0.851728	2.339432	3.662979	H	-3.020626	3.357342	3.603980
H	-1.837495	3.687916	3.070364	H	-1.514457	4.240704	3.901348
H	-0.944074	2.672687	1.918806	H	-1.791114	2.680815	4.696307
C	-3.574612	1.723794	4.010629	C	0.230612	2.317636	2.831655
H	-4.408004	1.016396	3.936039	H	0.741880	3.278934	2.961607
H	-3.995759	2.719789	4.190357	H	0.692748	1.782102	1.995190
H	-2.967238	1.451598	4.881084	H	0.390144	1.726086	3.739886
C	0.872659	-2.918158	3.512650	C	-3.132398	-2.761152	3.866857
H	1.576583	-3.757436	3.544720	H	-3.001801	-2.228998	4.815693
H	0.567173	-2.710359	4.544047	H	-2.957337	-3.826957	4.053605
H	1.404908	-2.043530	3.128705	H	-4.173316	-2.644147	3.544509
C	-1.026466	-4.545162	3.189555	C	-0.693104	-2.350698	3.278267
H	-1.906963	-4.823482	2.600783	H	0.002711	-1.934222	2.542486
H	-1.331294	-4.419429	4.234495	H	-0.427331	-3.400952	3.448330
H	-0.319900	-5.381842	3.139683	H	-0.551592	-1.814365	4.223629
C	-2.292460	-3.715904	-2.914159	C	-2.763222	1.854723	-2.904237
H	-2.811725	-4.312710	-2.156010	H	-1.984692	2.425832	-3.422993
H	-1.593441	-4.376331	-3.440227	H	-3.417822	1.401022	-3.657838
H	-3.031547	-3.357992	-3.639926	H	-2.278413	1.052969	-2.340258
C	-0.841094	-1.682304	-3.346097	C	-4.368641	3.807477	-2.787601
H	-1.552111	-1.373306	-4.119766	H	-3.712395	4.395652	-3.438416
H	-0.037376	-2.243439	-3.836109	H	-4.915002	4.498217	-2.137050
H	-0.408943	-0.780794	-2.901669	H	-5.091694	3.296992	-3.432672
C	-6.051832	0.393063	-2.430398	C	-2.100179	-1.820303	-3.080781
H	-6.822030	0.251343	-1.664848	H	-2.350343	-1.206381	-3.953666
H	-6.131798	-0.422783	-3.157060	H	-1.751857	-2.797452	-3.436450
H	-6.269363	1.325468	-2.962773	H	-1.278164	-1.339383	-2.540883
C	-3.568053	0.662414	-2.884291	C	-4.522984	-2.575202	-2.913778
H	-2.564604	0.635097	-2.444266	H	-5.385725	-2.696902	-2.250007
H	-3.707240	1.647341	-3.344900	H	-4.283081	-3.556341	-3.338535
H	-3.624481	-0.097832	-3.671966	H	-4.813537	-1.918847	-3.741698
O	0.820437	1.850255	-1.181346	H	3.656090	-1.875443	-1.286953
C	2.668119	3.258253	-0.678872	C	1.496375	-2.268674	-1.525786
C	1.847161	4.094559	0.094000	C	1.823778	-2.744577	-2.948904
C	3.985311	3.665346	-0.947374	H	0.668643	-1.543892	-1.579526
C	2.337601	5.294989	0.605487	H	0.939357	-3.194612	-3.413299
H	0.824563	3.785096	0.277139	H	2.160991	-1.927800	-3.596890
C	4.473719	4.868648	-0.438418	H	2.616086	-3.503530	-2.925523
H	4.624924	3.053292	-1.575009	C	3.909255	-0.817795	1.191617
C	3.653712	5.684901	0.344884	C	3.848344	0.122798	2.230737
H	1.693294	5.927199	1.207616	C	5.151779	-1.375904	0.856315
H	5.491738	5.172890	-0.658709	C	5.006508	0.522470	2.894763
H	4.035990	6.618889	0.743003	H	2.880971	0.535185	2.493161
H	4.010902	1.035897	-1.495637	C	6.309525	-0.978043	1.521841
C	2.425068	-0.317057	-2.211406	H	5.221411	-2.117637	0.068736
C	2.131015	0.185273	-3.640305	C	6.242812	-0.021683	2.537558

<pre> H  1.481799  -0.662418  -1.765836 H  1.764062  -0.632613  -4.271089 H  3.044329  0.582115   -4.100780 H  1.376476  0.977495  -3.627074 C  3.389646  -1.508443  -2.261192 H  3.470040  -2.009181  -1.294892 H  3.032682  -2.245932  -2.989618 H  4.396752  -1.193046  -2.561888 H  -4.232031  -1.110418  2.288318 H  -3.172215  -3.205259  1.801363 </pre>	<pre> H  4.946240  1.259798  3.688922 H  7.264835  -1.409806  1.243226 H  7.146156  0.291246  3.050869 O  1.538974  -0.785683  1.000566 C  0.989033  -3.450622  -0.678908 H  1.766875  -4.218014  -0.580773 H  0.699648  -3.116453  0.321037 H  0.110814  -3.905971  -1.149377 H  -5.151152  -0.575510  -0.017495 H  -5.028055  1.771006  0.510445 </pre>
<b>TS2b-Me</b>	<b>TS4b-Me</b>
	<p>Optimization leads to TS4a-Me.</p>
<pre> Gas phase energy=          -466.411246510 Gas phase free energy correction=  0.896751 SMD energy=                -2139.94285643 </pre>	
<pre> C  3.089745  1.633840  -1.286003 C  1.808099  2.216402  -1.236852 C  3.145520  0.757726  0.606698 H  3.086541  1.740505  1.073873 C  2.054818  -0.098667  0.884639 C  0.781285  0.344183  1.290642 H  2.193516  -1.172082  0.779854 H  0.687102  1.394614  1.574488 Pd -0.432905  0.281944  -0.523464 C  4.531080  0.208947  0.593125 C  5.603276  1.053426  0.922691 C  4.816214  -1.122141  0.244803 C  6.917790  0.586225  0.913675 H  5.398531  2.086883  1.191245 C  6.129714  -1.590088  0.237609 H  4.011778  -1.793644  -0.037662 C  7.187431  -0.740335  0.571831 H  7.729790  1.256663  1.175694 H  6.329046  -2.621530  -0.034943 H  8.208220  -1.107624  0.563236 H  0.194576  -0.326817  1.912068 C  -2.859064  -2.873595  1.170280 C  -3.835634  -1.689678  1.279815 H  -3.181192  -3.618701  0.432584 H  -4.797030  -1.877377  0.795076 C  -1.813821  -0.929315  0.294267 N  -1.621786  -2.214723  0.704941 N  -3.101420  -0.620208  0.578059 C  -3.702068  0.652891  0.316816 C  -3.591117  1.677906  1.272217 C  -4.386119  0.836779  -0.899105 C  -4.200410  2.906492  0.992817 </pre>	

C	-4.970859	2.083346	-1.144089
C	-4.883252	3.108375	-0.203936
H	-4.131762	3.714585	1.714590
H	-5.490692	2.259965	-2.080017
C	-0.423686	-2.953218	0.432784
C	-0.146219	-3.333542	-0.895294
C	0.453131	-3.266554	1.490918
C	1.068210	-3.977113	-1.157051
C	1.648502	-3.926631	1.184760
C	1.963385	-4.262464	-0.129999
H	1.314432	-4.258628	-2.175933
H	2.347272	-4.167971	1.978799
C	-1.138982	-3.116233	-2.031261
H	-1.991622	-2.549510	-1.641781
C	0.108628	-2.947245	2.939754
H	-0.700455	-2.205789	2.929977
C	-4.430623	-0.262931	-1.950396
H	-4.158111	-1.204607	-1.458891
C	-2.826137	1.481530	2.572322
H	-2.305046	0.519531	2.511139
H	-5.343958	4.069076	-0.407847
H	2.902763	-4.757921	-0.351368
C	-1.753393	2.566783	2.763400
H	-1.119575	2.327372	3.624363
H	-2.204250	3.549629	2.943417
H	-1.118098	2.643209	1.876751
C	-3.784299	1.431933	3.777578
H	-4.540265	0.648156	3.655630
H	-4.309756	2.387016	3.894549
H	-3.228644	1.236403	4.701487
C	1.284973	-2.345756	3.728882
H	2.076951	-3.085726	3.890158
H	0.939577	-2.017994	4.715630
H	1.724076	-1.486203	3.215257
C	-0.403839	-4.215352	3.655415
H	-1.240168	-4.677898	3.120771
H	-0.730490	-3.977179	4.673902
H	0.396486	-4.961641	3.720821
C	-1.674055	-4.469427	-2.540009
H	-2.115283	-5.053388	-1.724656
H	-0.870955	-5.067806	-2.985304
H	-2.440597	-4.309981	-3.306695
C	-0.541519	-2.289162	-3.178640
H	-1.281047	-2.158315	-3.976098
H	0.341449	-2.772174	-3.611939
H	-0.243458	-1.299650	-2.818961
C	-5.829304	-0.447927	-2.561520
H	-6.585418	-0.605032	-1.785036
H	-5.833876	-1.315878	-3.229972
H	-6.128542	0.423125	-3.154895
C	-3.377062	0.001895	-3.042165
H	-2.375463	0.088722	-2.605241
H	-3.594531	0.936873	-3.571525
H	-3.367510	-0.814181	-3.773585
O	0.759636	1.544341	-1.619187
C	1.558274	3.503865	-0.523653
C	0.227612	3.892619	-0.287895
C	2.586912	4.337245	-0.049611
C	-0.065569	5.065843	0.402831
H	-0.569324	3.253291	-0.649826
C	2.292412	5.511210	0.645075
H	3.626571	4.085943	-0.229350
C	0.965788	5.880361	0.876767
H	-1.101684	5.338733	0.575611
H	3.101140	6.140955	1.001443
H	0.739629	6.793628	1.416951

H 3.914247 2.311176 -1.065843 C 3.510473 0.603380 -2.327375 C 2.568492 -0.589302 -2.539331 H 4.478418 0.208244 -1.991438 H 3.077281 -1.360662 -3.131165 H 1.670831 -0.273245 -3.073516 H 2.244512 -1.036899 -1.595743 H -4.024038 -1.396376 2.319136 H -2.700964 -3.378291 2.124504 C 3.758049 1.322835 -3.670682 H 4.485800 2.134672 -3.560530 H 4.143448 0.617362 -4.416543 H 2.822085 1.748553 -4.050161	
<b>TS2c-Me</b>	<b>TS4c-Me</b>
	
Gas phase energy= -466.409914631 Gas phase free energy correction= 0.897083 SMD energy= -2139.94121615	Gas phase energy= -466.407528073 Gas phase free energy correction= 0.894563 SMD energy= -2139.93931902
C 3.035935 1.374067 -1.443761 C 1.835589 2.110983 -1.366389 C 3.134370 0.719884 0.531185 H 3.078942 1.746304 0.892701 C 2.033128 -0.090886 0.893988 C 0.775952 0.407746 1.276070 H 2.136449 -1.170974 0.838411 H 0.707353 1.472727 1.507947 Pd -0.488684 0.333887 -0.530819 C 4.531660 0.188719 0.588882 C 5.599013 1.102903 0.577784 C 4.838704 -1.179016 0.666554 C 6.923782 0.671086 0.603942 H 5.382237 2.167764 0.546610 C 6.164407 -1.613825 0.691496 H 4.043997 -1.915533 0.712137 C 7.214183 -0.694175 0.651622 H 7.728342 1.398843 0.588725 H 6.376695 -2.676688 0.745953 H 8.243534 -1.036167 0.667648 H 0.165531 -0.220649 1.918710 C -2.961470 -2.757819 1.200605 C -3.902733 -1.548988 1.336161 H -3.315309 -3.486863 0.461375 H -4.879508 -1.708945 0.872710 C -1.879175 -0.836798 0.319771 N -1.713816 -2.128306 0.721334 N -3.155176 -0.497393 0.621868 C -3.740236 0.780718 0.351509	C 3.171293 -1.460315 -1.313034 C 2.553230 -1.598245 -0.054771 C 2.950637 0.613981 -1.575705 H 2.658803 0.456631 -2.613480 C 1.968282 1.257594 -0.780406 C 0.608427 1.397890 -1.113286 H 2.291197 1.697488 0.161528 H 0.314900 1.185763 -2.143371 Pd -0.313728 -0.276371 -0.074710 C 4.386349 0.988929 -1.418752 C 5.217206 1.002662 -2.551267 C 4.954232 1.299382 -0.171918 C 6.572765 1.315675 -2.445052 H 4.791609 0.766196 -3.523129 C 6.309888 1.607968 -0.065786 H 4.346285 1.274685 0.726516 C 7.126679 1.618288 -1.199460 H 7.195104 1.322971 -3.334171 H 6.730300 1.830155 0.909478 H 8.181523 1.856481 -1.111827 H 0.076475 2.235172 -0.671157 C -4.470787 -0.109537 0.892852 C -4.160944 1.382935 1.095914 H -4.805356 -0.605210 1.807905 H -4.128197 1.665431 2.155029 C -2.219401 0.312977 0.235110 N -3.161908 -0.637883 0.470749 N -2.811026 1.505771 0.507375 C -2.179552 2.782424 0.393523

C	-3.590255	1.822246	1.282940	C	-1.352282	3.243442	1.431229
C	-4.454925	0.950007	-0.849251	C	-2.407680	3.536313	-0.774751
C	-4.197214	3.051088	0.999194	C	-0.730752	4.488380	1.271914
C	-5.035545	2.197235	-1.099848	C	-1.765924	4.772413	-0.894228
C	-4.913463	3.237477	-0.180215	C	-0.931610	5.242784	0.119853
H	-4.100476	3.871377	1.703791	H	-0.075922	4.864267	2.051951
H	-5.578926	2.362973	-2.024224	H	-1.907891	5.372213	-1.786257
C	-0.546455	-2.903794	0.420541	C	-2.960709	-2.037755	0.248095
C	-0.309057	-3.292839	-0.913617	C	-3.207272	-2.564022	-1.033491
C	0.334073	-3.257072	1.462570	C	-2.517697	-2.843543	1.312359
C	0.860821	-4.007203	-1.192578	C	-3.014769	-3.934949	-1.230128
C	1.488610	-3.977910	1.136701	C	-2.345338	-4.211148	1.074745
C	1.758116	-4.337813	-0.181564	C	-2.593044	-4.753085	-0.183844
H	1.075235	-4.302591	-2.214514	H	-3.182841	-4.365981	-2.212337
H	2.186157	-4.256770	1.920031	H	-1.996801	-4.854546	1.876541
C	-1.301616	-3.012983	-2.037325	C	-1.107764	2.423422	2.689047
H	-2.090897	-2.361324	-1.648728	H	-1.619859	1.462644	2.569094
C	0.031509	-2.921040	2.917131	C	-3.277155	2.982041	-1.897642
H	-0.752140	-2.152938	2.920993	H	-4.026736	2.322293	-1.443643
C	-4.532653	-0.166850	-1.880981	C	-2.195284	-2.256771	2.678548
H	-4.281681	-1.107113	-1.375319	H	-2.322552	-1.170383	2.609370
C	-2.784104	1.643767	2.560402	C	-3.615390	-1.671656	-2.197306
H	-2.273713	0.676176	2.499937	H	-3.790377	-0.663303	-1.804542
H	-5.372438	4.198254	-0.387633	H	-0.434608	6.200226	0.007169
H	2.664914	-4.883425	-0.419869	H	-2.444245	-5.814028	-0.353984
C	-1.696091	2.723066	2.693636	C	-1.690337	3.122477	3.931043
H	-1.033835	2.493817	3.535637	H	-2.761577	3.317411	3.809621
H	-2.132757	3.712810	2.871052	H	-1.193392	4.082725	4.111744
H	-1.091205	2.775520	1.783843	H	-1.550705	2.497870	4.820459
C	-3.700888	1.625244	3.798099	C	0.386688	2.110062	2.870806
H	-4.464698	0.843907	3.716326	H	0.968382	3.018502	3.066549
H	-4.216499	2.585821	3.913999	H	0.784741	1.629071	1.972116
H	-3.115760	1.443467	4.706510	H	0.530734	1.428137	3.716909
C	1.243545	-2.356182	3.678702	C	-3.161361	-2.780747	3.756733
H	2.023632	-3.115016	3.807545	H	-2.950314	-2.306140	4.721657
H	0.934530	-2.034098	4.679314	H	-3.054495	-3.864224	3.884473
H	1.685988	-1.498716	3.164683	H	-4.204804	-2.575873	3.491757
C	-0.506809	-4.168739	3.649435	C	-0.728710	-2.521261	3.064948
H	-1.366507	-4.608076	3.132714	H	-0.048756	-2.207054	2.266729
H	-0.807256	-3.915195	4.672275	H	-0.554335	-3.587332	3.252613
H	0.271132	-4.939138	3.705091	H	-0.473174	-1.975320	3.980521
C	-1.967410	-4.325897	-2.495912	C	-2.439799	2.112161	-2.854725
H	-2.447451	-4.840920	-1.656167	H	-1.643588	2.706978	-3.317451
H	-1.229021	-5.009806	-2.930044	H	-3.073574	1.705130	-3.651248
H	-2.728211	-4.120363	-3.257358	H	-1.977418	1.276394	-2.321152
C	-0.661715	-2.275773	-3.224747	C	-4.034670	4.072286	-2.671102
H	-1.410843	-2.105258	-4.005678	H	-3.356215	4.686979	-3.272929
H	0.157387	-2.853795	-3.667069	H	-4.587827	4.733299	-1.995745
H	-0.263788	-1.304208	-2.914712	H	-4.748633	3.609436	-3.360771
C	-5.937415	-0.329085	-2.484175	C	-2.470264	-1.562702	-3.219882
H	-6.694922	-0.450759	-1.702701	H	-2.746081	-0.882126	-4.033467
H	-5.965410	-1.210913	-3.133579	H	-2.237745	-2.541325	-3.655770
H	-6.216705	0.535831	-3.095915	H	-1.564783	-1.181114	-2.737156
C	-3.477150	0.053171	-2.981162	C	-4.919370	-2.147694	-2.860963
H	-2.470812	0.117637	-2.550681	H	-5.728957	-2.230813	-2.127733
H	-3.671248	0.986955	-3.521466	H	-4.791714	-3.127744	-3.334378
H	-3.494759	-0.772621	-3.701652	H	-5.227987	-1.440676	-3.639126
O	0.709916	1.537617	-1.676903	H	4.259039	-1.457600	-1.285286
C	1.761437	3.450069	-0.720620	C	2.659254	-2.092592	-2.603326
C	0.501628	3.954310	-0.353532	C	3.340115	-1.358841	1.185935
C	2.899692	4.222349	-0.430492	C	2.710883	-0.724877	2.268275
C	0.384731	5.182117	0.293995	C	4.696024	-1.702890	1.299559
H	-0.378604	3.364595	-0.583528	C	3.426965	-0.409433	3.422040
C	2.781818	5.451037	0.219490	H	1.660052	-0.476360	2.183579
H	3.884956	3.877480	-0.725717	C	5.410053	-1.397369	2.457098
C	1.524585	5.934878	0.587927	H	5.195652	-2.211619	0.482303

H	-0.597736	5.549509	0.572319	C	4.780792	-0.740883	3.518542
H	3.672467	6.032378	0.434549	H	2.929608	0.095095	4.244402
H	1.434170	6.889940	1.094400	H	6.458220	-1.667215	2.530706
H	3.952630	1.950798	-1.345887	H	5.339741	-0.496542	4.415819
C	3.153205	0.238144	-2.468004	O	1.265701	-1.641419	0.058219
C	2.595644	-1.131696	-2.050655	C	3.057278	-3.583662	-2.616390
H	2.546972	0.561137	-3.327572	H	4.133632	-3.711171	-2.455580
H	2.522995	-1.780018	-2.932202	H	2.526094	-4.118511	-1.820614
H	1.600776	-1.045201	-1.608620	H	2.796807	-4.046027	-3.575772
H	3.249452	-1.630535	-1.330587	H	-5.219784	-0.285797	0.111440
H	-4.059615	-1.254322	2.380396	H	-4.868187	2.043389	0.588517
H	-2.802120	-3.275381	2.147649	H	3.210355	-1.601441	-3.421838
C	4.610631	0.092796	-2.941333	C	1.160181	-1.949522	-2.900421
H	4.681637	-0.661418	-3.733350	H	0.836370	-0.905498	-2.869490
H	4.996374	1.038589	-3.339037	H	0.944420	-2.342945	-3.901463
H	5.261112	-0.221063	-2.116699	H	0.559670	-2.497834	-2.170784

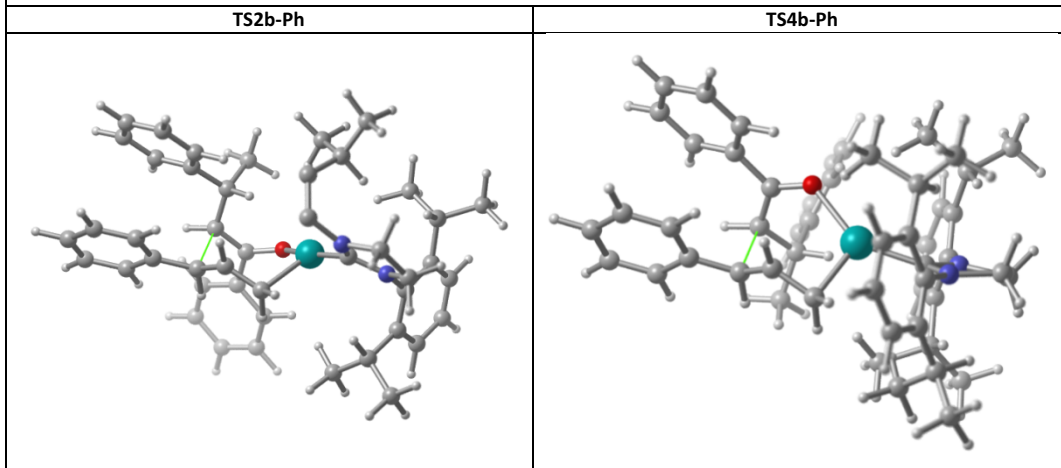
TS2a-Ph	TS4a-Ph
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C 3.024910 -0.630254 0.514988 C 2.149692 -1.729312 0.637245 C 2.674583 -0.274355 -1.532694 H 2.550167 -1.328421 -1.778951 C 1.497224 0.491692 -1.646851 C 0.220194 -0.069962 -1.856642 H 1.554298 1.569664 -1.510373 H 0.190121 -1.089651 -2.247697 Pd -0.635326 -0.455991 0.101334 C 4.002539 0.237452 -1.996541 C 5.108356 -0.629324 -1.995531 C 4.182081 1.536312 -2.496880 C 6.358372 -0.203449 -2.442600 H 4.979527 -1.650730 -1.646646 C 5.433233 1.966144 -2.939314 H 3.337534 2.215150 -2.552837 C 6.529453 1.101796 -2.909079 H 7.196979 -0.891952 -2.431599 H 5.549688 2.976062 -3.319082 H 7.500887 1.436960 -3.256738 H -0.529078 0.583069 -2.296891 C -3.727177 2.383280 -0.871533 C -4.498261 1.071311 -1.084979 H -4.081917 2.941646 0.003839 H -5.437786 1.026897 -0.528848	C -2.778342 0.890808 0.440035 C -2.406625 -0.119854 1.344052 C -2.605450 -0.283417 -1.361202 H -2.516188 0.647129 -1.917416 C -1.451064 -1.100073 -1.360695 C -0.162037 -0.685332 -1.768385 H -1.551275 -2.134960 -1.041180 H -0.080702 0.261500 -2.305389 Pd 0.532212 -0.288185 0.220787 C -3.978016 -0.857019 -1.402307 C -5.043581 -0.025271 -1.788758 C -4.265436 -2.183171 -1.045881 C -6.354000 -0.499919 -1.807690 H -4.836419 1.006708 -2.063244 C -5.576610 -2.657526 -1.061788 H -3.471068 -2.848597 -0.728849 C -6.627229 -1.819941 -1.439934 H -7.161096 0.160042 -2.109097 H -5.776533 -3.681580 -0.765091 H -7.646763 -2.191113 -1.448662 H 0.527737 -1.448029 -2.123036 C 4.721101 0.445085 0.769154 C 4.791503 -0.861622 -0.039532 H 5.129615 0.344667 1.777943 H 5.036189 -1.729684 0.584810

C	-2.295462	0.555570	-0.374019	C	2.529329	-0.139114	0.049672
N	-2.354189	1.895673	-0.629234	N	3.268417	0.693810	0.826237
N	-3.542936	0.068982	-0.574825	N	3.410111	-0.987928	-0.545755
C	-3.943577	-1.289354	-0.365254	C	3.030876	-2.047186	-1.428713
C	-3.753477	-2.240452	-1.381832	C	2.490085	-3.232432	-0.900600
C	-4.542747	-1.622632	0.864576	C	3.189679	-1.847819	-2.814762
C	-4.207350	-3.545240	-1.154860	C	2.079359	-4.223519	-1.801161
C	-4.972630	-2.939413	1.054307	C	2.769869	-2.864796	-3.677309
C	-4.813904	-3.891813	0.049344	C	2.212525	-4.040411	-3.174098
H	-4.076630	-4.299460	-1.924583	H	1.647932	-5.144705	-1.422077
H	-5.426690	-3.227923	1.996616	H	2.868772	-2.740304	-4.749613
C	-1.269213	2.786710	-0.338679	C	2.723583	1.729576	1.650968
C	-0.905464	2.997108	1.007529	C	2.563734	3.018142	1.109283
C	-0.585364	3.416592	-1.397408	C	2.374253	1.429397	2.980167
C	0.211041	3.798334	1.269920	C	2.048333	4.020664	1.936727
C	0.519779	4.217545	-1.086145	C	1.862743	2.462341	3.773722
C	0.928222	4.390817	0.233851	C	1.703920	3.746104	3.258700
H	0.516633	3.967552	2.297568	H	1.900748	5.021019	1.542445
H	1.068752	4.707957	-1.883662	H	1.579468	2.257573	4.801484
C	-1.723099	2.439481	2.166893	C	2.351246	-3.464201	0.597915
H	-2.435730	1.710857	1.769054	H	2.646111	-2.542318	1.110555
C	-1.059928	3.296882	-2.840261	C	3.746407	-0.532094	-3.350220
H	-1.743529	2.440353	-2.893126	H	4.476387	-0.158482	-2.622005
C	-4.650342	-0.601272	1.988337	C	2.538512	0.030950	3.557621
H	-4.516541	0.395378	1.551388	H	2.870915	-0.628392	2.747636
C	-3.065109	-1.889288	-2.691765	C	2.868243	3.300335	-0.355371
H	-2.643663	-0.883511	-2.589907	H	3.479176	2.473994	-0.738234
H	-5.155019	-4.908940	0.210133	H	1.881195	-4.814668	-3.857649
H	1.798731	4.998270	0.456795	H	1.299842	4.533279	3.886172
C	-1.893757	-2.843849	-2.981359	C	3.293987	-4.589366	1.065489
H	-1.327075	-2.495576	-3.852005	H	4.336039	-4.366554	0.810309
H	-2.246277	-3.858949	-3.197365	H	3.030840	-5.543961	0.595315
H	-1.216464	-2.891779	-2.122591	H	3.222902	-4.717174	2.151369
C	-4.067665	-1.871248	-3.860931	C	0.895871	-3.752666	1.005129
H	-4.880690	-1.160450	-3.675788	H	0.527813	-4.681508	0.553176
H	-4.515610	-2.861294	-4.006121	H	0.240983	-2.928812	0.699454
H	-3.564789	-1.586253	-4.791826	H	0.823324	-3.854692	2.093699
C	0.075057	3.046753	-3.848267	C	3.620378	0.011558	4.654374
H	0.757415	3.902359	-3.904795	H	3.772277	-1.009426	5.022122
H	-0.346094	2.899425	-4.848875	H	3.324127	0.635336	5.505728
H	0.659721	2.159173	-3.591087	H	4.577448	0.391385	4.278904
C	-1.843431	4.565889	-3.240408	C	1.205418	-0.532023	4.081723
H	-2.647199	4.787460	-2.530371	H	0.431761	-0.516970	3.307284
H	-2.280925	4.450396	-4.238379	H	0.842113	0.045906	4.939925
H	-1.173981	5.433777	-3.259669	H	1.343197	-1.567533	4.414247
C	-2.535793	3.568342	2.832343	C	2.636767	0.532010	-3.456778
H	-3.173934	4.083221	2.105295	H	1.856427	0.202477	-4.152531
H	-1.870128	4.314754	3.281384	H	3.050794	1.477731	-3.825634
H	-3.172918	3.160027	3.625077	H	2.172489	0.713181	-2.483386
C	-0.863611	1.701977	3.202731	C	4.479099	-0.685077	-4.692208
H	-1.503589	1.236231	3.959348	H	3.782670	-0.909177	-5.507865
H	-0.186045	2.384424	3.725679	H	5.229476	-1.481467	-4.652474
H	-0.262267	0.915134	2.735011	H	4.985271	0.252274	-4.946347
C	-6.020461	-0.617762	2.685247	C	1.560740	3.306318	-1.167459
H	-6.834549	-0.497053	1.962568	H	1.764448	3.469236	-2.232243
H	-6.080032	0.198234	3.413671	H	0.885178	4.097793	-0.822105
H	-6.186046	-1.554185	3.229027	H	1.047138	2.346122	-1.050797
C	-3.506178	-0.809236	2.998586	C	3.662300	4.600195	-0.561593
H	-2.530522	-0.750381	2.502545	H	4.579251	4.605203	0.037213
H	-3.584807	-1.793657	3.474189	H	3.072562	5.481577	-0.286530
H	-3.544621	-0.044440	3.782895	H	3.937136	4.707436	-1.616669
O	0.894866	-1.553738	0.917379	H	-3.838768	1.100548	0.338062
C	2.562424	-3.101613	0.233580	C	-1.851774	2.056013	0.129953
C	1.576037	-4.004193	-0.193931	H	-0.928109	1.646518	-0.306287
C	3.900926	-3.526466	0.261021	C	-3.409252	-1.074405	1.888483
C	1.921400	-5.290248	-0.605435	C	-2.983658	-2.364981	2.237701



H	0.542517	-3.676793	-0.188855	C	-4.767943	-0.750792	2.017906
C	4.244991	-4.815326	-0.146920	C	-3.900130	-3.319470	2.674726
H	4.676677	-2.858616	0.622209	H	-1.929195	-2.599842	2.148569
C	3.257244	-5.699816	-0.586833	C	-5.683462	-1.704194	2.458784
H	1.148575	-5.974960	-0.938721	H	-5.117435	0.244748	1.768176
H	5.282245	-5.132186	-0.113001	C	-5.254707	-2.993953	2.781190
H	3.525699	-6.701711	-0.904621	H	-3.559502	-4.317672	2.930783
H	4.082479	-0.855111	0.399465	H	-6.732968	-1.443745	2.544056
C	2.740172	0.642767	1.293460	H	-5.969847	-3.736828	3.118833
H	1.690562	0.922093	1.114274	O	-1.156125	-0.404641	1.528380
C	3.629567	1.816411	0.836881	C	-1.427726	2.814713	1.405535
H	3.324181	2.184712	-0.143435	H	-2.298693	3.223246	1.930504
H	3.559976	2.653229	1.537856	H	-0.893688	2.140003	2.081265
H	4.680898	1.512673	0.775400	H	-0.758918	3.642833	1.149457
H	-4.711952	0.877763	-2.142735	H	5.229505	1.280083	0.272913
H	-3.765236	3.041789	-1.740417	H	5.510542	-0.819974	-0.860613
C	2.898893	0.440990	2.808950	C	-2.473250	2.994570	-0.891853
C	2.522849	1.487212	3.666142	C	-1.863066	3.211978	-2.133866
C	3.423059	-0.720458	3.387800	C	-3.677487	3.660103	-0.616588
C	2.651838	1.377908	5.049050	C	-2.436980	4.067188	-3.078062
H	2.113163	2.397213	3.237242	H	-0.931792	2.702366	-2.363875
C	3.559756	-0.834966	4.774646	C	-4.254939	4.514202	-1.556747
H	3.715622	-1.555329	2.761574	H	-4.166234	3.508616	0.341958
C	3.174715	0.210728	5.612261	C	-3.636346	4.720779	-2.793098
H	2.343043	2.199887	5.687541	H	-1.948938	4.218321	-4.035352
H	3.965789	-1.748333	5.197218	H	-5.187371	5.019166	-1.326153
H	3.278772	0.118548	6.688318	H	-4.085243	5.384293	-3.524696

<b>TS2b-Ph</b>	<b>TS4b-Ph</b>
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Gas phase energy=	-495.970372296	Gas phase energy=	-495.966434487
Gas phase free energy correction=	0.945457	Gas phase free energy correction=	0.944433
SMD energy=	-2331.68980855	SMD energy=	-2331.68522243
C	2.547613	1.494591	-1.046823
C	1.465003	2.400979	-1.008949
C	2.593653	1.001337	0.971446
H	2.353180	2.008480	1.310312
C	1.585052	0.043349	1.227632
C	0.267653	0.382809	1.588505
H	1.809021	-1.012662	1.086908
H	0.099156	1.400236	1.949796
Pd	-0.865830	0.493253	-0.270318
C	4.043260	0.688193	1.171761
C	4.971538	1.742308	1.141516
C	4.520139	-0.608143	1.412318
C	6.335013	1.506486	1.310737
H	4.613697	2.757402	0.985970
C	5.883456	-0.845981	1.578192
C	-2.790826	0.500811	-0.734096
C	-2.618085	-0.045893	0.550946
C	-2.172998	-1.373092	-1.756545
H	-1.952809	-0.792828	-2.646799
C	-1.054937	-1.985288	-1.145167
C	0.296341	-1.726059	-1.487855
H	-1.230755	-2.746373	-0.388836
H	0.488616	-1.177964	-2.411300
Pd	0.478126	-0.362522	0.121491
C	-3.509308	-2.023765	-1.797578
C	-4.468905	-1.547762	-2.707724
C	-3.866688	-3.089498	-0.957345
C	-5.745360	-2.103803	-2.766430
H	-4.207613	-0.724626	-3.368632
C	-5.144836	-3.643564	-1.011054

H	3.831133	-1.442985	1.454199	H	-3.156272	-3.479020	-0.238271
C	6.798912	0.206417	1.522505	C	-6.091522	-3.153506	-1.912095
H	7.033918	2.336371	1.282074	H	-6.469422	-1.718771	-3.477253
H	6.231032	-1.860429	1.741729	H	-5.403808	-4.451616	-0.335502
H	7.859555	0.017257	1.650584	H	-7.086037	-3.585150	-1.950242
H	-0.313592	-0.367063	2.114974	H	1.031526	-2.502356	-1.281343
C	-3.405739	-2.756159	1.090149	C	4.423289	1.303639	0.562609
C	-4.384915	-1.573879	1.080239	C	4.700220	-0.171076	0.895218
H	-3.635326	-3.501763	0.318685	H	4.665599	1.982447	1.383651
H	-5.289232	-1.767146	0.497555	H	4.805713	-0.343256	1.973818
C	-2.258442	-0.818658	0.332232	C	2.443870	0.042387	0.194792
N	-2.116534	-2.100955	0.775759	N	2.969804	1.287607	0.316357
N	-3.575679	-0.516196	0.449968	N	3.470938	-0.827028	0.405586
C	-4.166203	0.727266	0.057625	C	3.342926	-2.250061	0.334650
C	-4.187652	1.803772	0.960071	C	2.733044	-2.950739	1.389468
C	-4.726386	0.822734	-1.230399	C	3.816827	-2.901771	-0.822695
C	-4.806406	2.991392	0.553273	C	2.569108	-4.334838	1.248924
C	-5.327007	2.029783	-1.600567	C	3.634276	-4.284398	-0.919683
C	-5.372492	3.103998	-0.713704	C	3.006781	-4.993862	0.104558
H	-4.836275	3.839036	1.231126	H	2.091647	-4.899360	2.043795
H	-5.755708	2.137490	-2.591615	H	3.976678	-4.815538	-1.800674
C	-0.938334	-2.903540	0.624841	C	2.218720	2.491578	0.135805
C	-0.575212	-3.352503	-0.662220	C	2.031095	2.990297	-1.165133
C	-0.214663	-3.290955	1.771581	C	1.675479	3.128483	1.265546
C	0.537430	-4.193442	-0.778343	C	1.246925	4.138410	-1.322998
C	0.896540	-4.125640	1.604701	C	0.916589	4.284790	1.064150
C	1.269302	-4.576528	0.342041	C	0.691157	4.778676	-0.218078
H	0.838102	-4.549847	-1.758729	H	1.062638	4.530782	-2.318767
H	1.470803	-4.431286	2.473328	H	0.460953	4.782847	1.913487
C	-1.358729	-2.981103	-1.915546	C	2.276000	-2.259789	2.666924
H	-2.184335	-2.324009	-1.624394	H	2.398009	-1.179934	2.531397
C	-0.635704	-2.876932	3.175539	C	4.467168	-2.109851	-1.954180
H	-1.386197	-2.083045	3.076598	H	4.983160	-1.252171	-1.506931
C	-4.620361	-0.328201	-2.221428	C	1.870175	2.567145	2.667274
H	-4.365314	-1.233689	-1.658113	H	2.541970	1.704210	2.590840
C	-3.541519	1.711821	2.333847	C	2.637819	2.296721	-2.376825
H	-3.036046	0.742322	2.403619	H	3.252743	1.464925	-2.015525
H	-5.842671	4.033830	-1.015412	H	2.862972	-6.064700	0.008160
H	2.130323	-5.227121	0.230902	H	0.057169	5.647654	-0.355367
C	-2.466000	2.797738	2.512456	C	3.155439	-2.688116	3.857837
H	-1.921254	2.643830	3.450584	H	4.214818	-2.488869	3.661326
H	-2.911217	3.799035	2.542980	H	3.047150	-3.760276	4.058908
H	-1.750422	2.764623	1.684957	H	2.861695	-2.143243	4.761939
C	-4.594641	1.781346	3.455197	C	0.786673	-2.509089	2.959960
H	-5.347543	0.993389	3.341940	H	0.589754	-3.569394	3.158921
H	-5.115755	2.745720	3.444466	H	0.167579	-2.187820	2.115211
H	-4.117761	1.666066	4.434943	H	0.475460	-1.936561	3.840533
C	0.533009	-2.320392	4.009536	C	2.532250	3.596177	3.601432
H	1.256783	-3.105744	4.255158	H	2.732581	3.145526	4.579906
H	0.155349	-1.916271	4.955266	H	1.880500	4.462616	3.760910
H	1.064931	-1.521985	3.484644	H	3.478394	3.959911	3.185696
C	-1.286101	-4.063672	3.917472	C	0.544205	2.053830	3.256430
H	-2.115443	-4.497429	3.349193	H	0.097770	1.282070	2.620535
H	-1.664870	-3.743082	4.894334	H	-0.180091	2.870995	3.359255
H	-0.549472	-4.858444	4.083225	H	0.711803	1.624751	4.251168
C	-1.972197	-4.228851	-2.578084	C	3.407610	-1.537288	-2.914195
H	-2.594015	-4.789400	-1.871202	H	2.828821	-2.345258	-3.376329
H	-1.195446	-4.905785	-2.951334	H	3.889156	-0.958736	-3.711401
H	-2.596660	-3.933572	-3.428854	H	2.713093	-0.881351	-2.382809
C	-0.489355	-2.191752	-2.908183	C	5.521055	-2.916683	-2.729088
H	-1.060129	-1.957935	-3.813355	H	5.061256	-3.706268	-3.333598
H	0.400467	-2.758691	-3.206154	H	6.247675	-3.380479	-2.053924
H	-0.162406	-1.247126	-2.461445	H	6.061788	-2.256477	-3.415521
C	-5.940832	-0.603319	-2.959512	C	1.546022	1.691191	-3.273079
H	-6.765897	-0.748847	-2.254089	H	1.994146	1.123288	-4.096564
H	-5.846623	-1.506603	-3.572222	H	0.912160	2.474245	-3.704324

H	-6.208772	0.220625	-3.629926	H	0.909686	1.019413	-2.688634
C	-3.469514	-0.071582	-3.212732	C	3.555337	3.241486	-3.172946
H	-2.520429	0.070825	-2.682854	H	4.339588	3.660359	-2.533196
H	-3.663969	0.830736	-3.804085	H	2.990374	4.076576	-3.602275
H	-3.359818	-0.917770	-3.901255	H	4.032851	2.701471	-3.998399
O	0.246042	1.976254	-1.159136	H	-3.802689	0.527088	-1.131895
C	1.635968	3.807798	-0.558099	C	-1.909499	1.641285	-1.241103
C	0.529042	4.478854	-0.014479	C	-1.946175	1.786134	-2.767797
C	2.863611	4.485564	-0.638012	H	-0.867039	1.441563	-0.947018
C	0.651593	5.783771	0.459466	H	-1.424029	2.696079	-3.079163
H	-0.420841	3.958185	0.020833	H	-1.442703	0.950231	-3.258560
C	2.984009	5.792875	-0.167001	H	-2.975405	1.831854	-3.144860
H	3.724850	4.003077	-1.088130	C	-3.719571	-0.772677	1.235902
C	1.880391	6.444701	0.389045	C	-3.389531	-1.757671	2.178689
H	-0.212109	6.285137	0.883598	C	-5.071659	-0.532185	0.950971
H	3.937406	6.305589	-0.240790	C	-4.386446	-2.510849	2.795412
H	1.977045	7.460097	0.758514	H	-2.342360	-1.919733	2.406482
H	3.544703	1.925169	-1.074153	C	-6.068698	-1.283990	1.569478
C	2.373918	0.196432	-1.817971	H	-5.349688	0.241993	0.245038
C	2.060571	0.476424	-3.305989	C	-5.729824	-2.281103	2.486912
H	1.502942	-0.318780	-1.390956	H	-4.117365	-3.276475	3.516025
H	1.921197	-0.467392	-3.844971	H	-7.110270	-1.094045	1.333671
H	2.885649	1.019579	-3.780937	H	-6.507545	-2.867870	2.964728
H	1.146987	1.071586	-3.393920	O	-1.439261	-0.119869	1.090122
H	-4.684006	-1.265767	2.089225	H	4.954669	1.641926	-0.335938
H	-3.360942	-3.261625	2.055749	H	5.587205	-0.567567	0.397625
C	3.557169	-0.747579	-1.707868	C	-2.330925	2.938471	-0.529446
C	3.338252	-2.084523	-1.361442	C	-2.146102	3.052020	0.857853
C	4.866157	-0.334352	-1.989295	C	-2.900809	4.022723	-1.208564
C	4.397291	-2.990892	-1.288057	C	-2.514564	4.208171	1.540175
H	2.327991	-2.409052	-1.133145	H	-1.697106	2.226883	1.397164
C	5.928550	-1.233721	-1.909482	C	-3.264674	5.189279	-0.526500
H	5.062115	0.700098	-2.256532	H	-3.068068	3.973578	-2.278552
C	5.698792	-2.567203	-1.559579	C	-3.072644	5.288634	0.850582
H	4.204961	-4.024075	-1.013850	H	-2.360047	4.268413	2.613343
H	6.938566	-0.892737	-2.111112	H	-3.705105	6.015948	-1.075376
H	6.527085	-3.265657	-1.497739	H	-3.358925	6.190934	1.381298