Supplementary Information

Mechanistic Insight into the Regioselectivity of Pd(II)-catalyzed C-H Functionalization of N-methoxy Cinnamamide

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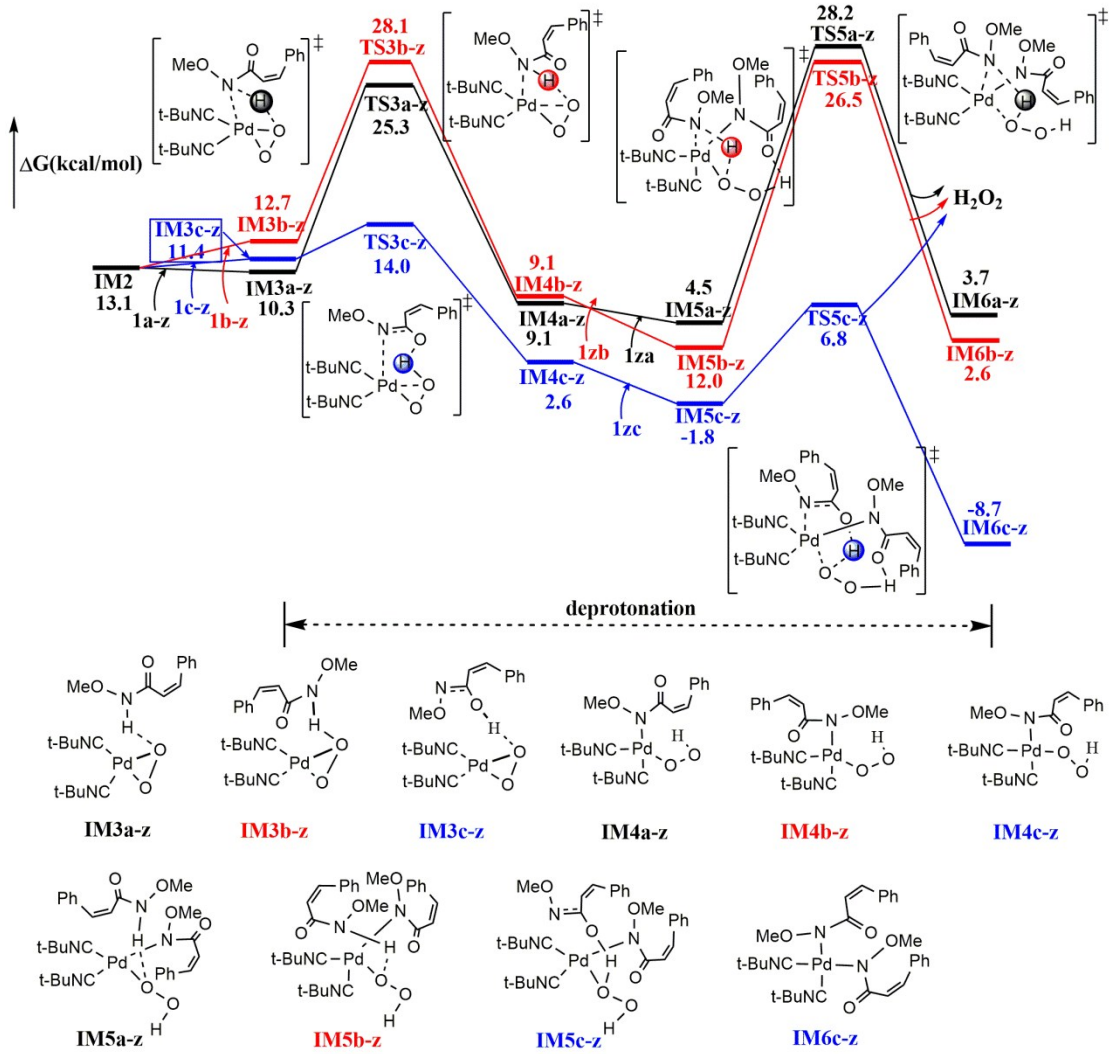

Figure S1. Energy profiles of the deprotonation of (Z)-N-methoxy amide steps. Δ G refer to the Gibbs free energy. All energies are relative to $Pd(t\text{-}BuNC)_2 + O_2$, and are mass balanced.

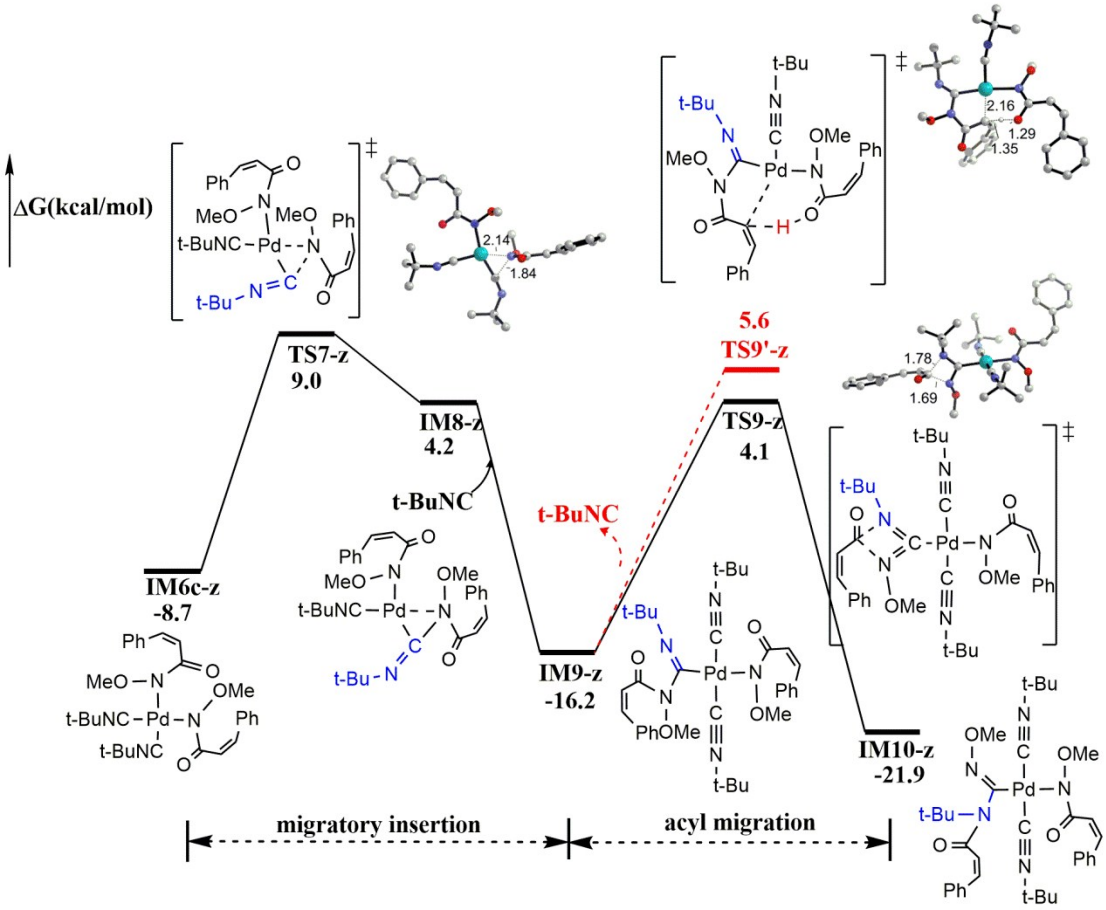

Figure S2. Energy profiles of the migratory insertion and acyl migration steps. Δ G refer to the Gibbs free energy. All energies are relative to $Pd(t\text{-}BuNC)_2 + O_2$, and are mass balanced.

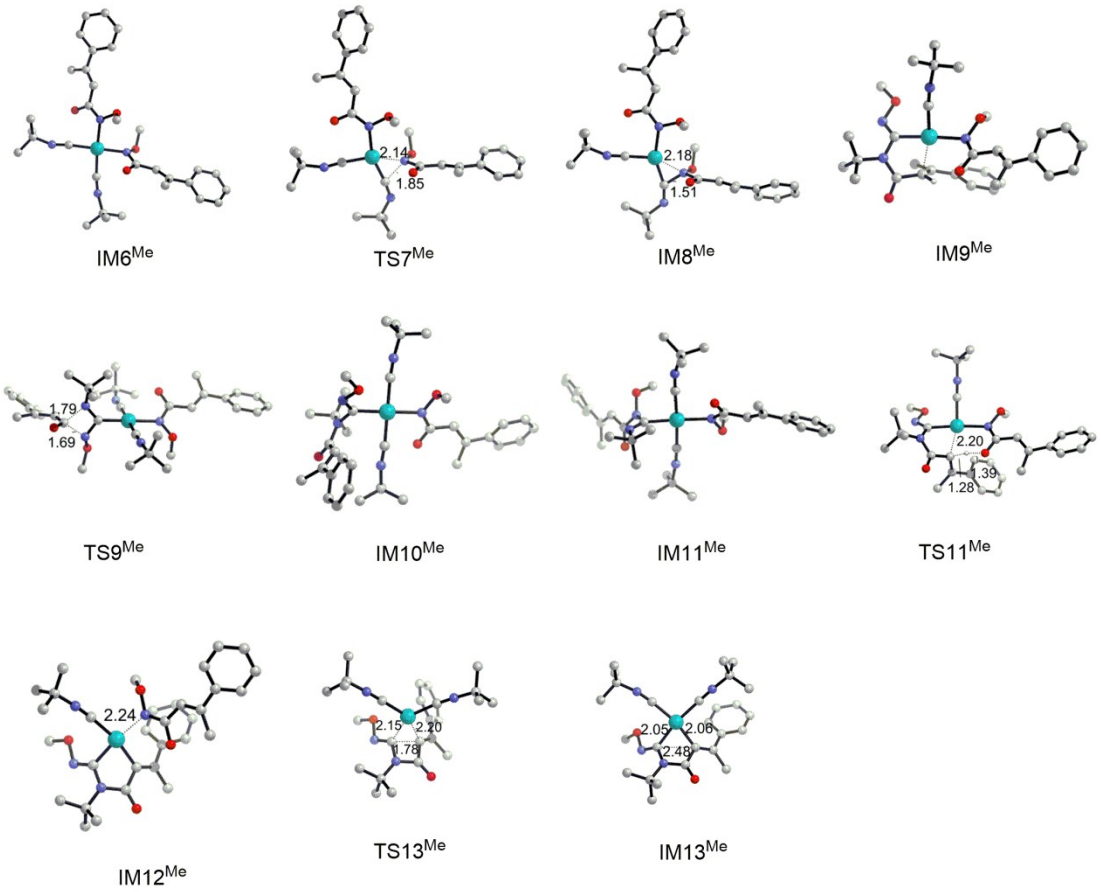

Figure S3. Optimized Structures of the stationary points of the reaction of Z-isomer.

Table 1. Atom coordinates and absolute energy of Pd(t-BuNC)$_2$ (Energy= -627.6975832 a.u.)

Atom	X	Y	Z
Pd	0.0000130	0.0007640	0.0033540
C	-5.0680960	0.3784390	1.4118020
C	-4.5878130	-0.0006710	-0.0022810
H	-4.7052640	-0.3424960	2.1495310
H	-4.7054380	1.3717970	1.6900360
H	-6.1619400	0.3858270	1.4398150
C	-5.0666820	1.0351010	-1.0375710
C	-5.0676930	-1.4149170	-0.3815410
H	-4.7041810	0.7784090	-2.0367700
H	-6.1605370	1.0571310	-1.0576010
H	-4.7023270	2.0340790	-0.7825200
H	-6.1616160	-1.4436150	-0.3875730
H	-4.7059850	-1.6928180	-1.3752940
H	-4.7034740	-2.1529050	0.3384560
C	-1.9716400	0.0010340	0.0024980
N	-3.1472970	-0.0005860	-0.0013210
C	5.0690360	-1.3939130	0.4465330
C	4.5878400	-0.0003310	-0.0020500
H	4.7106060	-1.6213700	1.4542720
H	4.7030770	-2.1679200	-0.2337690
H	6.1628950	-1.4222870	0.4507730
C	5.0614650	0.3058990	-1.4358470
C	5.0718130	1.0863630	0.9771930
H	4.7013770	1.2860100	-1.7606780
H	6.1551690	0.3064950	-1.4704190
H	4.6907160	-0.4486940	-2.1350180
H	6.1657800	1.1061820	0.9938090
H	4.7093150	2.0714650	0.6711020
H	4.7110710	0.8835670	1.9892350
C	1.9717100	-0.0000220	0.0035530
N	3.1473710	-0.0002560	0.0034020

Table 2. Atom coordinates and absolute energy of t-BuNC (Energy= -250.4382407a.u.)

Atom	X	Y	Z
C	0.7352650	1.4363050	-0.2802630

C	0.2565600	0.0001000	-0.0000120
H	0.3725780	1.7823130	-1.2518610
H	0.3712220	2.1227460	0.4888640
H	1.8288560	1.4673030	-0.2855050
C	0.7349340	-0.4748770	1.3840930
C	0.7368410	-0.9608740	-1.1029540
H	0.3711550	-1.4843520	1.5936000
H	1.8285600	-0.4854310	1.4143540
H	0.3715970	0.1933760	2.1693620
H	1.8304930	-0.9802880	-1.1255990
H	0.3744690	-1.9754910	-0.9170640
H	0.3739690	-0.6386060	-2.0826090
C	-2.3655280	-0.0004490	-0.0006880
N	-1.1873330	-0.0003990	-0.0006570

Table 3. Atom coordinates and absolute energy of O_2 (triplet)(Energy= -150.313267 a.u.)

Atom	X	Y	Z
O	0.0000000	0.0000000	0.6072620
O	0.0000000	0.0000000	-0.6072620

Table 4. Atom coordinates and absolute energy of IM1 (Energy=-778.0034879a.u.)

Atom	X	Y	Z
Pd	-0.0823630	0.4419630	-0.0706290
O	1.5011670	3.0879930	0.0684830
O	0.3053640	2.8572590	0.0654260
C	-2.0122090	0.0368700	0.0302830
C	1.8010180	-0.1445590	-0.0254030
C	-4.5280270	-0.6759220	0.0297230
C	4.2913090	-0.9442000	0.0253280
C	4.7159530	-1.0933530	1.4986570
H	5.7563920	-1.4281380	1.5496160
H	4.6305330	-0.1386810	2.0246380
H	4.0877280	-1.8277680	2.0099090
C	5.1519390	0.1164850	-0.6871630
H	6.2008360	-0.1949570	-0.6792210
H	4.8326610	0.2399170	-1.7255330
H	5.0711450	1.0831380	-0.1827690
C	4.3749070	-2.2969210	-0.7072370

H	5.4086500	-2.6554780	-0.7004690
H	3.7437890	-3.0426050	-0.2163400
H	4.0475210	-2.1952610	-1.7454270
C	-4.5915260	-2.1125340	0.5827930
H	-4.2291000	-2.1467990	1.6138230
H	-5.6259180	-2.4688830	0.5644100
H	-3.9779550	-2.7838580	-0.0235930
C	-5.3479420	0.2877410	0.9074520
H	-5.2791310	1.3110510	0.5284080
H	-6.3991110	-0.0157930	0.9031010
H	-4.9859580	0.2755480	1.9391440
C	-5.0105340	-0.6331240	-1.4328560
H	-4.4005570	-1.2915220	-2.0567850
H	-6.0522850	-0.9634590	-1.4868490
H	-4.9455660	0.3826070	-1.8323790
N	-3.1509680	-0.2507100	0.0555380
N	2.9200320	-0.5027560	-0.0034680

Table 5. Atom coordinates and absolute energy of TS1 (Energy=-777.9859192 a.u.)

Atom	X	Y	Z
Pd	0.0100220	1.3616280	0.0085670
O	-0.7844400	3.5450190	-0.0044690
O	0.4626650	3.7951950	-0.0266120
C	1.7395880	0.3533980	0.0173850
C	-1.6909800	0.2874790	0.0041510
C	3.6249950	-1.4592320	-0.0031250
C	-3.5774880	-1.5266280	-0.0027190
C	-4.1087540	-1.6817410	1.4342510
H	-4.8798210	-2.4575820	1.4599340
H	-3.3033840	-1.9679980	2.1154000
H	-4.5456400	-0.7442930	1.7883350
C	-2.9300080	-2.8363910	-0.4902740
H	-3.6768420	-3.6357290	-0.5044590
H	-2.5294710	-2.7159820	-1.4999180
H	-2.1134510	-3.1333790	0.1731880
C	-4.7036720	-1.0871370	-0.9562530
H	-5.4861580	-1.8514360	-0.9783280
H	-5.1463570	-0.1439160	-0.6245730
H	-4.3203160	-0.9516380	-1.9711240
C	3.8845780	-1.8994540	1.4507780
H	2.9668040	-2.2749040	1.9115220
H	4.6348640	-2.6960310	1.4667950

H	4.2537840	-1.0612960	2.0479350
C	3.0706700	-2.6299790	-0.8389210
H	2.8685100	-2.3091170	-1.8650550
H	3.7996750	-3.4460080	-0.8649360
H	2.1401020	-3.0067010	-0.4048300
C	4.9089920	-0.8933710	-0.6383300
H	5.2921350	-0.0526420	-0.0536080
H	5.6761270	-1.6724680	-0.6722810
H	4.7176110	-0.5470520	-1.6574190
N	2.6276990	-0.4185270	0.0153380
N	-2.5623460	-0.5029170	0.0027080

Table 6. Atom coordinates and absolute energy of $IM2_{trip}$ (Energy= -777.9906783a.u.)

Atom	X	Y	Z
Pd	0.0003640	1.1302090	0.0001320
O	-0.6156340	3.4146380	0.0000200
O	0.5943430	3.4220780	0.0000320
C	1.7698240	0.1857340	-0.0010030
C	-1.7699060	0.1862510	0.0022060
C	3.9231050	-1.3026420	-0.0006840
C	-3.9198380	-1.3067920	-0.0007170
C	-4.1992080	-1.7458570	1.4489250
H	-5.0938870	-2.3752430	1.4777010
H	-3.3574640	-2.3173000	1.8488460
H	-4.3638510	-0.8768190	2.0912930
C	-3.6481780	-2.5280590	-0.8989740
H	-4.5310990	-3.1741060	-0.9209410
H	-3.4211240	-2.2132320	-1.9209500
H	-2.8021120	-3.1066710	-0.5194440
C	-5.0900220	-0.4718090	-0.5528220
H	-6.0020770	-1.0760510	-0.5629650
H	-5.2625330	0.4098830	0.0694850
H	-4.8806010	-0.1392430	-1.5729370
C	4.2830480	-1.6194210	1.4638780
H	3.4695350	-2.1614980	1.9538680
H	5.1843810	-2.2388840	1.4963880
H	4.4725450	-0.6991740	2.0234580
C	3.6123610	-2.5954640	-0.7794110
H	3.3299800	-2.3673850	-1.8111970
H	4.4972710	-3.2389880	-0.7942720
H	2.7910090	-3.1427490	-0.3085480

C	5.0565280	-0.5127330	-0.6828580
H	5.2581560	0.4177270	-0.1448320
H	5.9705160	-1.1142600	-0.6943240
H	4.7893130	-0.2651860	-1.7141210
N	2.7385490	-0.4816640	-0.0013100
N	-2.7386410	-0.4811070	0.0021380

Table 7. Atom coordinates and absolute energy of IM2(Energy=-777.98989544a.u.)

Atom	X	Y	Z
Pd	-0.0000240	1.3808270	-0.0009260
C	-3.7667860	-2.1422470	1.3544950
C	-3.6877060	-1.4137680	0.0001590
H	-2.8951360	-2.7858120	1.5021170
H	-3.8132320	-1.4252050	2.1784270
H	-4.6665930	-2.7636230	1.3823320
C	-4.8941130	-0.4759530	-0.1919430
C	-3.5814930	-2.4197100	-1.1607820
H	-4.8200710	0.0619120	-1.1406990
H	-5.8168380	-1.0636300	-0.1944150
H	-4.9482640	0.2562290	0.6178520
H	-4.4782820	-3.0455500	-1.1843130
H	-3.4950630	-1.8994830	-2.1184680
H	-2.7091160	-3.0672270	-1.0364360
C	-1.5575850	0.1034420	-0.0010710
N	-2.4916470	-0.6026800	-0.0006040
C	3.7608570	-2.1558790	-1.3465360
C	3.6881200	-1.4132220	0.0004170
H	2.8881370	-2.8003200	-1.4836560
H	3.8043030	-1.4475910	-2.1781690
H	4.6600830	-2.7782060	-1.3716550
C	4.8957560	-0.4740190	0.1773050
C	3.5867610	-2.4069360	1.1723110
H	4.8265250	0.0733330	1.1209770
H	5.8182630	-1.0620250	0.1811410
H	4.9462070	0.2499970	-0.6400390
H	4.4835500	-3.0326740	1.1985460
H	3.5045600	-1.8766080	2.1248190
H	2.7137440	-3.0555590	1.0586320
C	1.5583010	0.1044150	-0.0022480
N	2.4923670	-0.6017040	-0.0017090
O	0.6856530	3.2841200	0.0013830

O	-0.6880760	3.2831230	0.0022600

Table 8. Atom coordinates and absolute energy of 1a (Energy= -592.4188991a.u.)

Atom	X	Y	Z
O	-2.2855060	1.3905980	-0.1400280
C	-2.0032180	0.2013660	-0.1355690
C	-0.6205700	-0.3373700	-0.0734000
C	0.4236050	0.5096790	-0.0555390
C	1.8496210	0.1855990	-0.0074310
C	2.3427520	-1.1328750	0.0371760
C	3.7102670	-1.3798940	0.0826500
C	4.6199130	-0.3174800	0.0846270
C	4.1490180	0.9948940	0.0408080
C	2.7785880	1.2418590	-0.0045690
H	0.1719590	1.5689360	-0.0819580
H	1.6512380	-1.9697610	0.0368410
H	4.0715150	-2.4035370	0.1168570
H	5.6872510	-0.5142630	0.1201930
H	4.8479420	1.8259870	0.0419690
H	2.4132990	2.2647160	-0.0385290
N	-2.9746740	-0.7962400	-0.0934050
O	-4.2649050	-0.4365880	-0.5052170
C	-5.0289170	0.0160060	0.6171640
H	-5.0894640	-0.7574950	1.3917250
H	-6.0244800	0.2187670	0.2157870
H	-4.6015770	0.9332550	1.0311000
H	-0.4883550	-1.4163570	-0.0439310
H	-2.7396680	-1.6993480	-0.4897650

Table 9. Atom coordinates and absolute energy of 1b (Energy= -592.4194334 a.u.)

Atom	X	Y	Z
O	-2.1726310	-2.2804440	0.0282440
C	-2.1281840	-1.0563770	-0.0265030
C	-0.8852180	-0.2561180	-0.0421170
C	0.3024540	-0.8865050	0.0134440
C	1.6371700	-0.2875290	0.0051590
C	1.8614760	1.0991970	-0.0980240
C	3.1536920	1.6122940	-0.1002000
C	4.2542010	0.7549120	0.0007650

C	4.0504390	-0.6213960	0.1028160
C	2.7554330	-1.1352180	0.1040580
H	0.2657310	-1.9732220	0.0735830
H	1.0182470	1.7777130	-0.1800810
H	3.3069880	2.6844170	-0.1817240
H	5.2619790	1.1594560	-0.0013160
H	4.8990000	-1.2945550	0.1807070
H	2.5981440	-2.2075590	0.1828940
N	-3.3296320	-0.3468480	0.0020480
O	-3.3472530	0.9544320	-0.5402420
C	-3.8256390	1.8750820	0.4433940
H	-4.8498060	1.6328600	0.7514050
H	-3.8124560	2.8521880	-0.0453960
H	-3.1773010	1.8880280	1.3265530
H	-0.9777870	0.8207030	-0.1140780
H	-4.1211720	-0.8940330	-0.3276540

Table 10. Atom coordinates and absolute energy of 1c (Energy= -592.409805 a.u.)

Atom	X	Y	Z
O	-2.0565800	2.2274030	-0.0013830
C	-2.1008520	0.8668890	-0.0005900
C	-0.8179210	0.1850990	-0.0003310
C	0.3598870	0.8415470	-0.0005360
C	1.6984410	0.2487510	-0.0003020
C	1.9304520	-1.1407830	-0.0018910
C	3.2258350	-1.6460820	-0.0014830
C	4.3236470	-0.7795570	0.0004790
C	4.1124480	0.5993980	0.0019750
C	2.8144940	1.1055110	0.0015450
H	0.3313960	1.9286220	-0.0007710
H	1.0914350	-1.8292720	-0.0035910
H	3.3830480	-2.7207860	-0.0027580
H	5.3336410	-1.1784770	0.0007720
H	4.9578570	1.2811590	0.0034510
H	2.6535960	2.1804170	0.0027020
N	-3.2774290	0.3348440	-0.0001400
O	-3.2240140	-1.0713840	0.0006360
C	-4.5537840	-1.5701760	0.0015980
H	-5.1006970	-1.2466800	0.8951160
H	-4.4581210	-2.6583630	0.0018500
H	-5.1017860	-1.2471760	-0.8914260
H	-0.8812060	-0.8959070	0.0001600

Table 11. Atom coordinates and absolute energy of IM3a (Energy= −1370. 413043 a.u.)

Atom	X	Y	Z
Pd	-1.4962590	0.2835650	-0.8886990
C	-6.7022580	-0.1983030	-1.1060990
C	-5.8739430	-0.9134460	-0.0227970
H	-6.5644290	0.8845140	-1.0488840
H	-6.4088460	-0.5334970	-2.1044020
H	-7.7625760	-0.4235660	-0.9601580
C	-6.0273720	-2.4416310	-0.1274830
C	-6.2529200	-0.4141620	1.3834390
H	-5.4163680	-2.9472290	0.6252910
H	-7.0741230	-2.7138560	0.0351210
H	-5.7264960	-2.7958440	-1.1170760
H	-7.3035810	-0.6460200	1.5796820
H	-5.6412500	-0.9005520	2.1481760
H	-6.1147980	0.6673780	1.4623850
C	-3.3725580	-0.2888640	-0.4632200
N	-4.4812110	-0.5898950	-0.2479310
C	0.2469420	-3.7654040	2.2284890
C	1.0952430	-2.6713050	1.5562380
H	-0.4882910	-3.3266950	2.9086930
H	-0.2807780	-4.3649550	1.4813870
H	0.9004600	-4.4267120	2.8043620
C	2.1009980	-3.2822050	0.5632630
C	1.8097390	-1.7967850	2.6029940
H	2.6850040	-2.5032920	0.0669140
H	2.7882680	-3.9381230	1.1052790
H	1.5851580	-3.8739980	-0.1981360
H	2.5132380	-2.4141330	3.1690410
H	2.3619330	-0.9868320	2.1202300
H	1.0907640	-1.3595840	3.3012720
C	-0.4586100	-1.0684840	0.1926250
N	0.2005500	-1.8122890	0.8064060
O	-0.2436450	1.5510780	-1.8835840
O	-1.5675550	1.8614110	-2.1303160
O	2.4583000	3.1344340	1.8685970
C	1.9300460	2.6348240	0.8768110
C	2.5767870	1.5856430	0.0332030
C	3.8053310	1.1397410	0.3467480
C	4.6047580	0.1428960	-0.3734270

C	4.1912580	-0.4496850	-1.5842080
C	4.9888000	-1.3948000	-2.2236360
C	6.2193110	-1.7714790	-1.6749680
C	6.6461870	-1.1906170	-0.4799850
C	5.8474580	-0.2446030	0.1609390
H	4.2587910	1.5739520	1.2371070
H	3.2473500	-0.1568120	-2.0339660
H	4.6541600	-1.8342470	-3.1592280
H	6.8403960	-2.5059900	-2.1795460
H	7.6028200	-1.4710820	-0.0481280
H	6.1847450	0.2091290	1.0894000
N	0.6656040	2.9331910	0.4510600
O	0.0338390	4.0594850	0.9689380
C	-0.5915270	3.7573060	2.2178660
H	-1.3444620	2.9668680	2.1015560
H	-1.0787880	4.6862600	2.5252840
H	0.1546250	3.4654610	2.9628120
H	2.0317940	1.2316720	-0.8377410
H	0.2890580	2.6136840	-0.4531410

Table12. Atom coordinates and absolute energy of IM3b (Energy= -1370.408941 a.u.)

Atom	X	Y	Z
Pd	2.2893790	-0.2346490	-1.1022300
C	6.4153440	0.0386210	2.2223720
C	5.3165410	-1.0376820	2.2897540
H	6.9185220	0.0199340	1.2519880
H	5.9939420	1.0355660	2.3771470
H	7.1580070	-0.1499600	3.0028960
C	4.5741380	-0.9866610	3.6377200
C	5.8989760	-2.4396290	2.0324040
H	3.7751190	-1.7320930	3.6698660
H	5.2779250	-1.1959210	4.4483770
H	4.1359940	0.0011790	3.8038500
H	6.6299670	-2.6781580	2.8103930
H	5.1109420	-3.1970730	2.0507450
H	6.3979900	-2.4809580	1.0606490
C	3.5881090	-0.5605820	0.3854860
N	4.3569830	-0.7578690	1.2439640
C	-0.5699410	3.9646420	-1.4407790
C	0.2950040	3.7910350	-0.1782680
H	0.0560500	4.1663050	-2.3149690

H	-1.1546230	3.0588810	-1.6157290
H	-1.2470830	4.8123070	-1.2967300
C	-0.5833740	3.4644210	1.0437990
C	1.1842330	5.0197790	0.0743640
H	0.0322990	3.3085930	1.9350390
H	-1.2583470	4.3047250	1.2336630
H	-1.1713710	2.5653970	0.8451460
H	0.5505350	5.8948270	0.2444000
H	1.8150380	4.8737670	0.9561760
H	1.8279200	5.2216370	-0.7865330
C	1.6800480	1.6311090	-0.6392870
N	1.1587980	2.6478350	-0.4044970
O	1.2735260	-0.8265550	-2.7507580
O	2.0321010	-1.8777590	-2.2598170
O	-1.6643160	0.8489970	-0.7691340
C	-2.0276840	-0.3321540	-0.8946580
C	-3.3316470	-0.8389050	-0.3943670
C	-4.1893390	0.0047210	0.2048900
C	-5.5109680	-0.3040120	0.7569360
C	-6.0887680	-1.5879240	0.7072620
C	-7.3476210	-1.8244880	1.2499150
C	-8.0633870	-0.7867720	1.8564060
C	-7.5070800	0.4916180	1.9136510
C	-6.2459080	0.7277430	1.3690760
H	-3.8656160	1.0410450	0.2893390
H	-5.5483640	-2.4038600	0.2375870
H	-7.7758540	-2.8217100	1.1999160
H	-9.0463760	-0.9755440	2.2782500
H	-8.0549990	1.3049160	2.3811130
H	-5.8152560	1.7248590	1.4138740
N	-1.2084910	-1.2380000	-1.4895070
O	-1.6759590	-2.5177300	-1.8077870
C	-0.8379290	-3.4964950	-1.1772190
H	0.2103430	-3.3381200	-1.4540200
H	-1.1892940	-4.4609790	-1.5524450
H	-0.9446350	-3.4584960	-0.0851180
H	-3.5491370	-1.8890680	-0.5471320
H	-0.3473940	-0.9678230	-2.0016500

Table 13. Atom coordinates and absolute energy of IM3c (Energy= -1370.403333 a.u.)

Atom	X	Y	Z
Pd	-1.9706360	-0.7199560	-1.0698080

O	-0.6186000	-1.9042620	-2.0480170
O	-1.6449620	-2.6544420	-1.5024110
C	-3.7046540	-0.5414790	-0.0934650
C	-1.3382150	1.1948550	-1.0242040
C	-6.0086960	-0.4362270	1.1391170
C	0.0171330	3.4007660	-0.7011920
C	1.3570940	3.1568720	-1.4203760
H	2.0089760	4.0231860	-1.2740690
H	1.8550300	2.2716300	-1.0173610
H	1.2031040	3.0142470	-2.4934480
C	0.2276060	3.5406780	0.8181330
H	0.8885630	4.3904950	1.0138060
H	-0.7252590	3.7213340	1.3247050
H	0.6781270	2.6320960	1.2273700
C	-0.7117870	4.6236090	-1.2835270
H	-0.1026010	5.5182270	-1.1262020
H	-0.8806270	4.5037340	-2.3573000
H	-1.6780440	4.7727140	-0.7932930
C	-5.8779870	-1.2660900	2.4296010
H	-5.1116890	-0.8459580	3.0865700
H	-6.8332950	-1.2627220	2.9622910
H	-5.6100340	-2.3006380	2.1999960
C	-6.3427110	1.0323080	1.4582370
H	-6.4073070	1.6248460	0.5416100
H	-7.3062930	1.0830660	1.9733350
H	-5.5796160	1.4729720	2.1056850
C	-7.0578130	-1.0485990	0.1927610
H	-6.8000130	-2.0813320	-0.0559740
H	-8.0365260	-1.0408530	0.6811580
H	-7.1268610	-0.4743640	-0.7350180
N	-4.7311280	-0.4671430	0.4619440
N	-0.8115920	2.2325090	-0.9186790
N	0.7189540	-0.6292400	0.8539150
O	1.0195620	0.2463270	1.9428900
C	0.0134280	0.0718180	2.9260920
H	-0.9845930	0.2486300	2.5058260
H	0.0418460	-0.9379780	3.3550570
H	0.2243660	0.8077210	3.7075180
C	1.7996860	-1.0017090	0.2331040
O	1.6878670	-1.7541520	-0.8597830
H	0.7302910	-1.8566180	-1.1757130
C	3.1680370	-0.6665900	0.6374790
C	4.2387940	-1.0015370	-0.1086450
H	3.2577310	-0.1362260	1.5769890

H	4.0505980	-1.5246370	-1.0434380
C	5.6466500	-0.7363470	0.2004080
C	6.6273440	-1.1252350	-0.7309770
C	7.9815520	-0.8973770	-0.4923330
C	8.3877020	-0.2743530	0.6884120
C	7.4268610	0.1171100	1.6267600
C	6.0754350	-0.1101990	1.3877380
H	6.3146280	-1.6122570	-1.6510690
H	8.7188730	-1.2075430	-1.2274210
H	9.4420610	-0.0961700	0.8792830
H	7.7356410	0.5998090	2.5499320
H	5.3448440	0.1962900	2.1299280

Table 14. Atom coordinates and absolute energy of TS3a (Energy= -1370.389514 a.u.)

Atom	X	Y	Z
Pd	1.3110860	-0.6544830	0.2447790
C	6.5200220	-0.0939330	-0.3327740
C	5.5259980	-0.0752630	-1.5083030
H	6.3387350	0.7451230	0.3442450
H	6.4338600	-1.0245690	0.2339260
H	7.5396930	-0.0143870	-0.7201870
C	5.7502250	-1.2775740	-2.4436270
C	5.6062230	1.2529830	-2.2819850
H	5.0228970	-1.2772270	-3.2598190
H	6.7548390	-1.2194430	-2.8721950
H	5.6581050	-2.2187210	-1.8955380
H	6.6071940	1.3634920	-2.7083210
H	4.8776980	1.2743600	-3.0970190
H	5.4157140	2.1020930	-1.6199250
C	3.1227680	-0.3243690	-0.5070540
N	4.1905580	-0.1890320	-0.9587380
C	-0.2554070	4.4608510	-0.8373730
C	-1.0556620	3.2790120	-0.2632380
H	0.6412480	4.6520400	-0.2412130
H	0.0447700	4.2677310	-1.8713040
H	-0.8786290	5.3592690	-0.8203430
C	-2.2870460	2.9677370	-1.1328370
C	-1.4547840	3.5280320	1.2041330
H	-2.8258870	2.1009380	-0.7440800
H	-2.9577870	3.8316630	-1.1264520
H	-1.9940820	2.7637210	-2.1666660
H	-2.1541410	4.3685500	1.2449560

H	-1.9249160	2.6434460	1.6433270
H	-0.5757030	3.7826900	1.8032910
C	0.3929980	1.1060870	-0.1898270
N	-0.1991630	2.1066790	-0.2843950
O	0.3952230	-2.8153950	0.7016500
O	1.7390660	-2.4806890	0.8362700
O	-2.0541230	0.4725680	2.7983500
C	-1.5856460	-0.3850840	2.0397780
C	-2.3087260	-0.8471490	0.8150420
C	-3.5516140	-0.4030640	0.5566340
C	-4.4201910	-0.7662550	-0.5677470
C	-4.0371760	-1.6664280	-1.5820480
C	-4.9010860	-1.9699420	-2.6295260
C	-6.1698980	-1.3842710	-2.6941790
C	-6.5665810	-0.4918500	-1.6975240
C	-5.7006880	-0.1880260	-0.6480700
H	-3.9645970	0.3039770	1.2754420
H	-3.0578940	-2.1339050	-1.5465110
H	-4.5861270	-2.6687210	-3.3995480
H	-6.8417810	-1.6250150	-3.5130220
H	-7.5510680	-0.0338570	-1.7352570
H	-6.0148650	0.5040380	0.1293300
N	-0.3682700	-1.0101050	2.1918070
O	0.2094890	-0.8479850	3.4690780
C	0.8460130	0.4137480	3.6221640
H	1.6224680	0.5537910	2.8539170
H	1.3177360	0.3827310	4.6084950
H	0.1227520	1.2337020	3.5823670
H	-1.8132030	-1.5776370	0.1815820
H	-0.0645450	-2.1259200	1.5633550

Table 15. Atom coordinates and absolute energy of TS3b (Energy= -1370.383509 a.u.)

Atom	X	Y	Z
Pd	1.8008510	-0.4494430	-0.7612530
C	6.6079280	1.1844930	0.6833280
C	5.9297750	-0.0952290	1.2050390
H	6.7018180	1.1591710	-0.4055050
H	6.0348820	2.0722200	0.9644970
H	7.6086940	1.2658220	1.1167980
C	5.7525890	-0.0466450	2.7333970
C	6.7090370	-1.3516410	0.7755850
H	5.2410120	-0.9427350	3.0944570

H	6.7353880	0.0082750	3.2099870
H	5.1725790	0.8309380	3.0314980
H	7.7121450	-1.3202040	1.2103170
H	6.2071570	-2.2587130	1.1222550
H	6.8015770	-1.3995690	-0.3124760
C	3.5586530	-0.2584410	0.1127260
N	4.6111840	-0.1712500	0.6091240
C	-1.0156630	3.6838960	-1.4492700
C	-0.3973320	3.5038010	-0.0504220
H	-0.2516280	3.9696840	-2.1782870
H	-1.4820970	2.7487240	-1.7665130
H	-1.7684640	4.4772530	-1.4075770
C	-1.4697270	3.0740400	0.9671060
C	0.3527170	4.7629250	0.4104250
H	-1.0299720	2.9131200	1.9559020
H	-2.2250340	3.8614800	1.0484700
H	-1.9453660	2.1503250	0.6307250
H	-0.3517530	5.5958320	0.4871420
H	0.8131880	4.6102210	1.3910190
H	1.1339070	5.0376950	-0.3042470
C	1.0573410	1.3776900	-0.3468970
N	0.5561180	2.4110540	-0.1472980
O	1.0841240	-1.8908780	-2.4302870
O	2.0985390	-2.2413010	-1.5301990
O	-1.4246940	0.3617790	-1.2909670
C	-1.6209820	-0.7136110	-0.6756950
C	-2.9465690	-1.0158760	-0.0625220
C	-3.9943140	-0.1994090	-0.2717490
C	-5.3569650	-0.3425630	0.2511150
C	-5.7580900	-1.4057870	1.0841670
C	-7.0640490	-1.4899680	1.5563760
C	-8.0067730	-0.5160210	1.2106630
C	-7.6281140	0.5435430	0.3853480
C	-6.3192540	0.6266830	-0.0871980
H	-3.8152960	0.6661090	-0.9081300
H	-5.0396950	-2.1712400	1.3602790
H	-7.3513600	-2.3194810	2.1967650
H	-9.0257240	-0.5856200	1.5806820
H	-8.3520750	1.3048690	0.1080740
H	-6.0285620	1.4523810	-0.7319910
N	-0.6112630	-1.6159210	-0.5702960
O	-0.9928590	-2.8263790	0.1076350
C	-0.0656730	-3.0960900	1.1427540
H	0.9552000	-3.1691310	0.7475150

H	-0.3621910	-4.0597290	1.5693550
H	-0.0941430	-2.3256960	1.9283780
H	-3.0195440	-1.9200740	0.5288360
H	0.2258360	-1.9252350	-1.7864060

Table 16. Atom coordinates and absolute energy of TS3c (Energy= -1370.398606 a.u.)

Atom	X	Y	Z
Pd	-1.5775030	-0.4959680	-0.5689490
O	-0.5287220	-1.9426120	-2.0319200
O	-1.2883210	-2.4074790	-0.9717720
C	-3.4337230	-0.7769530	0.1015360
C	-1.4713070	1.5246260	-0.5850680
C	-5.8945680	-1.3750570	0.7523370
C	-0.7651710	4.0276710	-0.4054680
C	0.2035320	4.2826180	-1.5752050
H	0.5942530	5.3021220	-1.5071110
H	1.0423340	3.5829310	-1.5405540
H	-0.3066640	4.1688520	-2.5355360
C	-0.0330390	4.1196350	0.9468250
H	0.4234470	5.1087580	1.0481300
H	-0.7331030	3.9742140	1.7746630
H	0.7423880	3.3523590	1.0120580
C	-1.9655080	4.9874210	-0.4616280
H	-1.6130280	6.0172600	-0.3550460
H	-2.4931100	4.8986250	-1.4154030
H	-2.6703020	4.7773610	0.3477480
C	-5.8592080	-2.1856290	2.0609590
H	-5.4326740	-1.5934010	2.8751360
H	-6.8772920	-2.4749060	2.3374080
H	-5.2600270	-3.0916860	1.9387030
C	-6.7020100	-0.0762550	0.9289430
H	-6.7010950	0.5106740	0.0063980
H	-7.7370050	-0.3226360	1.1825720
H	-6.2840560	0.5361270	1.7327620
C	-6.4555830	-2.2219050	-0.4052360
H	-5.8577100	-3.1255710	-0.5484310
H	-7.4845600	-2.5148740	-0.1767260
H	-6.4535920	-1.6532520	-1.3389050
N	-4.5356890	-1.0132960	0.4154710
N	-1.2572660	2.6721480	-0.5338520
N	0.7381110	-0.3359030	0.2760270
O	1.0193970	0.6558480	1.2702060

C	0.3584240	0.2900920	2.4712110
H	-0.7180790	0.1547310	2.3012350
H	0.7687720	-0.6383220	2.8900890
H	0.5227090	1.1139910	3.1725810
C	1.8311880	-0.8632980	-0.2400700
O	1.7325490	-1.7108310	-1.2184030
H	0.6401030	-1.8576410	-1.5897080
C	3.1862090	-0.5412620	0.2470270
C	4.2761330	-1.0898640	-0.3205280
H	3.2458780	0.1512770	1.0766370
H	4.1067570	-1.7693550	-1.1531420
C	5.6758820	-0.8735260	0.0572690
C	6.6817730	-1.5354660	-0.6708030
C	8.0298490	-1.3674000	-0.3587280
C	8.4043990	-0.5303190	0.6929900
C	7.4180110	0.1353550	1.4284470
C	6.0728450	-0.0331540	1.1162340
H	6.3933920	-2.1884140	-1.4905420
H	8.7870090	-1.8900850	-0.9364790
H	9.4537090	-0.3965740	0.9399900
H	7.7017210	0.7879300	2.2496610
H	5.3208610	0.4900130	1.6987870

Table 17. Atom coordinates and absolute energy of H_2O_2 (Energy= -151.5245893 a.u.)

Atom	X	Y	Z
O	-0.7183520	-0.1176190	-0.0544080
O	0.7183520	0.1176150	-0.0544110
H	1.0139480	-0.6666120	0.4352850
H	-1.0139420	0.6666410	0.4352680

Table 18. Atom coordinates and absolute energy of IM4a (Energy= -1370.414084 a.u.)

Atom	X	Y	Z
Pd	1.1982420	-0.3917710	-0.7649310
C	4.6531710	3.2211980	0.4751080
C	4.7631680	1.8250960	1.1152500
H	4.6589920	3.1485420	-0.6152200
H	3.7303670	3.7188910	0.7844060
H	5.5029430	3.8321860	0.7930000
C	4.6878080	1.9072510	2.6499550

C	6.0447800	1.1044310	0.6589300
H	4.7342340	0.9108420	3.0980960
H	5.5319290	2.4942120	3.0225730
H	3.7611400	2.3919950	2.9690770
H	6.9169280	1.6755210	0.9896380
H	6.1031980	0.1008970	1.0892120
H	6.0751760	1.0202460	-0.4303760
C	2.7288880	0.4723690	0.1920140
N	3.6329620	1.0454200	0.6530710
C	-0.8222690	-2.4466100	3.8454170
C	-1.0982800	-2.8293910	2.3816500
H	0.2066720	-2.6876860	4.1276750
H	-0.9891610	-1.3782240	4.0066970
H	-1.4995280	-3.0046900	4.4978740
C	-2.5335570	-2.4612090	1.9608300
C	-0.8128150	-4.3217790	2.1342310
H	-2.6887530	-2.6503520	0.8951070
H	-3.2408440	-3.0610600	2.5412810
H	-2.7322860	-1.4035930	2.1530590
H	-1.4775170	-4.9236040	2.7603610
H	-0.9925470	-4.5813330	1.0880610
H	0.2216990	-4.5711970	2.3866070
C	0.4072190	-1.4652280	0.7409120
N	-0.1968260	-2.0649310	1.5386980
O	0.7183840	1.3159490	-2.9180400
O	1.8595320	0.6650380	-2.3378090
O	-2.4717900	-2.0160970	-1.6758760
C	-1.6410060	-1.1019750	-1.6130750
C	-1.9799620	0.2600460	-1.1019780
C	-3.1911040	0.5084470	-0.5726350
C	-3.6964570	1.7851140	-0.0596490
C	-2.9538970	2.9822190	-0.1024930
C	-3.4815390	4.1663910	0.4025100
C	-4.7627210	4.1894490	0.9638680
C	-5.5131210	3.0139090	1.0120420
C	-4.9848390	1.8278020	0.5046950
H	-3.8804360	-0.3340200	-0.5294020
H	-1.9610890	2.9851360	-0.5419530
H	-2.8935920	5.0789060	0.3553000
H	-5.1714230	5.1167020	1.3552260
H	-6.5112380	3.0207070	1.4412380
H	-5.5743930	0.9149510	0.5388030
N	-0.3264470	-1.1692480	-2.0368890
O	0.0118850	-2.3577190	-2.7130930

C	0.0462590	-3.5323300	-1.9056560
H	0.8166010	-3.4503470	-1.1253030
H	0.3238150	-4.3376950	-2.5910940
H	-0.9310910	-3.7405330	-1.4632940
H	-1.2285840	1.0345880	-1.2304830
H	0.1994100	0.5342120	-3.1965150

Table 19. Atom coordinates and absolute energy of IM4b (Energy= -1370.416442a.u.)

Atom	X	Y	Z
Pd	-1.4227840	-0.5440070	-0.1238490
C	-6.3502000	-0.3003250	1.6811900
C	-5.9868820	-0.6080790	0.2169650
H	-5.8181190	-0.9705300	2.3612380
H	-6.0967070	0.7319340	1.9379050
H	-7.4255970	-0.4395500	1.8238910
C	-6.6974980	0.3593680	-0.7458420
C	-6.2963630	-2.0746940	-0.1351540
H	-6.4120100	0.1574380	-1.7817330
H	-7.7797640	0.2324160	-0.6533560
H	-6.4490060	1.3980710	-0.5108720
H	-7.3679990	-2.2575310	-0.0130380
H	-6.0195130	-2.2918790	-1.1699770
H	-5.7442610	-2.7540280	0.5188380
C	-3.3974790	-0.3871450	-0.0235360
N	-4.5590340	-0.4198400	0.0690870
C	0.4304410	4.0183760	1.2029030
C	-0.4444360	3.9264860	-0.0611110
H	-0.1792540	3.9155760	2.1056230
H	1.1817590	3.2261900	1.1880200
H	0.9256140	4.9940590	1.2296180
C	0.4181730	4.0420450	-1.3316010
C	-1.5718250	4.9695100	-0.0457230
H	-0.2005760	3.9574410	-2.2300890
H	0.9145030	5.0174330	-1.3444140
H	1.1684040	3.2487890	-1.3393400
H	-1.1404140	5.9746330	-0.0384710
H	-2.2063330	4.8736230	-0.9317460
H	-2.1972040	4.8568660	0.8447950
C	-1.0631420	1.4291350	-0.0884360
N	-1.0424890	2.5996990	-0.0699770
O	-1.3778860	-3.0404450	1.0853610

O	-1.8429910	-2.5173370	-0.1744990
O	1.4668960	1.1131650	-0.1015800
C	1.6594000	-0.1208000	-0.1092820
C	3.0408690	-0.6732530	-0.0005190
C	4.0954660	0.1599810	0.0305050
C	5.5128900	-0.1990100	0.1354170
C	5.9713830	-1.5285190	0.2206470
C	7.3303220	-1.8102670	0.3166470
C	8.2693100	-0.7734440	0.3304690
C	7.8336390	0.5495290	0.2472930
C	6.4717200	0.8305920	0.1510200
H	3.8742420	1.2241930	-0.0283510
H	5.2569850	-2.3458200	0.2117760
H	7.6617310	-2.8429790	0.3814470
H	9.3295140	-0.9975190	0.4056170
H	8.5538080	1.3629250	0.2573890
H	6.1355990	1.8624030	0.0863620
N	0.6187720	-0.9870740	-0.2292910
O	0.9864040	-2.3608890	-0.1598670
C	0.9371140	-2.9516290	-1.4648040
H	-0.0674880	-2.8552150	-1.8824790
H	1.1788760	-4.0082480	-1.3183310
H	1.6803320	-2.4876850	-2.1242780
H	3.1489600	-1.7484490	0.0598930
H	-0.4155290	-3.0628310	0.9048040

Table 20. Atom coordinates and absolute energy of IM4c (Energy=-1370.416784 a.u.)

Atom	X	Y	Z
Pd	-1.4799350	-0.0302540	0.3400970
O	-1.4143730	-2.6194180	-0.5531000
O	-1.5692030	-2.0033330	0.7353090
C	-3.4269610	-0.3835680	0.0695080
C	-1.3032920	1.9206240	-0.1116540
C	-5.4121160	-1.9876190	-0.3083820
C	-0.6393880	4.3872600	-0.6398780
C	0.0964510	4.3696820	-1.9924250
H	0.4498660	5.3783840	-2.2247940
H	0.9570200	3.6968680	-1.9569950
H	-0.5704350	4.0418280	-2.7944290
C	0.3115470	4.7863170	0.5039140
H	0.7205160	5.7815310	0.3067940

H	-0.2209300	4.8116880	1.4586950
H	1.1335710	4.0709010	0.5855820
C	-1.8725080	5.3050880	-0.6913500
H	-1.5521130	6.3325650	-0.8854090
H	-2.5545170	4.9984600	-1.4891770
H	-2.4138150	5.2842820	0.2584370
C	-5.2850440	-2.8981200	0.9273560
H	-5.5935780	-2.3687570	1.8336010
H	-5.9281250	-3.7741000	0.8003800
H	-4.2481120	-3.2220790	1.0463330
C	-6.8193200	-1.3883690	-0.4355450
H	-6.8843910	-0.7184060	-1.2977160
H	-7.5455300	-2.1948150	-0.5703630
H	-7.0901920	-0.8278080	0.4638080
C	-4.9918630	-2.7366240	-1.5873000
H	-3.9596010	-3.0851660	-1.4988640
H	-5.6539430	-3.5952150	-1.7347410
H	-5.0698940	-2.0848240	-2.4623910
N	-4.4517070	-0.9080550	-0.1245660
N	-1.0893100	3.0376500	-0.3695880
N	0.5771100	-0.0540270	0.7092710
O	1.1355730	1.0487300	1.4135130
C	0.9322310	0.8653300	2.8106840
H	-0.1363990	0.7646390	3.0417230
H	1.4602390	-0.0234990	3.1774130
H	1.3310980	1.7621200	3.2946110
C	1.4657650	-0.8128180	0.0264350
O	1.0841250	-1.7227650	-0.7465110
H	-0.4481090	-2.4330350	-0.7058050
C	2.9220180	-0.5587730	0.2188090
C	3.8234850	-1.3335200	-0.4092410
H	3.2081960	0.2588690	0.8682490
H	3.4225040	-2.1216730	-1.0441810
C	5.2847370	-1.2374650	-0.3394680
C	6.0579740	-2.1343100	-1.0995320
C	7.4510150	-2.0896750	-1.0745100
C	8.1057660	-1.1437670	-0.2847940
C	7.3535380	-0.2447600	0.4786570
C	5.9632940	-0.2900610	0.4524400
H	5.5510500	-2.8727440	-1.7153270
H	8.0245760	-2.7938740	-1.6707690
H	9.1911300	-1.1058650	-0.2613990
H	7.8559710	0.4936340	1.0976680
H	5.3953430	0.4139940	1.0527760

Table 21. Atom coordinates and absolute energy of IM5a (Energy=−1962. 837872a.u.)

Atom	X	Y	Z
Pd	-0.1423540	-1.5663440	-0.6676710
C	2.3112190	-3.0108330	3.7353730
C	3.0264920	-2.1764410	2.6571750
H	1.4332280	-2.4851400	4.1220160
H	1.9962990	-3.9797600	3.3374410
H	3.0015980	-3.1862810	4.5649440
C	4.2480160	-2.9174270	2.0867470
C	3.4234930	-0.7890260	3.1931450
H	4.7119710	-2.3341500	1.2890200
H	4.9724330	-3.0663880	2.8930620
H	3.9599650	-3.8964750	1.6928320
H	4.0976960	-0.9257940	4.0438990
H	3.9453410	-0.2141530	2.4243920
H	2.5438930	-0.2357840	3.5355600
C	1.2974550	-1.8326100	0.7195140
N	2.0748500	-1.9805900	1.5723550
C	-3.7322500	-2.6089840	3.2471730
C	-3.8790490	-2.7340740	1.7213500
H	-2.9963740	-3.3210720	3.6314090
H	-3.4237780	-1.5983030	3.5274730
H	-4.6959700	-2.8196000	3.7188250
C	-4.8881550	-1.7123430	1.1646820
C	-4.2572610	-4.1694730	1.3137160
H	-4.9114780	-1.7397350	0.0719040
H	-5.8838090	-1.9479060	1.5518390
H	-4.6229210	-0.6987480	1.4758160
H	-5.2248160	-4.4231820	1.7555010
H	-4.3388290	-4.2553570	0.2272450
H	-3.5140060	-4.8883700	1.6697530
C	-1.6388020	-2.1434500	0.5141600
N	-2.5908290	-2.4337950	1.1200890
O	0.7785110	0.2630130	-2.6032900
O	1.2355810	-0.9821650	-2.0270950
O	-3.8697710	-0.9453370	-2.3075610
C	-2.7498870	-0.5910460	-1.9277550
C	-2.5235280	0.6597690	-1.1457480
C	-3.5719650	1.3896730	-0.7237950
C	-3.5542110	2.6455850	0.0300680

C	-2.3684140	3.3160100	0.3900590
C	-2.4128230	4.5065330	1.1090700
C	-3.6412280	5.0575900	1.4893430
C	-4.8260570	4.4082770	1.1396040
C	-4.7807890	3.2172360	0.4169190
H	-4.5561650	1.0001430	-0.9817540
H	-1.4045330	2.9103410	0.0990420
H	-1.4847040	5.0087630	1.3656640
H	-3.6722890	5.9873870	2.0501770
H	-5.7852560	4.8304680	1.4259460
H	-5.7054540	2.7169650	0.1399070
N	-1.5604490	-1.2481580	-2.2084140
O	-1.6889320	-2.3305770	-3.0966290
C	-2.3647280	-3.4712120	-2.5682090
H	-1.8158510	-3.8867900	-1.7106250
H	-2.3582030	-4.2032330	-3.3797050
H	-3.3939640	-3.2321570	-2.2902330
H	-1.4937600	0.9627000	-0.9764200
H	-0.0865320	-0.0323840	-2.9580690
O	5.0785920	0.1686950	0.3903220
C	4.1840900	0.2359520	-0.4585140
C	3.2852920	1.4042150	-0.6441950
C	3.4624050	2.5200660	0.0843070
C	2.6681410	3.7495900	0.0169410
C	1.5431880	3.8903140	-0.8212600
C	0.8306640	5.0854950	-0.8560870
C	1.2187120	6.1667570	-0.0560140
C	2.3274100	6.0409690	0.7821430
C	3.0420770	4.8444130	0.8168700
H	4.2890300	2.5163330	0.7937220
H	1.2275800	3.0602470	-1.4466020
H	-0.0323730	5.1769510	-1.5091290
H	0.6617150	7.0987200	-0.0914650
H	2.6377660	6.8743050	1.4062240
H	3.9080160	4.7499380	1.4672850
N	3.9383950	-0.7496750	-1.3819080
O	4.5501060	-1.9902620	-1.1625380
C	5.8162710	-2.0330700	-1.8255890
H	5.7008420	-1.8624560	-2.9020100
H	6.2005580	-3.0411810	-1.6496950
H	6.5024640	-1.2948660	-1.3989300
H	2.5005530	1.3152210	-1.3894270
H	2.9772910	-0.8595300	-1.7516630

Table 22. Atom coordinates and absolute energy of IM5b (Energy=-1962.83439a.u.)

Atom	X	Y	Z
Pd	-0.8797530	1.0213880	0.5749350
O	0.4442110	-0.4382380	1.0316090
C	0.6918280	2.2364370	0.3887650
C	-2.1961250	2.3930570	-0.0179750
C	2.7599450	3.8271250	0.2092800
C	-4.0949090	3.8292730	-1.0217530
C	-4.0147470	3.4682230	-2.5165510
H	-4.8816670	3.8883090	-3.0356420
H	-3.1078450	3.8803510	-2.9687010
H	-4.0102910	2.3826420	-2.6354540
C	-4.0241920	5.3469110	-0.7968930
H	-4.8829010	5.8257750	-1.2758080
H	-4.0463220	5.5874070	0.2699590
H	-3.1109930	5.7658750	-1.2294310
C	-5.3532950	3.2158750	-0.3807120
H	-6.2430520	3.6329660	-0.8619790
H	-5.3416540	2.1318560	-0.5144450
H	-5.3981020	3.4457860	0.6878940
C	3.6664260	3.5208580	1.4148470
H	3.9900750	2.4787800	1.3785480
H	4.5448320	4.1719110	1.3705140
H	3.1403490	3.7128090	2.3547910
C	3.4765680	3.5147180	-1.1168000
H	2.8146780	3.6974680	-1.9687890
H	4.3464620	4.1721970	-1.2085480
H	3.8113720	2.4756850	-1.1247130
C	2.2418370	5.2760490	0.2433300
H	1.7062950	5.4807840	1.1748330
H	3.0920350	5.9605440	0.1759790
H	1.5719540	5.4742850	-0.5984960
N	1.6025250	2.9537360	0.3010140
N	-2.9466010	3.2114760	-0.3767140
O	0.2113630	-0.8920490	2.3842240
H	-0.6204980	-1.3884240	2.2455820
C	4.1989460	-0.6500280	0.2568750
O	2.9967560	-2.6545360	0.7452390
C	2.8240800	-3.1455820	2.0806910
H	1.9465170	-2.6852790	2.5454970
H	2.6756690	-4.2232430	1.9735930
H	3.7148460	-2.9498110	2.6910670

N	3.0999410	-1.2593840	0.7726700
H	2.1851840	-0.7785850	0.8324730
O	4.2073050	0.5816480	0.0977170
N	-2.4808740	-0.2971450	0.8183560
C	-3.4588340	-0.4770810	-0.1088430
O	-3.5764480	0.3246530	-1.0583790
O	-2.4228040	-1.2802860	1.8448500
C	-2.9672660	-0.7456380	3.0563590
H	-4.0319170	-0.5170790	2.9330130
H	-2.8390880	-1.5248690	3.8130670
H	-2.4262580	0.1578970	3.3578400
C	-4.3899920	-1.6309570	0.0482370
C	-5.4002100	-1.7958210	-0.8236020
H	-4.2062890	-2.3202080	0.8629960
H	-5.4806060	-1.0518580	-1.6145060
C	6.4997370	-0.9551400	-0.5127160
C	5.3650990	-1.5137520	-0.0567450
H	6.4917300	0.1284720	-0.6214440
H	5.2501950	-2.5808690	0.0893030
C	-6.4360340	-3.9108750	0.1032990
C	-7.4152720	-4.8970290	0.0407450
C	-8.3889700	-4.8651180	-0.9632140
C	-8.3721090	-3.8360440	-1.9053980
C	-7.3904150	-2.8485870	-1.8418050
C	-6.4039950	-2.8636860	-0.8386350
H	-5.6862680	-3.9522490	0.8872560
H	-7.4208460	-5.6965260	0.7764050
H	-9.1515120	-5.6372990	-1.0089580
H	-9.1223280	-3.8024980	-2.6904280
H	-7.3789240	-2.0492920	-2.5784610
C	10.0531570	-1.4403370	-1.6520770
C	10.1969170	-2.8273310	-1.5999580
C	9.1186090	-3.6183650	-1.1894350
C	7.9096160	-3.0297750	-0.8331900
C	7.7469420	-1.6311300	-0.8780680
C	8.8411050	-0.8515500	-1.2956610
H	10.8839050	-0.8170370	-1.9706770
H	11.1391630	-3.2908410	-1.8777670
H	9.2230230	-4.6990040	-1.1491640
H	7.0816650	-3.6583310	-0.5205310
H	8.7313910	0.2291270	-1.3374080

Table 23. Atom coordinates and absolute energy of IM5c (Energy= -1962.831614a.u.)

Atom	X	Y	Z
Pd	-0.9680150	-1.2245190	-0.2452520
O	-0.2473620	0.5769590	-2.2125190
O	-0.0620320	0.5106440	-0.7771640
C	0.7023840	-2.1432040	-0.8804730
C	-1.9880610	-2.8819960	0.1690300
C	3.0224210	-2.9029150	-1.7987080
C	-3.4579590	-5.0136190	0.5328310
C	-4.9245740	-4.5457130	0.5344350
H	-5.5795560	-5.4103640	0.6747340
H	-5.1060780	-3.8363010	1.3459830
H	-5.1803720	-4.0629740	-0.4122520
C	-3.0771770	-5.6541650	1.8797780
H	-3.6940020	-6.5418670	2.0453410
H	-2.0261050	-5.9553480	1.8858820
H	-3.2449680	-4.9566060	2.7047240
C	-3.1842880	-5.9769640	-0.6363830
H	-3.8047410	-6.8702930	-0.5221410
H	-3.4255730	-5.5057870	-1.5927890
H	-2.1347730	-6.2832320	-0.6521390
C	3.5154310	-1.7027320	-2.6286220
H	3.5024500	-0.7864760	-2.0341030
H	4.5357110	-1.9002940	-2.9707070
H	2.8759210	-1.5525570	-3.5026880
C	3.9234350	-3.1542550	-0.5756690
H	3.5648500	-4.0124520	0.0004560
H	4.9400500	-3.3679750	-0.9181910
H	3.9445300	-2.2814590	0.0800490
C	2.8957060	-4.1669090	-2.6660560
H	2.2254250	-3.9936970	-3.5124870
H	3.8816490	-4.4360340	-3.0553510
H	2.5138700	-5.0091850	-2.0816810
N	1.7007820	-2.5653450	-1.3033430
N	-2.6226780	-3.8448810	0.3453290
N	-2.5758540	-0.0701760	0.4051340
O	-2.5306720	0.3486350	1.7590950
C	-3.0541470	0.8576170	-0.4637120
O	-2.9110490	0.6820760	-1.6968590
H	-1.2214510	0.7475690	-2.2323400
C	-3.2777130	-0.5448310	2.5684240
H	-2.8651880	-1.5623350	2.5276740
H	-3.1915720	-0.1659220	3.5907270
H	-4.3343330	-0.5725520	2.2703310

H	1.4711090	0.7012150	-0.5838500
N	2.3518940	-0.2885310	1.3853460
C	3.0209520	0.5200820	0.6184980
O	2.4651890	0.9262050	-0.5275820
O	3.1041420	-0.6604000	2.5323270
C	2.2169430	-1.2396640	3.4703380
H	1.7124090	-2.1215500	3.0536210
H	2.8358940	-1.5390330	4.3210000
H	1.4561290	-0.5221500	3.8024460
C	-3.8011870	2.0258530	0.0692640
C	-4.3442060	2.9144060	-0.7819160
H	-3.8739730	2.1253090	1.1449870
H	-4.1963840	2.7180750	-1.8425210
C	-5.1130840	4.1162170	-0.4476640
C	-5.6056980	4.9158680	-1.4953330
C	-5.3887100	4.5168360	0.8746860
C	-6.3451700	6.0690390	-1.2379260
H	-5.4000990	4.6221820	-2.5214540
C	-6.1266530	5.6675300	1.1326650
H	-5.0184570	3.9231540	1.7046920
C	-6.6094430	6.4498810	0.0782500
H	-6.7139070	6.6700420	-2.0644440
H	-6.3263580	5.9592330	2.1601080
H	-7.1845840	7.3482510	0.2835510
C	4.3742270	1.0138410	0.8818720
C	5.0034000	1.8671630	0.0498390
H	4.8287220	0.6570750	1.7974850
H	4.4646880	2.1842420	-0.8402440
C	6.3468500	2.4294270	0.2136220
C	6.8331690	3.3123650	-0.7685680
C	7.1846960	2.1329930	1.3072480
C	8.1027970	3.8784500	-0.6672040
H	6.1993950	3.5536050	-1.6181620
C	8.4519430	2.6977600	1.4090200
H	6.8396850	1.4570480	2.0835000
C	8.9188050	3.5732670	0.4228860
H	8.4539000	4.5582130	-1.4385270
H	9.0808080	2.4563790	2.2616010
H	9.9087250	4.0125540	0.5064170

Table 24. Atom coordinates and absolute energy of TS5a (Energy=-1962.811802a.u.)

Atom	X	Y	Z

Pd	0.1736010	0.5047480	-0.2342080
O	0.5300440	1.2160870	-2.5027610
C	-0.3787010	2.2431310	0.6021830
C	0.8467690	-0.2128910	1.4448760
C	-1.6395960	4.2000720	1.7790770
C	2.0086020	-1.3639970	3.4822590
C	3.4832010	-0.9240190	3.4328270
H	4.0370050	-1.4396760	4.2223500
H	3.9315330	-1.1750030	2.4684420
H	3.5752750	0.1539300	3.5918840
C	1.8647480	-2.8738080	3.2137980
H	2.4344670	-3.4259860	3.9665950
H	0.8174330	-3.1808390	3.2797610
H	2.2388490	-3.1330170	2.2198830
C	1.3476500	-0.9611280	4.8108000
H	1.8487990	-1.4807080	5.6319980
H	1.4312790	0.1158120	4.9810650
H	0.2899110	-1.2376240	4.8210540
C	-2.8018470	3.5129200	2.5213580
H	-2.4285010	2.8469930	3.3058330
H	-3.4248710	4.2809030	2.9893860
H	-3.4060160	2.9435070	1.8100180
C	-0.7234110	4.9746430	2.7402330
H	0.1154560	5.4269340	2.2036290
H	-1.2987590	5.7734020	3.2161820
H	-0.3279490	4.3213690	3.5240610
C	-2.1766900	5.0930290	0.6481590
H	-2.7727570	4.4896840	-0.0391200
H	-2.7945220	5.8799960	1.0920640
H	-1.3556590	5.5603950	0.0976040
N	-0.8498960	3.1395890	1.1711270
N	1.3161330	-0.6722250	2.4067700
O	0.8622890	0.1305070	-3.4038050
H	0.7285100	-0.6363930	-2.7955320
N	-1.8786680	1.6225310	-1.6923760
H	-0.4774500	1.2546940	-2.5229810
N	0.5185600	-1.3777070	-1.0867550
C	1.7335650	-2.0278390	-0.8093880
O	1.8359490	-3.2110980	-0.4903930
O	-0.6130300	-2.2000640	-1.0732630
C	-0.9593460	-2.7857150	0.1925130
H	-1.1414570	-2.0007050	0.9367860
H	-1.8951640	-3.3137710	0.0026050
H	-0.1865330	-3.4759190	0.5304860

O	-1.6256420	3.0406330	-1.7603810
C	-2.1640580	3.5462270	-2.9739590
H	-3.2582210	3.4695370	-2.9865930
H	-1.8725000	4.6004810	-3.0181880
H	-1.7500970	3.0212090	-3.8455130
C	-3.0355710	1.3688490	-1.0094600
O	-3.7770610	2.2141720	-0.4753500
C	-3.3566970	-0.0893800	-0.9969590
C	-4.4889900	-0.5304100	-0.4216530
H	-2.6521440	-0.7566140	-1.4853720
H	-5.1089650	0.2256060	0.0587670
C	-4.9813240	-1.9107740	-0.3669230
C	-6.0467700	-2.2226840	0.4975880
C	-4.4443800	-2.9506440	-1.1529870
C	-6.5431410	-3.5219150	0.5946770
H	-6.4829400	-1.4304230	1.1009110
C	-4.9402540	-4.2483690	-1.0565990
H	-3.6453810	-2.7337870	-1.8554030
C	-5.9896620	-4.5425380	-0.1799630
H	-7.3648380	-3.7364750	1.2725640
H	-4.5143510	-5.0328250	-1.6762620
H	-6.3771170	-5.5549960	-0.1108500
C	2.9013390	-1.1326350	-1.0218580
C	4.1451010	-1.5637570	-0.7378410
H	2.7090260	-0.1574220	-1.4572130
H	4.2279700	-2.5764880	-0.3443710
C	5.4033400	-0.8355350	-0.9122070
C	6.6054610	-1.4646010	-0.5387330
C	5.4707940	0.4695610	-1.4398150
C	7.8316260	-0.8177370	-0.6822190
H	6.5699260	-2.4742880	-0.1371740
C	6.6947670	1.1144690	-1.5831690
H	4.5616280	0.9779740	-1.7454180
C	7.8804510	0.4753210	-1.2047510
H	8.7473420	-1.3234930	-0.3897600
H	6.7270570	2.1189260	-1.9951990
H	8.8339490	0.9824190	-1.3203580

Table 25. Atom coordinates and absolute energy of TS5b (Energy=-1962.808271a.u.)

Atom	X	Y	Z
Pd	0.3722490	-1.7793610	-0.5488580

O	0.9630640	-1.7167950	-2.8500870
C	2.2937200	-2.2463210	-0.3189090
C	-0.0967900	-2.4163860	1.2280340
C	4.8686710	-2.5340610	-0.2164000
C	-0.8961140	-2.7937850	3.6582880
C	-0.5690170	-1.4351490	4.3051720
H	-1.0046230	-1.4007140	5.3083750
H	0.5123130	-1.2952750	4.3922290
H	-0.9842580	-0.6258230	3.7008250
C	-0.2587500	-3.9607730	4.4263460
H	-0.6707410	-3.9953430	5.4387470
H	-0.4684100	-4.9155110	3.9356050
H	0.8254290	-3.8363850	4.4998460
C	-2.4173620	-2.9740880	3.5050640
H	-2.8815130	-2.9689910	4.4958420
H	-2.8277720	-2.1560680	2.9087150
H	-2.6508950	-3.9258960	3.0189210
C	5.3026890	-2.0974660	-1.6277590
H	4.8706790	-1.1207820	-1.8550990
H	6.3947180	-2.0358360	-1.6604910
H	4.9722890	-2.8222070	-2.3774940
C	5.3163800	-1.5061380	0.8389670
H	4.9902420	-1.8071830	1.8393700
H	6.4090580	-1.4472820	0.8360900
H	4.8939380	-0.5281930	0.5978020
C	5.3554830	-3.9513980	0.1216240
H	4.9983120	-4.6762400	-0.6154520
H	6.4489540	-3.9656270	0.1169120
H	5.0116790	-4.2611650	1.1130090
N	3.4135350	-2.5380720	-0.2104060
N	-0.3369690	-2.7655770	2.3141170
O	-0.0591490	-1.5908190	-3.8737200
H	-0.8533850	-1.4152890	-3.3208690
C	2.2104920	1.0561240	-0.9784980
O	-0.0275950	1.3538130	-1.6188780
C	-0.1784320	1.8246770	-2.9521670
H	-0.2417360	0.9916520	-3.6635680
H	-1.1128780	2.3943590	-2.9680830
H	0.6536950	2.4807040	-3.2459080
N	1.1112170	0.4818100	-1.5450630
H	1.1615140	-0.7378560	-2.5828770
O	3.2701840	0.3995850	-0.8718660
N	-1.6107380	-1.3456810	-0.7939890
C	-2.3298570	-0.5658550	0.0650880

O	-1.9205790	-0.3838320	1.2247620
O	-2.1316010	-1.4937990	-2.1001400
C	-2.6710240	-2.8145890	-2.2688170
H	-3.5214580	-2.9634450	-1.5959280
H	-2.9970380	-2.8733800	-3.3101020
H	-1.9030320	-3.5703130	-2.0753520
C	-3.6179930	0.0043280	-0.4143800
C	-4.3941830	0.6995950	0.4354920
H	-3.8805540	-0.1469160	-1.4539580
H	-4.0241970	0.7993650	1.4544760
C	3.2282580	3.0827040	-0.0266710
C	2.1286780	2.4632320	-0.4898530
H	4.1524150	2.5068860	-0.0437580
H	1.1578970	2.9419280	-0.5237960
C	-6.2854010	1.3318310	-1.1216310
C	-7.5091950	1.9582810	-1.3336110
C	-8.1598570	2.6136770	-0.2828490
C	-7.5728300	2.6373440	0.9827920
C	-6.3464090	2.0095830	1.1941150
C	-5.6786720	1.3440080	0.1497700
H	-5.7928780	0.8309750	-1.9493230
H	-7.9594220	1.9385330	-2.3221320
H	-9.1149990	3.1022340	-0.4524870
H	-8.0686740	3.1453940	1.8050410
H	-5.8902480	2.0309550	2.1805440
C	4.7443880	6.2113450	1.4213160
C	3.6397000	7.0565330	1.5329480
C	2.3802590	6.6001410	1.1298630
C	2.2259920	5.3145770	0.6208480
C	3.3299370	4.4473230	0.4997870
C	4.5885310	4.9234190	0.9112280
H	5.7276710	6.5545400	1.7311200
H	3.7558230	8.0609910	1.9299960
H	1.5147670	7.2516370	1.2147970
H	1.2408080	4.9756640	0.3161780
H	5.4513990	4.2676340	0.8253210

Table 26. Atom coordinates and absolute energy of TS5c (Energy=-1962.81828a.u.)

Atom	X	Y	Z
Pd	-0.4334890	-1.5289050	-0.2833210
O	-0.6276390	-0.0899850	-3.1045530

O	0.3243550	-0.4763730	-2.0800780
C	0.7960880	-2.9539550	-0.9208460
C	-1.6847700	-2.6790270	0.6798570
C	2.9618590	-4.1341490	-1.7272200
C	-3.5969280	-4.0927280	1.7634610
C	-4.7819600	-3.1268170	1.9459890
H	-5.6318350	-3.6725400	2.3657780
H	-4.5197470	-2.3131120	2.6273600
H	-5.0811230	-2.6941800	0.9880040
C	-3.1340770	-4.6684760	3.1136030
H	-3.9478230	-5.2471860	3.5595650
H	-2.2717080	-5.3278720	2.9820590
H	-2.8587820	-3.8678960	3.8055280
C	-3.9462490	-5.2170820	0.7713940
H	-4.7784910	-5.8047700	1.1690500
H	-4.2423190	-4.8027560	-0.1957420
H	-3.0922180	-5.8829090	0.6200850
C	3.5587210	-3.0936620	-2.6927230
H	3.6612330	-2.1266340	-2.1952350
H	4.5453100	-3.4332940	-3.0216820
H	2.9197460	-2.9645790	-3.5699950
C	3.8226880	-4.2721380	-0.4574960
H	3.4037970	-5.0269200	0.2150630
H	4.8329550	-4.5833250	-0.7389910
H	3.8712260	-3.3167350	0.0719390
C	2.7451470	-5.4884900	-2.4189040
H	2.1072600	-5.3798850	-3.3003320
H	3.7114540	-5.8885240	-2.7383180
H	2.2823040	-6.2080610	-1.7373600
N	1.6702270	-3.6192820	-1.3040790
N	-2.4993360	-3.3336960	1.1995890
N	-1.5671090	0.0616990	0.3652410
O	-1.0312540	0.8602380	1.3872090
C	-2.4530910	0.6555010	-0.4671090
O	-2.8095910	0.0618140	-1.5134750
H	-1.4702550	-0.0351320	-2.5873720
C	-1.3835280	0.3364830	2.6609520
H	-0.9946210	-0.6814570	2.7908490
H	-0.9143970	0.9986280	3.3931140
H	-2.4721310	0.3326170	2.8055550
H	0.8023150	0.4152710	-1.6866050
N	1.8523260	-0.5263260	0.2901760
C	2.2662360	0.6723550	-0.1170530
O	1.5987770	1.3001250	-1.0120890

O	2.7931910	-1.1812310	1.1605000
C	2.1916550	-1.3967990	2.4216220
H	1.2593100	-1.9730550	2.3247510
H	2.9118380	-1.9691720	3.0155530
H	1.9648540	-0.4496510	2.9307060
C	-3.0110670	1.9778590	-0.0899700
C	-3.9311250	2.5603960	-0.8797020
H	-2.6388550	2.4390960	0.8160220
H	-4.2203780	2.0086120	-1.7724770
C	-4.5906840	3.8527410	-0.6768510
C	-5.5628510	4.2671970	-1.6057490
C	-4.3002830	4.7088270	0.4037230
C	-6.2241620	5.4858800	-1.4631830
H	-5.7948120	3.6200570	-2.4477000
C	-4.9592890	5.9255440	0.5462570
H	-3.5484080	4.4211190	1.1319110
C	-5.9252300	6.3203640	-0.3854540
H	-6.9703500	5.7843710	-2.1941160
H	-4.7183850	6.5726410	1.3850910
H	-6.4365960	7.2719300	-0.2716570
C	3.4858570	1.3089500	0.4385060
C	3.8982450	2.5057190	-0.0156200
H	4.0142010	0.7648860	1.2116260
H	3.3006450	2.9566060	-0.8055800
C	5.0640170	3.2738290	0.4330780
C	5.3366080	4.5102040	-0.1810960
C	5.9344490	2.8394000	1.4524180
C	6.4314950	5.2832180	0.2022570
H	4.6753650	4.8613550	-0.9690610
C	7.0276410	3.6098880	1.8358860
H	5.7512050	1.8905470	1.9472520
C	7.2830900	4.8362590	1.2133170
H	6.6191430	6.2342590	-0.2884950
H	7.6856180	3.2547870	2.6245380
H	8.1374860	5.4352980	1.5154290

Table 27. Atom coordinates and absolute energy of IM6a(Energy=-1811.310292a.u.)

Atom	X	Y	Z
Pd	-1.1904880	-0.6563340	-0.2520150
C	-0.2125840	-4.8138670	3.1896330
C	0.3228180	-4.4174040	1.8050670

H	0.1204840	-4.1096320	3.9575420
H	-1.3058620	-4.8468780	3.1931780
H	0.1628520	-5.8078640	3.4473720
C	-0.1648560	-5.3745320	0.7001500
C	1.8583010	-4.3141310	1.7954550
H	0.1718300	-5.0209030	-0.2779610
H	0.2475980	-6.3704650	0.8881470
H	-1.2564780	-5.4443960	0.6997640
H	2.2777330	-5.2903220	2.0566130
H	2.2084820	-4.0327700	0.7994640
H	2.2088180	-3.5795540	2.5261060
C	-0.5773620	-2.1125220	0.9856380
N	-0.2058320	-3.1010480	1.4754700
C	-4.2474310	1.6342740	3.6303760
C	-4.4157920	1.6028900	2.1022670
H	-4.2771480	0.6249890	4.0504180
H	-3.2991090	2.1018430	3.9089030
H	-5.0619480	2.2163980	4.0700880
C	-4.3475990	3.0165120	1.4943180
C	-5.7197970	0.8906040	1.6984170
H	-4.3555690	2.9747010	0.4013260
H	-5.2096370	3.5950660	1.8389590
H	-3.4381440	3.5307840	1.8176840
H	-6.5706560	1.4422950	2.1077270
H	-5.8195610	0.8547910	0.6107660
H	-5.7468980	-0.1300580	2.0901840
C	-2.4812760	0.2763930	0.9525660
N	-3.3150100	0.8363930	1.5434430
O	-3.2925800	2.4588040	-1.9282330
C	-2.2434030	1.9265410	-1.5411390
C	-1.2377780	2.7576350	-0.8109130
C	0.0886410	2.7067000	-1.0318710
C	1.0984060	3.6223470	-0.4820600
C	0.8539460	4.4569530	0.6258200
C	1.8310240	5.3314700	1.0915320
C	3.0804110	5.3931820	0.4654030
C	3.3442260	4.5645190	-0.6263460
C	2.3654280	3.6854640	-1.0898950
H	0.4538280	1.9515590	-1.7252920
H	-0.1061370	4.4099510	1.1309820
H	1.6217390	5.9655940	1.9486240
H	3.8404480	6.0787010	0.8291060
H	4.3119100	4.6000950	-1.1182170
H	2.5750870	3.0448000	-1.9423760

N	-1.8531650	0.6315700	-1.7748110
O	-2.6518450	-0.0424950	-2.7183470
C	-3.9504330	-0.4045660	-2.2454010
H	-3.8764820	-1.0670630	-1.3712350
H	-4.4116490	-0.9557370	-3.0692090
H	-4.5435560	0.4823960	-2.0100710
H	-1.6754350	3.5550710	-0.2153570
O	1.6605340	-3.2948580	-1.6031210
C	1.2407850	-2.1535660	-1.3673650
C	2.1206420	-1.0882610	-0.8043010
C	3.4136230	-1.3601950	-0.5505520
C	4.4380270	-0.4790460	0.0154900
C	4.1753790	0.8316520	0.4584700
C	5.1895620	1.6208270	0.9926740
C	6.4918090	1.1219810	1.1010560
C	6.7703350	-0.1753010	0.6679620
C	5.7539580	-0.9646740	0.1328570
H	3.7402840	-2.3678070	-0.8052160
H	3.1727290	1.2390620	0.3819920
H	4.9615060	2.6308310	1.3205340
H	7.2809450	1.7405220	1.5192420
H	7.7785600	-0.5725230	0.7461420
H	5.9740720	-1.9741560	-0.2052760
N	-0.0390060	-1.7180900	-1.6349230
O	-0.8740140	-2.7869600	-2.0533210
C	-0.9812210	-2.7793380	-3.4785300
H	-1.3637650	-1.8172030	-3.8297580
H	-1.6903430	-3.5772870	-3.7191910
H	-0.0123340	-3.0051240	-3.9381510
H	1.6818450	-0.1112820	-0.6216250

Table 28. Atom coordinates and absolute energy of IM6b (Energy=-1811.319895a.u.)

Atom	X	Y	Z
Pd	0.0636850	0.9656440	0.1673680
C	-1.4544040	2.2327210	0.3113160
C	1.4492570	2.3820230	-0.0632230
C	-3.7707990	3.3961510	0.1245920
C	3.3894890	4.0626870	-0.2754880
C	3.9854370	4.0325090	1.1439970
H	4.9401980	4.5674740	1.1451480
H	3.3151470	4.5203120	1.8579310
H	4.1461460	2.9984080	1.4556540

C	3.0699570	5.4950890	-0.7275900
H	3.9932050	6.0801790	-0.7662430
H	2.6168760	5.4999820	-1.7232010
H	2.3826110	5.9821850	-0.0297220
C	4.3192050	3.3455230	-1.2716080
H	5.2780150	3.8712520	-1.3149410
H	4.4819990	2.3161600	-0.9447450
H	3.8832650	3.3379210	-2.2749740
C	-4.1472070	3.1326050	-1.3460710
H	-4.0284630	2.0716320	-1.5812360
H	-5.1859080	3.4342550	-1.5111480
H	-3.5063190	3.7102410	-2.0183690
C	-4.7050090	2.6304950	1.0795890
H	-4.3948730	2.7624950	2.1199080
H	-5.7231180	3.0150790	0.9689990
H	-4.7067060	1.5630320	0.8452320
C	-3.7485650	4.8979310	0.4497180
H	-3.0502130	5.4288100	-0.2032790
H	-4.7479370	5.3148950	0.2975850
H	-3.4562940	5.0709730	1.4893970
N	-2.4315570	2.8665260	0.3132810
N	2.1485710	3.3034570	-0.2315770
C	-2.4640470	-0.5899900	-0.2980290
O	-1.5369560	-0.9361640	1.8298800
C	-0.5725490	-1.9421440	2.1475350
H	0.4457870	-1.5515000	2.0574340
H	-0.7767210	-2.2177360	3.1858040
H	-0.6807760	-2.8138360	1.4931510
N	-1.3708590	-0.4938160	0.5001010
O	-2.4835160	-0.0048380	-1.4024100
N	1.5132430	-0.4798500	-0.1471590
C	2.8222960	-0.3436460	0.1832480
O	3.2490700	0.7238610	0.6771250
O	1.1276930	-1.7535790	-0.6057560
C	0.6712320	-1.6813200	-1.9570520
H	1.4732350	-1.3411680	-2.6257240
H	0.3788700	-2.7019180	-2.2192120
H	-0.1977660	-1.0191590	-2.0451050
C	3.7355060	-1.4943020	-0.0640350
C	5.0376530	-1.3998230	0.2573250
H	3.3030930	-2.3881360	-0.4950410
H	5.3615220	-0.4588950	0.6988810
C	-4.6721370	-1.6095250	-0.6335920
C	-3.6042610	-1.4302420	0.1650190

H	-4.6353990	-1.1186810	-1.6050680
H	-3.5284210	-1.8749830	1.1497540
C	5.8239990	-3.6958690	-0.4606650
C	6.8480350	-4.6273000	-0.5989990
C	8.1503620	-4.3130930	-0.1963540
C	8.4172700	-3.0559740	0.3472340
C	7.3903310	-2.1236390	0.4857650
C	6.0746280	-2.4217620	0.0860760
H	4.8191040	-3.9569690	-0.7774700
H	6.6321240	-5.6043640	-1.0223810
H	8.9471820	-5.0431710	-0.3057280
H	9.4247500	-2.8011880	0.6641590
H	7.6013920	-1.1456490	0.9109630
C	-8.0563760	-3.1863760	-1.1164640
C	-8.2455140	-3.8660520	0.0874670
C	-7.2537260	-3.8121530	1.0725540
C	-6.0862540	-3.0867140	0.8576120
C	-5.8782880	-2.3934750	-0.3512720
C	-6.8863160	-2.4596300	-1.3307790
H	-8.8191590	-3.2223460	-1.8892310
H	-9.1554540	-4.4338880	0.2590230
H	-7.3933870	-4.3396760	2.0120930
H	-5.3270200	-3.0560420	1.6328800
H	-6.7414220	-1.9323030	-2.2703160

Table 29. Atom coordinates and absolute energy of IM6c (Energy=-1811.312273a.u.)

Atom	X	Y	Z
Pd	0.0678620	1.2392180	0.6915760
C	-1.4604220	2.3979910	0.2106450
C	1.4847510	2.5772230	0.2601190
C	-3.6616080	3.2638630	-0.8643330
C	3.4758840	4.0061160	-0.5403910
C	4.6660210	3.3171800	0.1521610
H	5.6009210	3.7191430	-0.2501770
H	4.6474280	3.4987000	1.2308670
H	4.6236870	2.2412490	-0.0311090
C	3.4462780	5.5141820	-0.2528450
H	4.3519980	5.9789610	-0.6526620
H	2.5796480	5.9866220	-0.7243840
H	3.4055150	5.7077130	0.8229750
C	3.4820960	3.7121330	-2.0520750

H	4.3987930	4.1144750	-2.4941720
H	3.4396710	2.6338110	-2.2195370
H	2.6256230	4.1828870	-2.5437140
C	-3.5798390	2.6545460	-2.2771850
H	-3.3600360	1.5854120	-2.2171210
H	-4.5337050	2.8056330	-2.7915030
H	-2.7898910	3.1362690	-2.8604200
C	-4.8079320	2.6325420	-0.0532950
H	-4.8244560	3.0222160	0.9683470
H	-5.7607490	2.8745070	-0.5331570
H	-4.7019490	1.5456010	-0.0133870
C	-3.7868710	4.7948050	-0.9084540
H	-2.9478080	5.2401020	-1.4503260
H	-4.7129140	5.0668550	-1.4226420
H	-3.8154300	5.2159270	0.1005530
N	-2.4180270	2.9239510	-0.1941920
N	2.2651150	3.4063870	0.0002550
N	1.5951320	-0.1333570	1.0161400
O	1.4370520	-1.1719200	1.9591010
C	2.5839270	-0.3078520	0.0998030
O	2.7978860	0.5555560	-0.7775930
C	2.1008460	-0.8245620	3.1694470
H	1.7391100	0.1363210	3.5583530
H	1.8681000	-1.6213340	3.8822720
H	3.1881740	-0.7642960	3.0280130
N	-1.4170290	-0.1755350	1.0654350
C	-2.1654900	-0.5809890	-0.0025230
O	-1.7926630	-0.3275940	-1.1626130
O	-2.1519310	-0.0901410	2.2749440
C	-1.4445450	-0.7071400	3.3436230
H	-0.5479610	-0.1343660	3.6058080
H	-2.1358900	-0.7027390	4.1916470
H	-1.1540080	-1.7319180	3.0907210
C	3.4163990	-1.5420600	0.1825810
C	4.4633670	-1.7009160	-0.6456590
H	3.1252810	-2.2940790	0.9052930
H	4.6552200	-0.8882060	-1.3442350
C	5.3748200	-2.8462610	-0.7240040
C	6.4334270	-2.8054470	-1.6499260
C	5.2472850	-3.9948390	0.0818560
C	7.3321410	-3.8643300	-1.7685450
H	6.5444800	-1.9283590	-2.2824980
C	6.1433750	-5.0524560	-0.0359320
H	4.4371620	-4.0595680	0.8014880

C	7.1910450	-4.9934980	-0.9610200
H	8.1407340	-3.8082500	-2.4920150
H	6.0251620	-5.9296490	0.5942390
H	7.8880170	-5.8218280	-1.0505570
C	-3.4027790	-1.3683820	0.2695070
C	-4.1339310	-1.8393260	-0.7569980
H	-3.6672240	-1.5451920	1.3048020
H	-3.7652090	-1.6084420	-1.7553960
C	-5.3603640	-2.6394670	-0.6892760
C	-5.9494960	-3.0769090	-1.8899500
C	-5.9878800	-2.9950690	0.5210570
C	-7.1159550	-3.8401380	-1.8871580
H	-5.4775860	-2.8132300	-2.8330530
C	-7.1526910	-3.7558230	0.5249480
H	-5.5591960	-2.6709210	1.4643250
C	-7.7234520	-4.1830670	-0.6786410
H	-7.5494590	-4.1674080	-2.8280780
H	-7.6199000	-4.0187240	1.4700660
H	-8.6325630	-4.7775370	-0.6715470

Table 30. Atom coordinates and absolute energy of TS7 (Energy=-1811.291366a.u.)

Atom	X	Y	Z
Pd	-0.0169950	1.0428040	0.0586500
C	-1.3819280	2.3937700	-0.3422630
C	1.6588420	1.9699110	0.4024280
C	-3.3916760	3.9375950	-0.8120750
C	2.8427200	4.1314080	0.5782180
C	1.5735640	4.8954800	0.1678570
H	1.7751250	5.9712750	0.1438120
H	1.2361330	4.5860160	-0.8256230
H	0.7614860	4.7137380	0.8779260
C	3.9738880	4.3719180	-0.4365860
H	4.2202620	5.4377840	-0.4747170
H	4.8711730	3.8152270	-0.1532610
H	3.6715680	4.0494980	-1.4371470
C	3.2933110	4.5417060	1.9907380
H	3.5340190	5.6093510	2.0098790
H	2.5010820	4.3525570	2.7211400
H	4.1802260	3.9777150	2.2916420
C	-4.1445930	3.1450570	-1.8966210
H	-4.2773610	2.1118470	-1.5681980

H	-5.1229190	3.6055090	-2.0658260
H	-3.5903030	3.1542230	-2.8398890
C	-4.1533060	3.8896670	0.5255230
H	-3.6073960	4.4320240	1.3033920
H	-5.1327310	4.3613760	0.3985580
H	-4.2849510	2.8516600	0.8375400
C	-3.1102860	5.3809670	-1.2545670
H	-2.5411830	5.4012350	-2.1885610
H	-4.0574890	5.9031040	-1.4171800
H	-2.5449580	5.9227220	-0.4905920
N	-2.1193560	3.2629610	-0.5997330
N	2.6139850	2.6775370	0.6136940
C	-2.7447280	-0.4516130	0.0454230
O	-0.8455610	-1.8088420	-0.2268420
C	-0.4714000	-2.1002580	-1.5746900
H	0.2647940	-1.3781080	-1.9448080
H	-0.0221310	-3.0975580	-1.5473720
H	-1.3498500	-2.1092490	-2.2333690
N	-1.4027860	-0.5047800	-0.1489520
O	-3.3222750	0.6458350	0.2051150
N	1.8488720	0.1524170	0.6170180
C	2.6844090	-0.4079170	-0.3584810
O	2.4402240	-0.1666280	-1.5395980
O	2.1503410	-0.1271220	1.9582380
C	1.1811090	-1.0291260	2.5100460
H	1.1720780	-1.9810460	1.9697520
H	1.4909930	-1.1777650	3.5471580
H	0.1782630	-0.5892410	2.4760510
C	-4.8481280	-1.7107690	0.2075760
C	-3.5126820	-1.7300940	0.0547790
H	-5.3080070	-0.7302860	0.3196840
H	-2.9521470	-2.6502070	-0.0526250
C	-7.6003690	-4.9967200	0.3339630
C	-6.2346670	-5.2469400	0.1633910
C	-5.3258880	-4.1945350	0.1194780
C	-5.7583770	-2.8594990	0.2453590
C	-7.1355350	-2.6271940	0.4160670
C	-8.0471960	-3.6808490	0.4601760
H	-8.3069150	-5.8210870	0.3679000
H	-5.8787860	-6.2688240	0.0646430
H	-4.2696540	-4.4070520	-0.0130340
H	-7.4870990	-1.6032950	0.5151980
H	-9.1055210	-3.4743340	0.5933010
C	3.8196630	-1.2335310	0.1030370

C	4.6143450	-1.8303330	-0.8065490
H	3.9733720	-1.3212210	1.1709910
H	4.3605160	-1.6650260	-1.8526090
C	8.0476860	-4.3091060	-0.1874630
C	7.6026710	-4.0107160	-1.4759960
C	6.4822000	-3.2018460	-1.6555310
C	5.7829690	-2.6735970	-0.5544770
C	6.2464560	-2.9847540	0.7392860
C	7.3643150	-3.7923170	0.9186980
H	8.9204220	-4.9392990	-0.0429660
H	8.1272340	-4.4075170	-2.3403240
H	6.1364590	-2.9700530	-2.6595400
H	5.7277730	-2.5906860	1.6075840
H	7.7070510	-4.0214970	1.9236620

Table 31. Atom coordinates and absolute energy of TS7' (Energy=−1560. 826995a.u.)

Atom	X	Y	Z
Pd	-1.5921060	0.3879550	-0.0083030
C	-2.8047560	-1.1596890	0.2537350
N	-3.5209030	-2.0757170	0.3461010
C	-4.3975500	-3.2269150	0.3999130
C	-5.8240670	-2.7206530	0.6793190
C	-4.3177080	-3.9354930	-0.9649000
C	-3.9021910	-4.1446390	1.5319330
H	-4.6339900	-3.2660520	-1.7690300
H	-4.9755590	-4.8093100	-0.9583600
H	-3.2972050	-4.2691090	-1.1704960
H	-2.8754060	-4.4706970	1.3465610
H	-4.5443250	-5.0281370	1.5886110
H	-3.9368250	-3.6285220	2.4952590
H	-5.8695550	-2.1896400	1.6340670
H	-6.5083210	-3.5726810	0.7232860
H	-6.1591020	-2.0456770	-0.1125390
N	-2.9170520	1.6714990	-0.8824590
O	-4.0304500	1.2994370	-1.6436850
C	-5.2153030	1.5467410	-0.9007100
H	-5.2341320	0.9600750	0.0287950
H	-5.3163850	2.6100610	-0.6547680
H	-6.0415850	1.2369540	-1.5469410
C	-1.9991700	2.4842180	-1.5336190
O	-2.1711560	3.2075620	-2.4991410

H	0.1351090	1.3118200	-0.9217210
N	0.1482060	-0.6108460	0.6037910
O	0.1884170	-1.7421310	1.4464590
C	0.0206630	-1.3330930	2.7996520
H	0.8565220	-0.7066480	3.1361750
H	-0.9181470	-0.7799080	2.9292530
H	-0.0099190	-2.2549480	3.3862760
O	1.1888900	0.4703850	-1.0827700
C	1.2082590	-0.4572440	-0.1987900
C	2.3995650	-1.3090170	-0.0583410
C	3.4824970	-1.1084170	-0.8340240
H	2.3496570	-2.0873990	0.6921490
H	3.4232770	-0.2996410	-1.5593730
C	4.7407450	-1.8565320	-0.8098250
C	5.7675140	-1.4729450	-1.6922770
C	4.9798400	-2.9434610	0.0543300
C	6.9882970	-2.1448960	-1.7129580
H	5.5978670	-0.6365840	-2.3652670
C	6.1978550	-3.6146240	0.0336090
H	4.2060490	-3.2647590	0.7446190
C	7.2082410	-3.2187510	-0.8494510
H	7.7664190	-1.8305400	-2.4024750
H	6.3631940	-4.4508030	0.7071470
H	8.1580170	-3.7455090	-0.8626100
C	-0.7295960	2.3014190	-0.7248870
C	-0.0826640	3.4165680	-0.2991310
H	-0.4844710	4.3593920	-0.6803060
C	1.1166420	3.5710610	0.5230520
C	1.8049070	4.7990420	0.4740480
C	1.6042550	2.5667110	1.3801360
C	2.9582870	5.0070200	1.2262920
H	1.4302480	5.5883290	-0.1726150
C	2.7541930	2.7775320	2.1352970
H	1.0611410	1.6332140	1.4674890
C	3.4389580	3.9941790	2.0588020
H	3.4791450	5.9583890	1.1668030
H	3.1168160	1.9928000	2.7936020
H	4.3347220	4.1543040	2.6522060

Table 32. Atom coordinates and absolute energy of IM8 (Energy=-1811.29799a.u.)

Atom	X	Y	Z

Pd	0.0014350	1.1117090	0.0382650
C	-1.3517340	2.4721110	-0.3294740
C	1.7509040	1.9284800	0.4433370
C	-3.4628620	3.8936980	-0.7728510
C	2.5534130	4.2274890	0.5586030
C	1.1612150	4.7617720	0.1948120
H	1.1846420	5.8561020	0.1603730
H	0.8384860	4.3967680	-0.7836760
H	0.4144290	4.4596100	0.9338240
C	3.5822020	4.6585980	-0.5047840
H	3.6301930	5.7509330	-0.5635410
H	4.5760970	4.2768000	-0.2552720
H	3.3044720	4.2709080	-1.4897480
C	2.9788690	4.7534890	1.9431210
H	3.0211970	5.8475560	1.9354750
H	2.2643510	4.4415260	2.7113080
H	3.9644430	4.3658370	2.2150150
C	-4.1644340	3.0905840	-1.8838540
H	-4.2482330	2.0444980	-1.5808130
H	-5.1630820	3.5056880	-2.0522280
H	-3.6025630	3.1513280	-2.8208020
C	-4.2322540	3.7718110	0.5557320
H	-3.7237960	4.3250970	1.3511820
H	-5.2350400	4.1919810	0.4298330
H	-4.3090270	2.7205570	0.8405850
C	-3.2540230	5.3608810	-1.1764200
H	-2.6780020	5.4348510	-2.1034250
H	-4.2264120	5.8353600	-1.3362630
H	-2.7256010	5.9122820	-0.3932390
N	-2.1593960	3.2823020	-0.5644220
N	2.6518680	2.7610650	0.6378320
C	-2.7064040	-0.5004710	0.0000110
O	-0.7387750	-1.7608230	-0.2890860
C	-0.3791340	-2.0337520	-1.6416540
H	0.2947860	-1.2632360	-2.0350370
H	0.1382220	-2.9981980	-1.6269070
H	-1.2681400	-2.1028360	-2.2824290
N	-1.3664880	-0.4787010	-0.2086550
O	-3.3406810	0.5649720	0.1590460
N	2.0015450	0.4460480	0.6031990
C	2.8361470	-0.1825920	-0.3932960
O	2.6181810	0.0851570	-1.5624520
O	2.2799360	0.1071340	1.9477130
C	1.3079720	-0.8289180	2.4407120

H	1.3070480	-1.7514000	1.8520490
H	1.6149100	-1.0288240	3.4696740
H	0.3045850	-0.3899950	2.4240440
C	-4.7389920	-1.8665410	0.1964700
C	-3.4062560	-1.8190790	0.0283390
H	-5.2448440	-0.9084400	0.3048280
H	-2.8005400	-2.7106450	-0.0769650
C	-7.3224690	-5.2843370	0.3952890
C	-5.9499870	-5.4675270	0.1964320
C	-5.0955710	-4.3716780	0.1282590
C	-5.5903160	-3.0587570	0.2573260
C	-6.9735160	-2.8941560	0.4559830
C	-7.8307770	-3.9912910	0.5247650
H	-7.9865310	-6.1423590	0.4482560
H	-5.5460550	-6.4711330	0.0944780
H	-4.0331260	-4.5325620	-0.0261760
H	-7.3730910	-1.8883280	0.5580630
H	-8.8949790	-3.8363050	0.6795750
C	3.8795320	-1.0939090	0.0956600
C	4.6262670	-1.7729030	-0.8007060
H	4.0212580	-1.1717090	1.1650830
H	4.3906110	-1.6091680	-1.8513200
C	7.8358760	-4.5119750	-0.1205690
C	7.4088230	-4.2183200	-1.4163960
C	6.3606320	-3.3226700	-1.6162850
C	5.7183790	-2.7030910	-0.5276850
C	6.1629720	-3.0102800	0.7740330
C	7.2089130	-3.9042030	0.9729960
H	8.6528910	-5.2093270	0.0397190
H	7.8914430	-4.6856200	-2.2695740
H	6.0282250	-3.0933660	-2.6252580
H	5.6883110	-2.5445460	1.6318260
H	7.5401760	-4.1295930	1.9824240

Table 33. Atom coordinates and absolute energy of IM9 (Energy=-2061.765766a.u.)

Atom	X	Y	Z
Pd	0.4046760	0.0818620	0.3984910
C	0.9559130	1.9866920	0.1246930
C	-0.2993560	-1.7769210	0.7085900
N	1.2840880	3.0936170	-0.0447520
C	2.1328590	4.2590000	-0.2277740

N	-0.7821950	-2.8217240	0.8795280
C	-1.5298740	-4.0432080	1.1048680
C	3.0078960	3.9871470	-1.4654110
C	1.2365370	5.4911040	-0.4211910
C	3.0051680	4.3809400	1.0355370
H	3.5864090	3.4665470	1.1713470
H	3.6831620	5.2327840	0.9236810
H	2.3852910	4.5475900	1.9215350
H	2.3901080	3.8759420	-2.3617910
H	3.6898090	4.8292670	-1.6188410
H	3.5846870	3.0725270	-1.3095550
H	0.5946220	5.6493400	0.4500740
H	1.8620350	6.3782850	-0.5558320
H	0.6011880	5.3791530	-1.3045150
C	-2.3001190	-3.8719800	2.4269110
C	-0.5288350	-5.2082520	1.1735750
C	-2.5075030	-4.2025420	-0.0744110
H	0.1821520	-5.0645800	1.9917830
H	-1.0731180	-6.1410480	1.3465520
H	0.0317000	-5.2997850	0.2391940
H	-1.9670520	-4.2782520	-1.0224810
H	-3.0905750	-5.1176430	0.0653580
H	-3.1876980	-3.3484340	-0.1115360
H	-2.9491490	-2.9953650	2.3691420
H	-2.9097290	-4.7633210	2.6034140
H	-1.6099620	-3.7538640	3.2670440
C	-1.4161260	0.6916720	1.1608470
N	-1.8238920	0.9812600	2.3159080
N	-2.4431600	0.6601370	0.1328450
O	-2.3520610	1.7129650	-0.7941660
C	-1.8835290	1.2428610	-2.0669650
H	-0.8999280	0.7723970	-1.9721620
H	-1.8115670	2.1373490	-2.6907130
H	-2.5958440	0.5378270	-2.5114940
C	-3.6305110	-0.0465430	0.2319030
O	-3.7205770	-1.0237270	0.9785340
C	-1.0707880	0.9914510	3.5784850
C	-1.2616530	-0.3979650	4.2195600
H	-0.8510890	-0.4066240	5.2349370
H	-0.7486760	-1.1658340	3.6331830
H	-2.3239320	-0.6536690	4.2669070
C	0.4273720	1.3232910	3.4664500
H	0.5801790	2.2891300	2.9761840
H	0.9804690	0.5661710	2.9033000

H	0.8650780	1.3814890	4.4691430
C	-1.7596820	2.0578030	4.4542970
H	-1.3123860	2.0877250	5.4535790
H	-2.8267660	1.8394560	4.5504100
H	-1.6578140	3.0497720	4.0021810
O	2.3022180	-1.9716540	-0.9219470
C	1.8430550	-1.9942520	-2.2637850
H	2.4991620	-1.4130920	-2.9265210
H	0.8205270	-1.5982670	-2.3405640
H	1.8492480	-3.0446170	-2.5725420
O	3.5449650	1.0970400	0.2553730
N	2.2529830	-0.6350060	-0.4193740
C	3.4603950	-0.0434220	-0.2540040
C	-4.7426480	0.4098680	-0.6405740
C	-5.8626840	-0.3316360	-0.7219690
H	-4.6260800	1.3528790	-1.1600110
H	-5.8688410	-1.2583420	-0.1499110
C	-8.4385950	1.3750940	-2.9247360
C	-9.4608420	0.4199900	-2.9182330
C	-9.2963620	-0.7619670	-2.1949100
C	-8.1180300	-0.9857170	-1.4851200
C	-7.0780320	-0.0380090	-1.4835880
C	-7.2623540	1.1506680	-2.2171550
H	-8.5630330	2.2988870	-3.4825620
H	-10.3781800	0.5994850	-3.4713570
H	-10.0854940	-1.5082280	-2.1816810
H	-7.9926980	-1.9057770	-0.9200940
H	-6.4816070	1.9047950	-2.2270440
C	5.8898990	-0.1802570	-0.5980770
C	4.6859410	-0.7678270	-0.7064360
H	5.9010190	0.8189710	-0.1657390
H	4.5600380	-1.7659550	-1.1068940
C	9.6087440	-0.4236700	-1.1414020
C	8.3460090	0.0461490	-0.7833740
C	7.1910040	-0.7298990	-0.9921420
C	7.3499880	-2.0019640	-1.5767880
C	8.6095450	-2.4721030	-1.9346760
C	9.7465350	-1.6861560	-1.7195780
H	10.4844570	0.1958990	-0.9687430
H	8.2426630	1.0300550	-0.3327440
H	6.4785420	-2.6253040	-1.7515510
H	8.7080670	-3.4565640	-2.3840780
H	10.7283560	-2.0564320	-2.0004810

Table 34. Atom coordinates and absolute energy of TS9 (Energy=−2061.735722a.u.)

Atom	X	Y	Z
Pd	-0.3880800	0.6283630	-0.1770420
C	-0.0834520	-1.3452610	-0.1472320
C	-0.6334620	2.6132670	-0.1710590
N	0.1155920	-2.4935690	-0.1414200
C	-0.1002750	-3.9245010	-0.0048370
N	-0.7787490	3.7675670	-0.1591490
C	-0.9808210	5.2016830	-0.1476050
C	-1.2621750	-4.2928550	-0.9460410
C	1.1969680	-4.6530610	-0.3854100
C	-0.4888750	-4.1791950	1.4634010
H	-1.3812200	-3.6023320	1.7158210
H	-0.6936990	-5.2452870	1.6010700
H	0.3248470	-3.8945420	2.1368900
H	-0.9970970	-4.0923640	-1.9883600
H	-1.4843750	-5.3595290	-0.8444740
H	-2.1464480	-3.7082390	-0.6818250
H	2.0204790	-4.3551830	0.2699450
H	1.0496590	-5.7322390	-0.2859320
H	1.4785470	-4.4366410	-1.4199010
C	-1.2561880	5.6209160	1.3080980
C	-2.1888730	5.5071070	-1.0511450
C	0.3033050	5.8601660	-0.6826400
H	-3.0806630	4.9845100	-0.6959110
H	-2.3831260	6.5834040	-1.0424660
H	-1.9913210	5.1982270	-2.0811270
H	0.5075090	5.5387940	-1.7074370
H	0.1802170	6.9469140	-0.6771170
H	1.1638380	5.6014860	-0.0605260
H	-0.4097630	5.3694230	1.9526060
H	-1.4126190	6.7025540	1.3468400
H	-2.1509720	5.1251740	1.6938120
C	1.5945010	0.9305270	0.1635040
N	2.3774420	0.8186580	1.2110460
N	2.4621910	1.3844160	-0.7826880
O	2.3531010	0.7936040	-2.0656110
C	2.7814700	1.7331050	-3.0464720
H	2.1468720	2.6279970	-3.0453390
H	2.6941930	1.2172250	-4.0061290
H	3.8236970	2.0303990	-2.8831910

C	3.7927890	1.2300320	0.2245420
O	4.4180760	2.2365670	0.5376840
C	2.1321320	1.0231420	2.6461030
C	1.9171200	2.5304460	2.8988880
H	1.8336640	2.7329760	3.9724700
H	0.9966990	2.8717190	2.4132770
H	2.7580160	3.0970260	2.4907710
C	0.9151280	0.2091040	3.1150480
H	1.0645320	-0.8583610	2.9262070
H	-0.0018650	0.5187610	2.6042100
H	0.7680900	0.3493900	4.1914470
C	3.4004570	0.5501390	3.3795030
H	3.2916180	0.7023370	4.4580250
H	4.2721450	1.1093390	3.0308070
H	3.5792040	-0.5139770	3.1973040
O	-3.1862110	1.3832580	-1.1921500
C	-3.0480630	1.2707600	-2.6030660
H	-3.4954340	0.3404060	-2.9775690
H	-1.9914350	1.3025840	-2.9009860
H	-3.5758750	2.1291620	-3.0305500
O	-2.6653610	-1.5741940	0.6351870
N	-2.4547760	0.3381380	-0.5553270
C	-3.2074820	-0.6479710	-0.0066660
C	4.4452680	-0.0882870	-0.0799970
C	5.7812070	-0.1998620	-0.0410940
H	3.7932030	-0.9138340	-0.3468720
H	6.3289870	0.6976380	0.2429600
C	6.8616880	-3.7019900	-1.0484680
C	8.2436340	-3.6205660	-0.8489110
C	8.8010780	-2.4251650	-0.3936490
C	7.9834670	-1.3247950	-0.1396700
C	6.5911750	-1.3897010	-0.3297630
C	6.0467700	-2.6030430	-0.7938560
H	6.4196160	-4.6273720	-1.4080600
H	8.8770390	-4.4798860	-1.0497720
H	9.8734890	-2.3482220	-0.2368530
H	8.4222780	-0.3954150	0.2144240
H	4.9770690	-2.6815220	-0.9633290
C	-5.4506790	-1.5966940	0.3051250
C	-4.6871890	-0.6110630	-0.1974730
H	-4.9262280	-2.3856960	0.8416400
H	-5.1036590	0.2327630	-0.7333610
C	-8.9026970	-3.0169330	0.7950440
C	-7.5213720	-2.8356930	0.8413360

C	-6.9080760	-1.7315660	0.2211900
C	-7.7351030	-0.8108730	-0.4520600
C	-9.1138750	-0.9907080	-0.4993240
C	-9.7059760	-2.0943360	0.1238200
H	-9.3512050	-3.8778320	1.2829510
H	-6.8987640	-3.5559550	1.3660200
H	-7.2925460	0.0509850	-0.9419060
H	-9.7325800	-0.2681010	-1.0244170
H	-10.7828160	-2.2313440	0.0847390

Table 35. Atom coordinates and absolute energy of TS9' (Energy=−1811. 287606a.u.)

Atom	X	Y	Z
Pd	-1.0724940	0.0236270	0.0194830
C	-1.5178050	1.9437610	-0.3128200
N	-1.5745880	3.1035930	-0.4361450
C	-1.4841260	4.5396790	-0.5983790
C	-0.0422500	4.9471230	-0.2412370
C	-2.5026230	5.1951240	0.3504600
C	-1.8061310	4.8676110	-2.0677510
H	-2.2942940	4.9260100	1.3893640
H	-2.4389500	6.2827280	0.2542300
H	-3.5222340	4.8839820	0.1075210
H	-2.8122320	4.5305770	-2.3315590
H	-1.7514790	5.9495250	-2.2180620
H	-1.0890520	4.3869060	-2.7385770
H	0.6748610	4.3963310	-0.8546850
H	0.0860240	6.0200880	-0.4115130
H	0.1699620	4.7327960	0.8096000
C	-2.8869140	-0.4361810	0.8680640
N	-4.1028640	-0.3345900	0.5738940
N	-2.5171410	-0.9285010	2.1571830
O	-3.5467320	-1.1397310	3.0822610
C	-1.4752640	-1.8732070	2.2276740
O	-1.3000330	-2.5694530	3.2104800
C	-4.7499300	0.0785100	-0.6723980
C	-5.1265760	1.5689770	-0.5562980
H	-5.7160290	1.8852200	-1.4241090
H	-4.2335340	2.1961250	-0.4986270
H	-5.7216520	1.7381920	0.3462450
C	-3.9161820	-0.1794580	-1.9437340
H	-3.6218520	-1.2323080	-1.9995240

H	-3.0079550	0.4263230	-1.9718530
H	-4.5094080	0.0553070	-2.8345930
C	-6.0446920	-0.7579500	-0.7542920
H	-6.6354740	-0.4797590	-1.6341840
H	-6.6511350	-0.6048930	0.1425240
H	-5.8060590	-1.8239050	-0.8203250
H	0.4843800	-1.3661930	0.9398400
O	1.3291940	1.5816290	-1.4200120
C	1.0976280	1.2581890	-2.7837450
H	0.0554510	0.9544490	-2.9476980
H	1.7629640	0.4541750	-3.1255420
H	1.3075480	2.1701790	-3.3502820
O	1.7872810	-0.9423440	0.9684910
N	0.9920750	0.4590200	-0.6091030
C	2.0044460	0.0057560	0.1355530
C	-3.3221030	-0.3438450	4.2461020
H	-3.3034110	0.7249970	3.9999190
H	-4.1723870	-0.5545020	4.8996150
H	-2.3931250	-0.6342760	4.7464390
C	-0.6692120	-1.9300600	0.9590280
C	-0.6647440	-3.1713040	0.3794010
H	-1.2013700	-3.9610900	0.9120370
C	0.0195300	-3.6525470	-0.8155150
C	0.0011560	-5.0395550	-1.0673000
C	0.7055630	-2.8165960	-1.7191390
C	0.6570680	-5.5788470	-2.1706780
H	-0.5281810	-5.6937280	-0.3793390
C	1.3625750	-3.3584030	-2.8185050
H	0.7100500	-1.7448880	-1.5586890
C	1.3428000	-4.7382820	-3.0494700
H	0.6340360	-6.6505810	-2.3447620
H	1.8904250	-2.7029990	-3.5057590
H	1.8543440	-5.1533330	-3.9133040
C	3.3696020	0.5521320	0.0068600
C	4.3766110	0.0600180	0.7530430
H	3.5062180	1.3550070	-0.7058680
H	4.1278160	-0.7456580	1.4408220
C	5.7776980	0.4870640	0.7453490
C	6.6891700	-0.1798450	1.5846270
C	6.2638770	1.5357790	-0.0602240
C	8.0348430	0.1813500	1.6194270
H	6.3293910	-0.9902960	2.2130940
C	7.6065670	1.8972400	-0.0253870
H	5.5843120	2.0721040	-0.7152840

C	8.4991410	1.2219720	0.8139630
H	8.7196150	-0.3487400	2.2751320
H	7.9618660	2.7092850	-0.6536330
H	9.5468700	1.5073320	0.8385610

Table 36. Atom coordinates and absolute energy of IM10 (Energy=−2061.779013a.u.)

Atom	X	Y	Z
Pd	-0.0222380	0.8442520	-0.0542020
C	0.4629380	-1.0678960	0.2736210
C	-0.5825620	2.7388220	-0.3547020
N	0.7194920	-2.1849560	0.4783310
C	0.6531630	-3.5836750	0.8613050
N	-1.0376430	3.8000440	-0.5028950
C	-1.7330570	5.0474120	-0.7332790
C	-0.4261830	-4.2378830	-0.0207510
C	2.0362470	-4.2152890	0.6433420
C	0.2382390	-3.6170380	2.3442430
H	-0.7221170	-3.1124790	2.4724990
H	0.1473320	-4.6581960	2.6685980
H	0.9887650	-3.1233970	2.9680020
H	-0.1430150	-4.1969090	-1.0767710
H	-0.5388100	-5.2877860	0.2662380
H	-1.3775710	-3.7179090	0.1150620
H	2.7966380	-3.7077130	1.2426100
H	2.0027530	-5.2679260	0.9386030
H	2.3329910	-4.1595520	-0.4077700
C	-2.5642340	5.3572310	0.5253870
C	-2.6422740	4.8403950	-1.9589720
C	-0.6839140	6.1428570	-0.9887570
H	-3.3143360	3.9941980	-1.7966170
H	-3.2356000	5.7435490	-2.1287580
H	-2.0454730	4.6425940	-2.8536600
H	-0.0690590	5.8973420	-1.8587140
H	-1.1901620	7.0937940	-1.1773930
H	-0.0280450	6.2643140	-0.1223700
H	-1.9196480	5.4590080	1.4026270
H	-3.1040040	6.2974000	0.3800680
H	-3.2906450	4.5629030	0.7155410
C	1.8737100	1.4430420	0.4894370
N	2.4829220	0.9655450	1.6946580
N	2.6478950	2.1806450	-0.2189080

O	2.0841530	2.5359740	-1.4587500
C	2.9913420	3.4031080	-2.1294070
H	3.1504950	4.3312490	-1.5669030
H	2.5250340	3.6299240	-3.0914670
H	3.9587440	2.9158910	-2.2946370
C	3.5795160	0.1102010	1.6279140
O	4.2374050	-0.1898900	2.6273080
C	2.0531580	1.5216350	3.0356550
C	3.1908200	2.3993200	3.5974100
H	2.8754520	2.8468770	4.5465380
H	3.4224290	3.2083550	2.8970040
H	4.0908500	1.8095170	3.7656280
C	0.8035340	2.4026760	2.8730580
H	-0.0554100	1.8345250	2.5055590
H	0.9789550	3.2458440	2.1994210
H	0.5448900	2.8060720	3.8572190
C	1.7027850	0.3687390	3.9964390
H	1.3702300	0.7828700	4.9542810
H	2.5645010	-0.2732090	4.1735830
H	0.8838870	-0.2307850	3.5856880
O	-2.7136610	1.0189370	-1.5691430
C	-2.3095170	0.6529340	-2.8823940
H	-2.5762900	-0.3882770	-3.1080730
H	-1.2263840	0.7797560	-3.0104900
H	-2.8408010	1.3239340	-3.5649470
O	-2.2025730	-1.3824090	0.9485630
N	-1.9924220	0.2369490	-0.6166730
C	-2.7234480	-0.6954490	0.0431060
C	3.8998560	-0.5001680	0.3036170
C	5.0077550	-1.2526230	0.1762440
H	3.2262210	-0.3421780	-0.5276750
H	5.6312400	-1.3512140	1.0630620
C	5.2770590	-2.6095420	-3.3616480
C	6.4441040	-3.3741590	-3.2609550
C	7.1253040	-3.4322280	-2.0444400
C	6.6419410	-2.7325550	-0.9399820
C	5.4683420	-1.9604230	-1.0217270
C	4.7948100	-1.9115270	-2.2588160
H	4.7432460	-2.5563770	-4.3065110
H	6.8179250	-3.9166650	-4.1245560
H	8.0337630	-4.0212390	-1.9552280
H	7.1754220	-2.7790960	0.0059140
H	3.8915340	-1.3174520	-2.3586550
C	-4.8957880	-1.8155910	0.2911010

C	-4.1522210	-0.8931220	-0.3436940
H	-4.3963310	-2.3784620	1.0780670
H	-4.5526260	-0.2633010	-1.1284210
C	-8.2531680	-3.4760990	0.6803410
C	-6.9164280	-3.1233600	0.8593640
C	-6.3044730	-2.1459940	0.0531280
C	-7.0857320	-1.5336610	-0.9468240
C	-8.4197630	-1.8850560	-1.1269120
C	-9.0116720	-2.8578550	-0.3144460
H	-8.7019730	-4.2332310	1.3173280
H	-6.3288000	-3.6061600	1.6360830
H	-6.6417490	-0.7777780	-1.5871830
H	-9.0034310	-1.3999410	-1.9045900
H	-10.0534830	-3.1298290	-0.4580110

Table 37. Atom coordinates and absolute energy of IM11 (Energy=-1811.323211a.u.)

Atom	X	Y	Z
Pd	-1.0308540	0.0103210	-0.1467510
C	-1.0469070	1.9815030	-0.3929860
N	-0.9282960	3.1332050	-0.5125180
C	-0.6278040	4.5332410	-0.7229390
C	0.8762990	4.7212050	-0.4516690
C	-1.4841190	5.3582980	0.2530430
C	-0.9762910	4.8669950	-2.1849590
H	-0.3789230	4.2623750	-2.8723000
H	-0.7654560	5.9232650	-2.3746270
H	-2.0349540	4.6807800	-2.3843820
H	1.1129670	4.4947210	0.5913400
H	1.1561590	5.7588540	-0.6561320
H	1.4659320	4.0575290	-1.0888280
H	-2.5500540	5.1971930	0.0700890
H	-1.2644560	6.4210110	0.1169730
H	-1.2624550	5.0884520	1.2889980
C	-3.0181670	-0.0838300	0.2546650
N	-3.2954590	-0.7562880	1.4770420
N	-3.9920360	0.2991370	-0.4794270
O	-3.5458000	0.9691820	-1.6462270
C	-4.6816220	1.2841450	-2.4376330
H	-5.3701760	1.9543550	-1.9077320
H	-4.2904350	1.7873000	-3.3256300
H	-5.2257990	0.3809190	-2.7395230

C	-2.4452200	-1.8179610	1.7466560
O	-2.5998230	-2.6352170	2.6438450
C	-4.5152580	-0.5108030	2.3525930
C	-5.5584750	-1.6031520	2.0610990
H	-6.4485280	-1.4451090	2.6797270
H	-5.8609840	-1.5702970	1.0102850
H	-5.1536610	-2.5920810	2.2875810
C	-5.1110980	0.8823430	2.0824590
H	-4.3526800	1.6647290	2.1884460
H	-5.5529660	0.9634410	1.0918790
H	-5.8864310	1.0632340	2.8330700
C	-4.0859690	-0.5288870	3.8368460
H	-4.9550010	-0.2736740	4.4513880
H	-3.7084850	-1.4996000	4.1475920
H	-3.3118230	0.2241630	4.0182280
H	-0.2965400	-2.0918780	1.3898640
O	1.5568990	0.9802220	-1.4835550
C	1.4846910	0.3714630	-2.7662550
H	2.1209470	-0.5205170	-2.8238720
H	0.4533510	0.0870920	-3.0133630
H	1.8357030	1.1239480	-3.4797290
N	1.0719730	0.0607570	-0.5001170
C	1.9803420	-0.2848150	0.4453210
O	1.6312660	-0.9934650	1.4170270
C	7.9173540	-0.1648060	2.2915030
C	8.5169970	0.6262900	1.3107760
C	7.7361400	1.1459660	0.2729650
C	6.3722040	0.8777240	0.2157440
C	5.7493120	0.0805420	1.1964990
C	6.5505010	-0.4325420	2.2332110
H	8.5134710	-0.5736230	3.1026030
H	9.5816650	0.8377750	1.3523530
H	8.1955030	1.7633250	-0.4943070
H	5.7811250	1.2900500	-0.5962490
H	6.0865070	-1.0486180	2.9991730
C	3.3993080	0.1452870	0.2838800
C	4.3181410	-0.2376130	1.1877660
H	3.6435450	0.7641020	-0.5705700
H	3.9564900	-0.8552320	2.0084770
C	1.8931700	-3.8926180	-1.7235640
C	1.4977670	-4.3275370	-2.9932320
C	0.1872940	-4.1132900	-3.4242620
C	-0.7198830	-3.4695030	-2.5856940
C	-0.3341570	-3.0302890	-1.3059560

C	0.9910680	-3.2478590	-0.8825530
H	2.9133190	-4.0545820	-1.3879850
H	2.2087210	-4.8317330	-3.6417270
H	-0.1278450	-4.4490580	-4.4078860
H	-1.7418250	-3.3052860	-2.9187410
H	1.3163770	-2.8890030	0.0888840
C	-1.2369490	-1.9931070	0.8530980
C	-1.3559430	-2.4014550	-0.4609470
H	-2.3529900	-2.3961570	-0.8992630

Table 38. Atom coordinates and absolute energy of TS11 (Energy=−1811. 298205a.u.)

Atom	X	Y	Z
Pd	-0.9712420	0.1061400	-0.2012260
C	-1.6806310	1.9395210	-0.4775810
N	-2.0521840	3.0388440	-0.5901170
C	-2.5885400	4.3740000	-0.7240140
C	-1.5410280	5.2365800	-1.4502440
C	-2.8607940	4.9127010	0.6927570
C	-3.8914070	4.2752250	-1.5381220
H	-3.6938890	3.8801680	-2.5382210
H	-4.3352060	5.2701260	-1.6368990
H	-4.6073430	3.6161370	-1.0411770
H	-0.6056490	5.2695350	-0.8854940
H	-1.9213250	6.2564290	-1.5583150
H	-1.3323300	4.8369490	-2.4464210
H	-3.5853370	4.2820410	1.2146730
H	-3.2661730	5.9263510	0.6240830
H	-1.9390830	4.9450850	1.2797880
C	-2.7460400	-0.5747750	0.4705090
N	-2.5509540	-1.3322400	1.6566280
N	-3.9309580	-0.4416450	0.0103180
O	-3.9783340	0.3822340	-1.1440390
C	-5.2670670	0.2485360	-1.7223770
H	-6.0573520	0.5487670	-1.0223730
H	-5.2723120	0.9131800	-2.5905340
H	-5.4569830	-0.7805630	-2.0513640
C	-1.5144550	-2.2591060	1.5344690
O	-1.3797490	-3.2353820	2.2622860
C	-3.5363670	-1.4019760	2.8001440
C	-4.4827090	-2.5969390	2.5869960
H	-5.2016050	-2.6594500	3.4115690

H	-5.0372110	-2.4788320	1.6521150
H	-3.9141590	-3.5288890	2.5520200
C	-4.3385680	-0.0906990	2.8878440
H	-3.6685960	0.7735390	2.9526440
H	-5.0023430	0.0470160	2.0360510
H	-4.9393990	-0.1199910	3.8020450
C	-2.7572790	-1.5435040	4.1258920
H	-3.4715610	-1.5156360	4.9551060
H	-2.1972270	-2.4744440	4.1739210
H	-2.0616210	-0.7068220	4.2505760
H	0.5117220	-1.3636180	0.5867620
O	1.4063860	1.9819780	-1.1402540
C	1.3139970	1.8973780	-2.5552970
H	2.0587550	1.2030720	-2.9677150
H	0.3119350	1.5759020	-2.8679390
H	1.5094850	2.9061890	-2.9300170
N	1.0692810	0.7244230	-0.5703180
C	2.0364690	0.1810540	0.1756430
O	1.7938380	-0.8983640	0.8190010
C	7.9125920	0.3338860	2.1904080
C	8.3999570	1.4816720	1.5641410
C	7.5543060	2.2297140	0.7379990
C	6.2354820	1.8347630	0.5396350
C	5.7263510	0.6787360	1.1637480
C	6.5909310	-0.0613160	1.9912200
H	8.5608850	-0.2538680	2.8339900
H	9.4292540	1.7932300	1.7166720
H	7.9274980	3.1245120	0.2476620
H	5.5929340	2.4269620	-0.1044920
H	6.2138060	-0.9557630	2.4801540
C	3.3813600	0.7833210	0.2503460
C	4.3484440	0.2120240	0.9926620
H	3.5351370	1.6940140	-0.3139100
H	4.0827210	-0.6974900	1.5277030
C	1.8848130	-2.5269960	-3.4005810
C	2.0165530	-3.8391470	-3.8672930
C	1.3417820	-4.8759310	-3.2198180
C	0.5462590	-4.5981300	-2.1117310
C	0.4118970	-3.2825710	-1.6218120
C	1.0889030	-2.2465100	-2.2950750
H	2.4030550	-1.7181460	-3.9083380
H	2.6364380	-4.0496620	-4.7342660
H	1.4353910	-5.8970330	-3.5777990
H	0.0249490	-5.4055900	-1.6041610

H	0.9784180	-1.2246910	-1.9525780
C	-0.5901100	-1.9893070	0.3653440
C	-0.4155940	-3.0848300	-0.4378730
H	-0.9290270	-3.9947880	-0.1182600

Table 39. Atom coordinates and absolute energy of TS11' (Energy=−1811.271908a.u.)

Atom	X	Y	Z
Pd	0.9181640	-0.1214980	-0.2859660
C	0.5346110	-1.7907650	-1.2917010
N	0.2848440	-2.7745620	-1.8670560
C	0.0640130	-4.0236900	-2.5598210
C	-1.1292220	-3.8357010	-3.5137030
C	-0.2397400	-5.0980800	-1.4991570
C	1.3505520	-4.3591250	-3.3361480
H	1.5666410	-3.5870170	-4.0794880
H	1.2258140	-5.3155880	-3.8520990
H	2.2020520	-4.4323540	-2.6551250
H	-2.0325880	-3.5680100	-2.9592330
H	-1.3145720	-4.7697560	-4.0517970
H	-0.9227280	-3.0488780	-4.2442830
H	0.6000090	-5.2082720	-0.8079760
H	-0.4131240	-6.0579960	-1.9940800
H	-1.1317180	-4.8357150	-0.9241760
C	2.6086130	-0.7720060	0.5776870
N	2.5451950	-0.3901810	1.9441750
N	3.6295050	-1.3932530	0.1339730
O	3.5019080	-1.7629580	-1.2247230
C	4.7665340	-2.2293400	-1.6725240
H	5.1049040	-3.0970040	-1.0923780
H	4.6200830	-2.5184230	-2.7165130
H	5.5288240	-1.4429610	-1.6154770
C	2.1406830	0.9343640	2.1461350
O	2.3050010	1.5502030	3.1905610
C	3.0580260	-1.2359850	3.0907090
C	4.4735710	-0.7644310	3.4671180
H	4.8598700	-1.3636860	4.2991040
H	5.1513870	-0.8778960	2.6161310
H	4.4565330	0.2835550	3.7741970
C	3.0775930	-2.7208820	2.6868810
H	2.0930540	-3.0431860	2.3322240
H	3.8131290	-2.9318170	1.9121030

H	3.3253190	-3.3096020	3.5753250
C	2.0868390	-1.1019950	4.2834280
H	2.4133200	-1.7814510	5.0773500
H	2.0606570	-0.0889340	4.6782590
H	1.0741110	-1.3877420	3.9819540
H	0.2648770	1.4906380	0.5464210
O	-1.5528860	1.9534310	-1.1455370
C	-1.8379760	3.2691360	-0.6704730
H	-2.6015280	3.2523780	0.1180080
H	-0.9352520	3.7618830	-0.2942950
H	-2.2159790	3.8205320	-1.5358890
N	-1.0024560	1.1527270	-0.1058540
C	-1.9111240	0.4279220	0.6475490
O	-1.4970930	-0.2873350	1.5670910
C	-7.8836350	-0.8773460	1.7498920
C	-8.5244780	-0.2718050	0.6682740
C	-7.7661830	0.4041970	-0.2936010
C	-6.3819660	0.4747350	-0.1756040
C	-5.7180500	-0.1302130	0.9098960
C	-6.4964980	-0.8065860	1.8671180
H	-8.4632800	-1.4043820	2.5024250
H	-9.6052220	-0.3243910	0.5729830
H	-8.2590110	0.8772920	-1.1384170
H	-5.8080240	1.0018620	-0.9314360
H	-5.9993830	-1.2783520	2.7107600
C	-3.3573840	0.5217860	0.3042200
C	-4.2642110	-0.0906900	1.0867050
H	-3.6288180	1.0745830	-0.5868890
H	-3.8711010	-0.6191630	1.9541340
C	1.2267900	3.8979710	-2.9379430
C	1.4654160	5.2722390	-2.8397430
C	1.9087100	5.8169890	-1.6319640
C	2.1089790	4.9899500	-0.5299240
C	1.8492800	3.6065170	-0.6058710
C	1.4197480	3.0704530	-1.8357850
H	0.8978310	3.4691200	-3.8799420
H	1.3189190	5.9132560	-3.7044760
H	2.1048070	6.8822510	-1.5525230
H	2.4593330	5.4110740	0.4089000
H	1.2557910	2.0008910	-1.9212200
C	1.5601090	1.5686810	0.9021100
C	2.0753360	2.7880550	0.5833970
H	2.7248600	3.2461960	1.3331590

Table 40. Atom coordinates and absolute energy of IM12 (Energy=−1811. 322231a.u.)

Atom	X	Y	Z
Pd	1.0324550	-0.0040100	0.2328140
C	1.4888330	1.9963720	0.3678010
N	1.7963770	3.1229180	0.3526720
C	2.3167700	4.4706640	0.3394410
C	1.1812680	5.4306720	0.7351800
C	2.8169190	4.7662830	-1.0868910
C	3.4754110	4.5301740	1.3520890
H	3.1166940	4.3204120	2.3635070
H	3.9209450	5.5292250	1.3399540
H	4.2422950	3.7945460	1.0984920
H	0.3505240	5.3645200	0.0274910
H	1.5565980	6.4580830	0.7371790
H	0.8052770	5.1968760	1.7349610
H	3.6052040	4.0652110	-1.3732290
H	3.2203190	5.7823000	-1.1278600
H	2.0002010	4.6867570	-1.8094350
C	2.9006090	-0.5402960	-0.3110740
N	2.8759450	-1.4127460	-1.4329590
N	4.0276000	-0.2247960	0.2056260
O	3.8872080	0.6686190	1.3059200
C	5.1273700	0.7019450	1.9921790
H	5.9432750	1.0377690	1.3386380
H	4.9955720	1.4146790	2.8112600
H	5.3881500	-0.2809120	2.4045810
C	1.8508430	-2.3565490	-1.3220080
O	1.7630000	-3.3675540	-2.0118280
C	3.9871410	-1.5659880	-2.4409080
C	4.9246460	-2.6994730	-1.9867890
H	5.7377240	-2.8314640	-2.7094550
H	5.3610520	-2.4615080	-1.0128240
H	4.3728920	-3.6396060	-1.9115210
C	4.7683620	-0.2463640	-2.5870230
H	4.0912930	0.5837630	-2.8159850
H	5.3305390	0.0045390	-1.6900500
H	5.4639150	-0.3540680	-3.4252640
C	3.3771060	-1.8765550	-3.8260470
H	4.1849530	-1.9028510	-4.5646090
H	2.8518170	-2.8281540	-3.8387200
H	2.6777480	-1.0858150	-4.1187600

H	-0.9804120	-1.3737020	-0.8683720
O	-1.4977370	1.6097400	1.2731860
C	-1.1419200	1.4347150	2.6425550
H	-1.7048110	0.6124260	3.0980710
H	-0.0674320	1.2424750	2.7442500
H	-1.3977890	2.3795640	3.1281840
N	-1.1339960	0.4578920	0.5361500
C	-2.1033470	0.0344340	-0.2297340
O	-1.8741070	-0.9953240	-1.0442250
C	-7.9398260	0.3648650	-2.3242840
C	-8.4255140	1.4617680	-1.6113940
C	-7.5838470	2.1372980	-0.7209460
C	-6.2692330	1.7203260	-0.5431660
C	-5.7627360	0.6138500	-1.2536370
C	-6.6222630	-0.0524160	-2.1469460
H	-8.5857480	-0.1648960	-3.0182680
H	-9.4514580	1.7911040	-1.7474720
H	-7.9568100	2.9928510	-0.1652710
H	-5.6291560	2.2579870	0.1492340
H	-6.2454270	-0.9066090	-2.7033960
C	-3.4413240	0.6086960	-0.2823580
C	-4.3911550	0.1254650	-1.1098140
H	-3.6147580	1.4428190	0.3832080
H	-4.1256340	-0.7175480	-1.7433550
C	-1.2950410	-2.3361950	3.7250240
C	-2.3180150	-3.2874120	3.7702360
C	-2.5034320	-4.1509350	2.6879360
C	-1.6731510	-4.0608240	1.5727890
C	-0.6562000	-3.0897790	1.4997090
C	-0.4739050	-2.2358260	2.6032090
H	-1.1260010	-1.6819170	4.5765680
H	-2.9542170	-3.3656730	4.6474010
H	-3.2887630	-4.9011680	2.7176580
H	-1.8114930	-4.7428180	0.7375400
H	0.3378060	-1.5159290	2.5770090
C	0.9078360	-2.0083190	-0.1996650
C	0.2110680	-3.0486450	0.3153150
H	0.3041750	-3.9972490	-0.2202940

Table 41. Atom coordinates and absolute energy of IM13 (Energy= -1469.358808a.u.)

Atom	X	Y	Z

Pd	0.1635940	0.1389500	-0.0514260
C	1.2933090	1.8609740	-0.0709090
N	2.0081380	2.7854240	-0.0790720
C	3.0635930	3.7643520	0.0659850
C	2.9274790	4.7999560	-1.0627220
C	4.4009070	3.0054300	-0.0250580
C	2.8977720	4.4263140	1.4463750
H	1.9297870	4.9293370	1.5240920
H	3.6878330	5.1687320	1.5921590
H	2.9668040	3.6789160	2.2406990
H	3.0052650	4.3202760	-2.0422030
H	3.7270120	5.5413220	-0.9758550
H	1.9663740	5.3187290	-1.0039550
H	4.4297330	2.2046230	0.7172840
H	5.2293160	3.6976260	0.1529170
H	4.5251540	2.5599980	-1.0159130
C	1.7877640	-1.0755680	0.2687550
N	1.7292480	-2.2129860	-0.5824530
N	2.7742500	-0.9655570	1.0773930
O	2.7084440	0.2417730	1.8428640
C	3.4864820	0.0451830	3.0117670
H	4.5243380	-0.2159670	2.7672060
H	3.4641190	0.9965140	3.5518620
H	3.0661930	-0.7423480	3.6503300
C	0.4270390	-2.7189720	-0.6661030
O	0.1466680	-3.8300120	-1.1061620
C	2.9152780	-3.0155640	-1.0530760
C	3.1707020	-4.1678160	-0.0643600
H	4.0249260	-4.7695640	-0.3950950
H	3.3912480	-3.7707550	0.9303430
H	2.2931620	-4.8159930	-0.0048240
C	4.1637210	-2.1200820	-1.1692190
H	3.9610460	-1.2495740	-1.8026870
H	4.5137780	-1.7676310	-0.2013770
H	4.9575210	-2.7047580	-1.6451370
C	2.6297310	-3.5604610	-2.4708360
H	3.5280990	-4.0688240	-2.8363260
H	1.7961110	-4.2580570	-2.4817080
H	2.4065060	-2.7355320	-3.1562210
C	-1.6078180	1.0185900	-0.6237530
C	-3.8750330	1.8871500	-1.5903660
C	-4.6493950	2.5632430	-0.4441650
H	-5.6219830	2.8997170	-0.8151070
H	-4.8099040	1.8630840	0.3794040

H	-4.1032000	3.4322500	-0.0662650
C	-3.6032270	2.8787580	-2.7357940
H	-3.0525860	3.7515810	-2.3736850
H	-3.0221560	2.4050520	-3.5317110
H	-4.5544030	3.2185440	-3.1555060
C	-4.6219910	0.6406550	-2.1003660
H	-4.7777540	-0.0756810	-1.2898990
H	-5.5959260	0.9409510	-2.4984640
H	-4.0571260	0.1488480	-2.8970380
N	-2.5981900	1.4508880	-1.0671140
C	-0.5777560	-1.7657500	-0.0830420
C	-1.7549720	-2.3011830	0.2992240
H	-1.9086170	-3.3507390	0.0370150
C	-2.8643580	-1.6716540	1.0239840
C	-2.6820370	-0.6046500	1.9252430
C	-4.1692210	-2.1802390	0.8619620
C	-3.7651800	-0.0471690	2.6042440
H	-1.6765870	-0.2379230	2.1055290
C	-5.2531680	-1.6183090	1.5342440
H	-4.3246830	-3.0238420	0.1938650
C	-5.0569950	-0.5439460	2.4076780
H	-3.5977850	0.7668240	3.3049820
H	-6.2499580	-2.0257980	1.3874450
H	-5.8977180	-0.1155500	2.9464070

Table 41. Atom coordinates and absolute energy of TS13 (Energy= -1469.338324a.u.)

Atom	X	Y	Z
Pd	0.2308700	0.4206900	-0.3547620
C	1.7410180	1.7437380	0.0423610
N	2.5860030	2.5262480	0.2709520
C	3.6307200	3.4762210	0.5650940
C	4.1975510	3.9916170	-0.7712190
C	4.7202820	2.7548370	1.3803780
C	3.0117810	4.6292960	1.3773990
H	2.2209640	5.1241120	0.8069600
H	3.7837050	5.3672290	1.6155020
H	2.5843100	4.2577460	2.3126120
H	4.6115670	3.1683930	-1.3596880
H	4.9943520	4.7158480	-0.5774260
H	3.4172120	4.4808640	-1.3605130
H	4.3097120	2.3664240	2.3161660

H	5.5273440	3.4550350	1.6160770
H	5.1379410	1.9187720	0.8131630
C	1.1072620	-1.4969100	0.2505640
N	1.5773960	-2.1672310	-0.9313320
N	1.6868620	-1.6795530	1.3895230
O	1.0692580	-0.9119970	2.4059290
C	1.5248020	-1.3887810	3.6614470
H	2.6176520	-1.3257230	3.7368860
H	1.0646960	-0.7387780	4.4100910
H	1.2144450	-2.4264660	3.8373890
C	0.3160400	-2.4322710	-1.4663220
O	-0.0279230	-3.1165650	-2.4100640
C	2.8799030	-2.8115640	-1.2066770
C	2.9336210	-4.1766020	-0.4901740
H	3.8980360	-4.6636090	-0.6718030
H	2.8053090	-4.0469400	0.5874720
H	2.1427030	-4.8350240	-0.8623280
C	4.0077890	-1.8927910	-0.7058530
H	3.9463410	-0.9130950	-1.1902990
H	3.9520220	-1.7504260	0.3743470
H	4.9747400	-2.3414740	-0.9557900
C	3.0099990	-2.9959560	-2.7298030
H	3.9741830	-3.4642030	-2.9528920
H	2.2079620	-3.6198800	-3.1254940
H	2.9717790	-2.0276310	-3.2389770
C	-1.4794290	1.3445930	-1.0454570
C	-3.9011050	2.1346200	-1.6328790
C	-4.5276440	2.6798020	-0.3355260
H	-5.5661760	2.9678560	-0.5245510
H	-4.5109490	1.9198910	0.4501010
H	-3.9818920	3.5592530	0.0177890
C	-3.8706460	3.2160070	-2.7278530
H	-3.3157100	4.0956360	-2.3897020
H	-3.3971830	2.8349020	-3.6368290
H	-4.8925680	3.5220370	-2.9703330
C	-4.6509700	0.8787760	-2.1165270
H	-4.6466390	0.1069150	-1.3425940
H	-5.6884050	1.1382440	-2.3489480
H	-4.1836690	0.4710350	-3.0170940
N	-2.5400740	1.7512600	-1.3385980
C	-0.4556970	-1.6802120	-0.4114950
C	-1.7013240	-2.0889260	-0.0431430
H	-2.1131600	-2.8746780	-0.6803420
C	-2.6041360	-1.6002690	0.9874430

C	-2.2505960	-0.6198630	1.9395240
C	-3.9195100	-2.1125200	1.0233700
C	-3.1822280	-0.1678190	2.8701920
H	-1.2357900	-0.2369380	1.9556070
C	-4.8493940	-1.6547410	1.9537920
H	-4.2054600	-2.8767470	0.3045400
C	-4.4864000	-0.6751210	2.8817280
H	-2.8879610	0.5840100	3.5979520
H	-5.8560430	-2.0640360	1.9575200
H	-5.2075210	-0.3177970	3.6115770

Table 42. Atom coordinates and absolute energy of IM14 (Energy=-1469.371939a.u.)

Atom	X	Y	Z
Pd	-2.4738580	0.8556860	-0.7846720
C	-3.5099850	-0.8156960	-0.7980220
N	-4.1346580	-1.8119900	-0.8178280
C	-4.9067500	-3.0272390	-0.8497260
C	-6.1898500	-2.8024900	-0.0271600
C	-4.0545500	-4.1539420	-0.2350030
C	-5.2483880	-3.3408100	-2.3189750
H	-5.8332030	-2.5297770	-2.7612380
H	-5.8342550	-4.2635060	-2.3727530
H	-4.3369930	-3.4714340	-2.9086280
H	-5.9459920	-2.5546630	1.0094410
H	-6.7976230	-3.7124260	-0.0348480
H	-6.7806230	-1.9848550	-0.4487650
H	-3.1319090	-4.2952060	-0.8044470
H	-4.6191740	-5.0912040	-0.2459460
H	-3.7899940	-3.9181150	0.7993490
C	1.8944770	-0.9149520	1.5560490
N	1.2068890	0.2000320	2.1116300
N	1.7899780	-2.1184580	1.9715100
O	2.6457730	-2.9927000	1.2790320
C	2.4795370	-4.3000930	1.8116900
H	1.4517430	-4.6580820	1.6789140
H	3.1689960	-4.9336080	1.2489200
H	2.7365600	-4.3285700	2.8769400
C	1.8939530	1.1146070	1.2981210
O	1.8901000	2.3243960	1.2139650
C	0.2178150	0.2869320	3.2074200
C	0.9027440	-0.1515470	4.5173090

H	0.1813980	-0.1206100	5.3402740
H	1.2878190	-1.1707830	4.4329660
H	1.7331960	0.5177800	4.7635730
C	-0.9665160	-0.6395110	2.8734420
H	-1.4446920	-0.3285290	1.9386180
H	-0.6362630	-1.6762230	2.7753890
H	-1.7070980	-0.5847110	3.6781780
C	-0.2683540	1.7402390	3.3140710
H	-0.9967670	1.8042770	4.1280790
H	0.5541680	2.4264550	3.5275700
H	-0.7558330	2.0595450	2.3898680
C	-1.4429970	2.5494750	-0.7988800
C	-0.0768950	4.7813370	-0.8244560
C	-0.8514560	5.8188650	-1.6580970
H	-0.2948710	6.7607320	-1.6781310
H	-0.9840240	5.4709480	-2.6863810
H	-1.8381120	6.0068430	-1.2255110
C	0.0831400	5.2478750	0.6348080
H	-0.8939510	5.4383850	1.0884640
H	0.6074190	4.4868950	1.2167030
H	0.6630510	6.1758720	0.6582940
C	1.2982750	4.4818970	-1.4511480
H	1.1840060	4.1076860	-2.4727270
H	1.8903600	5.4019910	-1.4829610
H	1.8301010	3.7390790	-0.8524230
N	-0.8414060	3.5568300	-0.8186980
C	2.6227270	-0.0131030	0.6132030
C	3.4965320	0.0819980	-0.4031350
H	3.7136890	1.1199940	-0.6621790
C	4.2025890	-0.8984940	-1.2278990
C	3.7637250	-2.2215220	-1.4191360
C	5.3536110	-0.4665890	-1.9163740
C	4.4734880	-3.0844640	-2.2503260
H	2.8715270	-2.5658770	-0.9131910
C	6.0670330	-1.3350570	-2.7376750
H	5.6900420	0.5597280	-1.7933040
C	5.6278910	-2.6499540	-2.9071130
H	4.1186910	-4.1011430	-2.3942760
H	6.9578700	-0.9853110	-3.2512130
H	6.1748240	-3.3281880	-3.5558920

Table 43. Atom coordinates and absolute energy of 2a (Energy=-841.6794009a.u.)

Atom	X	Y	Z
C	-0.8902330	0.3607440	-0.0138650
N	-2.0600510	-0.4433560	0.0673740
N	-0.8907140	1.6357340	-0.1008860
O	0.4084920	2.1599050	-0.2314240
C	0.3126900	3.5743330	-0.3506630
H	-0.1452460	4.0199770	0.5399250
H	1.3407770	3.9275730	-0.4557240
H	-0.2681310	3.8567600	-1.2359250
C	-1.3215050	-1.6437480	0.0027540
O	-1.6352670	-2.8100590	-0.0172980
C	-3.4928770	-0.0858480	0.0640900
C	-3.8276500	0.6071170	-1.2713210
H	-4.8825590	0.8991570	-1.2842470
H	-3.2179880	1.5034140	-1.4071150
H	-3.6485450	-0.0695730	-2.1122900
C	-3.7642130	0.8636860	1.2464860
H	-3.5297290	0.3723630	2.1956180
H	-3.1631250	1.7719370	1.1654790
H	-4.8218250	1.1453850	1.2577180
C	-4.3169150	-1.3733850	0.2208000
H	-5.3789800	-1.1106280	0.2247760
H	-4.1319970	-2.0733520	-0.5961760
H	-4.0838990	-1.8846150	1.1581420
C	-0.0308970	-0.8638060	-0.0251340
C	1.2118590	-1.3760610	-0.0340000
H	1.1964550	-2.4658660	-0.0955400
C	2.5569530	-0.8064070	0.0261850
C	2.8464650	0.4852460	0.5028140
C	3.6286460	-1.6323780	-0.3674600
C	4.1626820	0.9351820	0.5575770
H	2.0381940	1.1297570	0.8223880
C	4.9422210	-1.1754760	-0.3210950
H	3.4188390	-2.6390370	-0.7193460
C	5.2135830	0.1129720	0.1428990
H	4.3718660	1.9326470	0.9333090
H	5.7526620	-1.8250830	-0.6378240
H	6.2379420	0.4707600	0.1907860

Table 44. Atom coordinates and absolute energy of2a' (Energy= -841.6855311a.u.)

Atom	X	Y	Z

C	-1.2433880	0.6835690	0.0000880
N	-1.7355570	-0.6452410	-0.0000040
N	-1.9222430	1.7657640	0.0001640
O	-1.0481360	2.8802810	0.0003060
C	-1.8321830	4.0647150	-0.0004520
H	-2.4656950	4.1243100	0.8923860
H	-1.1160510	4.8896540	0.0004830
H	-2.4636530	4.1245940	-0.8947320
C	-0.4343550	-1.1962130	0.0000310
O	-0.0388000	-2.3401690	-0.0000520
C	-3.1129290	-1.1756010	0.0000080
C	-3.8301510	-0.6660220	-1.2652820
H	-4.8639240	-1.0256490	-1.2760060
H	-3.8426270	0.4262200	-1.2931800
H	-3.3292600	-1.0329520	-2.1662060
C	-3.8299460	-0.6665750	1.2656410
H	-3.3289100	-1.0339010	2.1663220
H	-3.8424080	0.4256550	1.2940210
H	-4.8637210	-1.0261990	1.2763800
C	-3.0543600	-2.7104750	-0.0003450
H	-4.0771640	-3.0987020	-0.0003520
H	-2.5373160	-3.0925970	-0.8832600
H	-2.5371610	-3.0930060	0.8822990
C	0.1558240	0.1987440	0.0001240
C	1.3518160	0.8157870	0.0001090
H	1.3056690	1.9022840	0.0001680
C	2.6946560	0.2418870	0.0000440
C	2.9516830	-1.1449490	-0.0001480
C	3.7877740	1.1301200	0.0001490
C	4.2622750	-1.6118310	-0.0002070
H	2.1244390	-1.8473950	-0.0002800
C	5.0967060	0.6565920	0.0001100
H	3.5999000	2.2005770	0.0002930
C	5.3377440	-0.7181750	-0.0000740
H	4.4474590	-2.6819750	-0.0003610
H	5.9261510	1.3575120	0.0002100
H	6.3573550	-1.0924250	-0.0001210

Table 45. Atom coordinates and absolute energy of 1a-z (Energy= -592.4090863a.u.)

Atom	X	Y	Z
N	-3.0096100	0.7109700	-0.0898830

O	-1.3962040	-0.9014600	-0.1086630
O	-3.9523050	-0.2130210	-0.5558390
C	-1.6764450	0.2903390	-0.0869530
C	0.5972950	1.5106090	0.0881120
C	1.7046040	0.5522680	0.0436970
C	1.5793910	-0.8494740	-0.0429790
C	2.7156030	-1.6538100	-0.0778880
C	3.9935260	-1.0922840	-0.0272410
C	4.1351980	0.2938480	0.0603120
C	3.0040340	1.1021190	0.0954800
C	-4.4762530	-0.9738430	0.5373970
H	0.9627960	2.5340870	0.1751790
H	0.5896160	-1.2857390	-0.0794970
H	2.6006600	-2.7318530	-0.1446180
H	4.8725700	-1.7298640	-0.0547770
H	5.1232640	0.7426400	0.1011600
H	3.1200510	2.1809780	0.1634610
H	-3.6926640	-1.5825420	0.9965590
H	-5.2344450	-1.6212890	0.0911060
H	-4.9376290	-0.3212220	1.2877340
C	-0.7551310	1.4417190	0.0408890
H	-1.2621730	2.4030860	0.1067920
H	-3.2176330	1.6218220	-0.4828570

Table 46. Atom coordinates and absolute energy of 1b-z (Energy=−592. 4095289a.u.)

Atom	X	Y	Z
N	-2.9992480	0.7706620	-0.0042550
O	-0.9902540	1.7539240	-0.0594930
O	-3.7834460	-0.2836080	-0.5118520
C	-1.6045400	0.6895630	-0.0838800
C	0.2269620	-1.1178720	-0.0977210
C	1.5592870	-0.5124560	-0.0274890
C	1.8383150	0.8670810	0.0606450
C	3.1557410	1.3140030	0.1234900
C	4.2211320	0.4111650	0.1005070
C	3.9630320	-0.9582470	0.0142520
C	2.6493980	-1.4100730	-0.0481160
C	-4.6474430	-0.7755370	0.5165490
H	0.2921330	-2.2053110	-0.1456150
H	1.0141300	1.5680080	0.0765220
H	3.3516540	2.3802980	0.1908140
H	5.2447630	0.7714440	0.1495870

H	4.7825060	-1.6706640	-0.0040070
H	2.4542890	-2.4774720	-0.1147190
H	-4.0742670	-1.1657110	1.3647400
H	-5.2212090	-1.5799090	0.0503410
H	-5.3304310	0.0058740	0.8702680
C	-1.0552190	-0.6762330	-0.1151510
H	-1.8162900	-1.4451230	-0.1831320
H	-3.3529290	1.6730380	-0.3127570

Table 47. Atom coordinates and absolute energy of 1c-z (Energy=−592. 3992102a.u.)

Atom	X	Y	Z
N	2.8713300	-0.6282950	0.2144050
O	0.8269210	-1.3105150	0.8392140
O	3.6241100	0.4125580	-0.3545910
C	1.6166900	-0.3348820	0.3166970
C	-0.2893060	1.3190790	-0.1100530
C	-1.5606450	0.5815360	-0.1039480
C	-1.7083380	-0.7538520	-0.5215050
C	-2.9617440	-1.3598140	-0.5293900
C	-4.0958070	-0.6526280	-0.1233870
C	-3.9698700	0.6782010	0.2780660
C	-2.7189120	1.2889680	0.2729200
C	5.0017060	0.0776130	-0.2541140
H	-0.4310180	2.3921310	-0.2397660
H	-0.8399470	-1.3123190	-0.8443390
H	-3.0552610	-2.3898890	-0.8612400
H	-5.0705300	-1.1316300	-0.1313090
H	-4.8456130	1.2422270	0.5855040
H	-2.6272430	2.3294720	0.5741100
H	5.3208710	0.0001090	0.7920920
H	5.5372070	0.8943990	-0.7431070
H	5.2169520	-0.8668850	-0.7667310
C	1.0064100	0.9492490	0.0011680
H	1.7523270	1.7267120	-0.1220850
H	1.4135990	-2.0634220	1.0203280

Table 48. Atom coordinates and absolute energy of IM3a-z(Energy=−1370. 403572a.u.)

Atom	X	Y	Z
Pd	1.3326580	-0.8595400	-0.5144060
C	6.2914040	-2.5803290	-0.3604280

C	5.8828680	-1.2138190	0.2198230
H	5.7502970	-3.3903130	0.1355250
H	6.0806950	-2.6265850	-1.4321300
H	7.3639290	-2.7329540	-0.2090900
C	6.6073800	-0.0655240	-0.5058860
C	6.1395240	-1.1582820	1.7369360
H	6.2915860	0.9045720	-0.1124240
H	7.6864510	-0.1652190	-0.3579840
H	6.3999140	-0.0914910	-1.5790060
H	7.2091550	-1.2815060	1.9288180
H	5.8207680	-0.1979230	2.1513100
H	5.5992620	-1.9569760	2.2519340
C	3.3092810	-0.9593440	-0.1736670
N	4.4612410	-1.0496240	0.0047690
C	1.8581030	4.4962820	-0.9274250
C	0.6520550	3.7256940	-0.3623200
H	2.7744840	4.2404240	-0.3876410
H	2.0033470	4.2738550	-1.9884200
H	1.6816230	5.5701430	-0.8200180
C	-0.6380090	4.0519930	-1.1364700
C	0.4594200	3.9971450	1.1414130
H	-1.4842780	3.5114260	-0.7051710
H	-0.8332170	5.1258690	-1.0611270
H	-0.5353950	3.7945280	-2.1948310
H	0.2616810	5.0632690	1.2879610
H	-0.3922920	3.4261400	1.5196980
H	1.3598910	3.7329440	1.7041390
C	1.1170380	1.1569860	-0.5898720
N	0.9272800	2.3076610	-0.5191610
O	-0.4497420	-1.8224930	-0.7729910
O	0.5592880	-2.7146520	-0.4805160
O	-2.3079390	1.9378850	1.0774160
C	-2.2761980	0.8300090	0.5331640
C	-2.5847550	0.6410600	-0.9246150
C	-3.6650970	0.0374210	-1.4477090
C	-4.8217870	-0.5615770	-0.7608260
C	-5.5538090	-1.5615380	-1.4259390
C	-6.6576370	-2.1639220	-0.8260300
C	-7.0647150	-1.7629630	0.4478290
C	-6.3623490	-0.7533620	1.1107140
C	-5.2543630	-0.1549010	0.5151400
H	-3.7085590	-0.0217510	-2.5350550
H	-5.2400010	-1.8752290	-2.4184670
H	-7.2015530	-2.9424570	-1.3536390

H	-7.9283730	-2.2260890	0.9166660
H	-6.6825360	-0.4245760	2.0953380
H	-4.7380720	0.6476610	1.0303450
N	-1.9690890	-0.3362790	1.1565790
O	-1.7380040	-0.3436700	2.5268610
C	-0.3869990	0.0075920	2.8416030
H	0.3217160	-0.6956560	2.3861470
H	-0.3211250	-0.0589270	3.9305810
H	-0.1609620	1.0287350	2.5198010
H	-1.8528640	1.0755310	-1.6000230
H	-1.5808370	-1.1292210	0.6253910

Table 49. Atom coordinates and absolute energy of IM3b-z (Energy=-1370.400146a.u.)

Atom	X	Y	Z
Pd	2.1043130	-0.3535100	-1.0615850
C	5.1546480	0.5797190	3.1808960
C	5.6693320	0.5568800	1.7298680
H	4.3974370	1.3571680	3.3135970
H	4.7162940	-0.3839440	3.4535440
H	5.9882120	0.7867900	3.8581040
C	6.7060850	-0.5635760	1.5290240
C	6.2489770	1.9255820	1.3281010
H	7.0468140	-0.5968090	0.4908460
H	7.5699890	-0.3788790	2.1739370
H	6.2808680	-1.5371390	1.7866750
H	7.1043400	2.1605080	1.9680190
H	6.5853810	1.9152870	0.2879450
H	5.5009650	2.7144850	1.4446760
C	3.6440970	0.0405170	0.1568850
N	4.5437590	0.2807230	0.8639300
C	-0.3359360	4.5542580	-0.6829390
C	-0.8706910	3.1129110	-0.6566930
H	0.3226990	4.7441360	0.1696000
H	0.2194290	4.7503590	-1.6045840
H	-1.1766910	5.2517100	-0.6308240
C	-1.7653760	2.8161920	-1.8747570
C	-1.6136320	2.8069750	0.6569080
H	-2.0718600	1.7680990	-1.8616910
H	-2.6535160	3.4541110	-1.8326440
H	-1.2330600	3.0234140	-2.8076930
H	-2.4818810	3.4677950	0.7385130
H	-1.9539870	1.7688880	0.6612610

H	-0.9642260	2.9819050	1.5201130
C	1.0327740	1.3400700	-0.8410260
N	0.2618780	2.2092000	-0.7357960
O	1.0721850	-1.5493070	-2.3278530
O	2.1854560	-2.2200390	-1.8469530
O	-2.1168840	-0.3429390	-0.5070180
C	-2.0425910	-1.5254460	-0.1288670
C	-2.9870060	-2.2050820	0.7896060
C	-4.1999570	-1.8282290	1.2563610
C	-5.1203970	-0.7077360	1.0211400
C	-4.9713820	0.2817680	0.0287770
C	-5.9335090	1.2775220	-0.1245970
C	-7.0580810	1.3217930	0.7037230
C	-7.2216860	0.3492570	1.6918310
C	-6.2678150	-0.6538800	1.8403790
H	-4.6170660	-2.5375640	1.9723440
H	-4.0915650	0.2570250	-0.6005770
H	-5.8044080	2.0272900	-0.9008050
H	-7.8016300	2.1039940	0.5775870
H	-8.0933330	0.3677930	2.3400110
H	-6.4074630	-1.4158850	2.6035580
N	-0.9688840	-2.2708010	-0.5158880
O	-0.9691260	-3.6606700	-0.3464870
C	0.2489390	-4.0617690	0.2957670
H	1.1168780	-3.7228930	-0.2810710
H	0.2121330	-5.1536700	0.3205970
H	0.3015760	-3.6661630	1.3186290
H	-2.6211420	-3.1606720	1.1485450
H	-0.3206410	-1.9422660	-1.2568950

Table 50. Atom coordinates and absolute energy of IM3c-z (Energy=−1370. 391911a.u.)

Atom	X	Y	Z
Pd	-1.4764630	-0.7322220	-0.9159250
O	0.2734800	-1.5510590	-1.5859320
O	-0.5961670	-2.5262400	-1.1287980
C	-3.3351910	-0.9685530	-0.2239180
C	-1.3673970	1.2805620	-0.9893060
C	-5.7732640	-1.3988710	0.6186850
C	-0.6199110	3.7724630	-0.8050560
C	0.8207640	3.7818990	-1.3496290
H	1.2406650	4.7868840	-1.2467760
H	1.4456980	3.0805380	-0.7915490

H	0.8398910	3.5027080	-2.4065990
C	-0.6401180	4.1122120	0.6968580
H	-0.2279410	5.1148740	0.8456600
H	-1.6642390	4.1005300	1.0818130
H	-0.0421560	3.3904100	1.2601840
C	-1.5261340	4.7196480	-1.6093340
H	-1.1574300	5.7446530	-1.5116620
H	-1.5285470	4.4519020	-2.6696120
H	-2.5545130	4.6852420	-1.2385900
C	-6.3780550	-0.0710200	1.1095520
H	-6.4116560	0.6638040	0.3005640
H	-7.3980640	-0.2445460	1.4639510
H	-5.7901530	0.3432250	1.9331150
C	-6.5736860	-1.9646890	-0.5690880
H	-6.1240920	-2.8921000	-0.9332880
H	-7.5982890	-2.1758040	-0.2494900
H	-6.6070220	-1.2469180	-1.3931190
C	-5.6862270	-2.4242960	1.7640410
H	-5.0922920	-2.0316620	2.5937030
H	-6.6925800	-2.6465990	2.1305220
H	-5.2275810	-3.3543210	1.4182670
N	-4.4278820	-1.1341530	0.1583000
N	-1.1275260	2.4233830	-0.9527760
N	0.8173060	0.2292900	1.2645810
O	0.7214150	1.2074180	2.2998980
C	-0.4255460	0.9049250	3.0766760
H	-1.3245150	0.8503250	2.4500250
H	-0.3089010	-0.0470780	3.6104820
H	-0.5233490	1.7201070	3.7994990
C	2.0525450	-0.0592550	0.9644410
O	2.2598070	-0.8959740	-0.0490720
H	1.4037520	-1.1654210	-0.5278350
C	3.2180230	0.4977540	1.6570730
C	4.5520600	0.3329980	1.4888190
H	2.9267570	1.1937310	2.4343760
H	5.1376760	0.9692310	2.1543080
C	5.4280740	-0.4788840	0.6298640
C	6.7638590	-0.0404450	0.5076410
C	7.6928970	-0.7393760	-0.2577710
C	7.3139660	-1.9170290	-0.9049490
C	6.0027610	-2.3805200	-0.7745550
C	5.0675460	-1.6755380	-0.0198010
H	7.0688950	0.8693240	1.0194830
H	8.7115650	-0.3709320	-0.3417480

H	8.0353100	-2.4725470	-1.4978420
H	5.7022880	-3.3025540	-1.2644300
H	4.0547480	-2.0414920	0.0682060

Table 51. Atom coordinates and absolute energy of TS3a-z (Energy= −1370. 379599a.u.)

Atom	X	Y	Z
Pd	0.9337160	-0.5831680	-0.2963140
C	5.4122170	-3.2359910	-0.6037010
C	5.3577530	-1.8084790	-0.0296530
H	4.7706500	-3.9103960	-0.0308260
H	5.0867970	-3.2488110	-1.6471920
H	6.4403130	-3.6059090	-0.5543210
C	6.2210580	-0.8418850	-0.8600930
C	5.7731880	-1.7902710	1.4526910
H	6.1543910	0.1765230	-0.4676640
H	7.2657860	-1.1621700	-0.8167630
H	5.9029270	-0.8356300	-1.9060500
H	6.8082910	-2.1319350	1.5420000
H	5.7044600	-0.7801260	1.8653530
H	5.1357380	-2.4532670	2.0434260
C	2.8630300	-1.0355760	-0.1725880
N	3.9834610	-1.3559070	-0.1091390
C	1.9668670	4.7582000	-0.9721210
C	0.7738700	4.0229360	-0.3395110
H	2.9062220	4.4704830	-0.4910510
H	2.0399700	4.5409340	-2.0415980
H	1.8313990	5.8360050	-0.8473450
C	-0.5529100	4.3894400	-1.0287470
C	0.6769160	4.2819010	1.1754190
H	-1.3789240	3.8514970	-0.5557810
H	-0.7211860	5.4650790	-0.9209000
H	-0.5196730	4.1523550	-2.0963790
H	0.5182580	5.3512220	1.3440660
H	-0.1676870	3.7260820	1.5901500
H	1.5984020	3.9838240	1.6842830
C	1.0526590	1.4311310	-0.5543970
N	0.9865880	2.5950000	-0.5173310
O	-0.8933630	-1.9946580	-0.6344190
O	0.2744540	-2.4124040	-0.0061530
O	-2.0533240	2.0933820	1.1214710
C	-1.9367820	1.0285700	0.4896380
C	-2.3576880	0.9704790	-0.9557700

C	-3.3795360	0.2650630	-1.4736860
C	-4.3377260	-0.6315930	-0.8049310
C	-5.0032020	-1.5968890	-1.5825870
C	-5.9261140	-2.4715990	-1.0134800
C	-6.2176590	-2.3871290	0.3491080
C	-5.5826390	-1.4184780	1.1304580
C	-4.6555440	-0.5465670	0.5641030
H	-3.5454210	0.3674670	-2.5465270
H	-4.7789930	-1.6652930	-2.6443640
H	-6.4189350	-3.2156560	-1.6332020
H	-6.9401080	-3.0636530	0.7971450
H	-5.8141720	-1.3362540	2.1886550
H	-4.1933870	0.2141500	1.1826870
N	-1.4226810	-0.1455590	0.9399450
O	-1.3420070	-0.2463440	2.3533710
C	-0.2165860	0.4231640	2.8990450
H	0.7185980	0.0562540	2.4473920
H	-0.2177590	0.1772530	3.9654940
H	-0.2898930	1.5075000	2.7708700
H	-1.8182690	1.6417630	-1.6201520
H	-1.3334130	-1.2967060	0.1453500

Table 52. Atom coordinates and absolute energy of TS3b-z (Energy=−1370.375517a.u.)

Atom	X	Y	Z
Pd	1.5623190	-0.5285970	-0.5805860
C	6.2288420	0.4371450	1.6945280
C	5.9078590	0.6964670	0.2112970
H	5.5961650	1.0483200	2.3438050
H	6.0760360	-0.6152540	1.9477730
H	7.2744740	0.6928180	1.8873700
C	6.7671060	-0.1921010	-0.7064520
C	6.0751850	2.1854380	-0.1411950
H	6.5158580	-0.0249980	-1.7570570
H	7.8231470	0.0502780	-0.5573130
H	6.6163220	-1.2500100	-0.4765640
H	7.1165880	2.4791490	0.0175920
H	5.8180240	2.3690680	-1.1877470
H	5.4385180	2.8104070	0.4908680
C	3.4122330	0.0325790	-0.2047570
N	4.5198360	0.3427580	-0.0092200
C	-0.4090900	4.4730200	0.7136810
C	-1.0435560	3.0985840	0.4508090

H	0.2578290	4.4395970	1.5802960
H	0.1623320	4.8138800	-0.1546440
H	-1.1981560	5.2029530	0.9145020
C	-1.9507050	3.1155030	-0.7929660
C	-1.8152910	2.5825640	1.6788510
H	-2.3414460	2.1128890	-0.9771170
H	-2.7835400	3.8034860	-0.6189710
H	-1.3976530	3.4547810	-1.6738300
H	-2.6408300	3.2665450	1.8969040
H	-2.2184470	1.5888450	1.4728320
H	-1.1649500	2.5325750	2.5572700
C	0.6304860	1.1886020	-0.0812570
N	0.0225400	2.1463620	0.1862860
O	0.7377190	-2.2499710	-1.9085640
O	1.9967690	-2.3138200	-1.2941700
O	-1.6746040	-0.3037340	-0.4588110
C	-1.6150230	-1.2871250	0.3273530
C	-2.6851650	-1.5909180	1.3162800
C	-3.9910500	-1.2404200	1.3405810
C	-4.9032470	-0.5625670	0.4061010
C	-4.5956630	-0.2066840	-0.9231110
C	-5.5553830	0.3972250	-1.7328790
C	-6.8376960	0.6679210	-1.2472920
C	-7.1597820	0.3206940	0.0657820
C	-6.2055140	-0.2916040	0.8747650
H	-4.5110430	-1.5589340	2.2454910
H	-3.5967000	-0.3918490	-1.2970240
H	-5.2986510	0.6579810	-2.7563790
H	-7.5786550	1.1398600	-1.8868690
H	-8.1539160	0.5191140	0.4571280
H	-6.4676680	-0.5719520	1.8924460
N	-0.5041920	-2.0610930	0.3116250
O	-0.5781750	-3.1841430	1.2038690
C	0.7104640	-3.4418000	1.7288850
H	1.4422160	-3.6083130	0.9287890
H	0.6110160	-4.3481440	2.3339730
H	1.0635110	-2.6159550	2.3653790
H	-2.3349380	-2.1831440	2.1551210
H	0.0968820	-2.3765310	-1.0705140

Table 53. Atom coordinates and absolute energy of TS3c-z (Energy=−1370. 387702a.u.)

Atom	X	Y	Z

Pd	-1.2324960	-0.4616270	-0.5458580
O	0.3918080	-1.5366420	-1.7408650
O	-0.3781590	-2.2207030	-0.8130900
C	-3.0086350	-1.1983960	-0.0359250
C	-1.6613400	1.5120500	-0.6500530
C	-5.2821180	-2.3914420	0.4599690
C	-1.6729090	4.1145640	-0.5028020
C	-0.5983830	4.5991250	-1.4938490
H	-0.5039820	5.6866730	-1.4229050
H	0.3698570	4.1474980	-1.2640710
H	-0.8698710	4.3397630	-2.5207680
C	-1.2591330	4.4147030	0.9501670
H	-1.1001910	5.4905800	1.0694870
H	-2.0422330	4.1006560	1.6464210
H	-0.3393230	3.8802310	1.2001600
C	-3.0462240	4.7218190	-0.8348530
H	-2.9961870	5.8097360	-0.7343140
H	-3.3428650	4.4820080	-1.8597770
H	-3.8139020	4.3465710	-0.1522890
C	-6.2426380	-1.4009880	1.1427370
H	-6.4350190	-0.5385770	0.4985930
H	-7.1939960	-1.8998730	1.3482740
H	-5.8264710	-1.0443170	2.0888730
C	-5.8461700	-2.8654320	-0.8922840
H	-5.1454360	-3.5418730	-1.3884320
H	-6.7878760	-3.3971130	-0.7273690
H	-6.0368230	-2.0159900	-1.5537200
C	-4.9760260	-3.5879040	1.3798620
H	-4.5508570	-3.2503360	2.3288470
H	-5.9012280	-4.1334000	1.5869390
H	-4.2667350	-4.2704340	0.9046890
N	-4.0367400	-1.7020130	0.2037230
N	-1.7666640	2.6751110	-0.6311390
N	0.8181500	0.3748320	0.6345140
O	0.6367790	1.4181120	1.5983330
C	-0.0215130	0.8791240	2.7337570
H	-0.9644400	0.3936240	2.4485600
H	0.6095700	0.1468110	3.2547400
H	-0.2265300	1.7245470	3.3979050
C	2.0858780	0.1209950	0.3592650
O	2.3483060	-0.7462460	-0.5706420
H	1.3881180	-1.1605830	-1.1187750
C	3.1859040	0.8141120	1.0556580
C	4.5288950	0.6369850	1.0406760

H	2.8307970	1.6231600	1.6823450
H	5.0497940	1.3729410	1.6554210
C	5.4848370	-0.2961820	0.4263740
C	6.8504870	0.0327980	0.5666550
C	7.8543130	-0.7808410	0.0492830
C	7.5168150	-1.9620410	-0.6139390
C	6.1711260	-2.3115680	-0.7508250
C	5.1637740	-1.4945760	-0.2423680
H	7.1214440	0.9464770	1.0907010
H	8.8963440	-0.4968900	0.1681270
H	8.2944180	-2.6051230	-1.0170410
H	5.8999180	-3.2315230	-1.2616070
H	4.1237820	-1.7635020	-0.3641420

Table 54. Atom coordinates and absolute energy of IM4a-z (Energy=-1370.405464a.u.)

Atom	X	Y	Z
Pd	0.7076050	-0.1498610	0.4528140
C	3.9083160	-3.9177360	-0.8187080
C	4.5115660	-2.6020260	-0.2927420
H	3.1747220	-4.3154140	-0.1131470
H	3.4129840	-3.7608190	-1.7805510
H	4.7064410	-4.6536880	-0.9526510
C	5.4933690	-1.9921260	-1.3081030
C	5.1843090	-2.8085930	1.0765850
H	5.8972120	-1.0442430	-0.9415300
H	6.3249920	-2.6840640	-1.4677510
H	5.0011400	-1.8149830	-2.2682380
H	6.0120750	-3.5153380	0.9691260
H	5.5806850	-1.8656780	1.4631910
H	4.4719030	-3.2119670	1.8006440
C	2.4607040	-1.0314060	0.0787200
N	3.4179860	-1.6701220	-0.1075560
C	2.1121320	4.6637990	-1.7614580
C	1.0016820	4.2730450	-0.7718970
H	3.1018140	4.4737760	-1.3364010
H	2.0180650	4.1022570	-2.6949370
H	2.0326790	5.7301230	-1.9904130
C	-0.3980280	4.5105220	-1.3707280
C	1.1637120	5.0162810	0.5667890
H	-1.1811160	4.1223600	-0.7129380
H	-0.5488830	5.5848040	-1.5119030
H	-0.4886750	4.0216740	-2.3450340

H	1.0842060	6.0929600	0.3920030
H	0.3822850	4.7197690	1.2706820
H	2.1395190	4.8082780	1.0146530
C	1.0652950	1.7233620	-0.2029740
N	1.1209930	2.8516350	-0.4973710
O	-0.8779940	-2.4210070	0.5043410
O	0.2462170	-1.9341310	1.2432870
O	-2.6539570	2.2862370	0.4962170
C	-1.9742350	1.3035410	0.1704010
C	-1.9235680	0.8667690	-1.2728360
C	-2.5811250	-0.1695750	-1.8225570
C	-3.4766020	-1.1469880	-1.1817950
C	-3.6685030	-2.3934530	-1.8055140
C	-4.5061610	-3.3572610	-1.2493250
C	-5.1855240	-3.0891340	-0.0592700
C	-5.0245340	-1.8476590	0.5603030
C	-4.1843810	-0.8821810	0.0073440
H	-2.4514140	-0.3199700	-2.8946030
H	-3.1386600	-2.6082750	-2.7302440
H	-4.6286030	-4.3168090	-1.7439570
H	-5.8415970	-3.8371170	0.3768010
H	-5.5629050	-1.6232390	1.4767840
H	-4.1047460	0.0900860	0.4803590
N	-1.2402180	0.5044060	0.9979320
O	-1.4118670	0.7902230	2.3731540
C	-0.7617930	1.9819110	2.7991670
H	0.3248480	1.9159810	2.6389270
H	-0.9565690	2.0504390	3.8730780
H	-1.1715860	2.8616690	2.2931960
H	-1.3703650	1.5273220	-1.9369800
H	-1.5806060	-1.8148530	0.8069530

Table 55. Atom coordinates and absolute energy of IM4b-z (Energy=-1370.405804a.u.)

Atom	X	Y	Z
Pd	-1.4822250	-0.5640830	-0.2600940
C	-6.6806380	-0.0104850	-0.1014260
C	-5.7405280	0.6994680	0.8898310
H	-6.5479350	0.3811460	-1.1136420
H	-6.4874190	-1.0861170	-0.1150240
H	-7.7181840	0.1553500	0.2023960
C	-5.8961390	0.1248430	2.3100540
C	-5.9655820	2.2215520	0.8765380

H	-5.2090780	0.6143870	3.0053530
H	-6.9202900	0.2906390	2.6566330
H	-5.6909650	-0.9485110	2.3176500
H	-6.9878380	2.4392540	1.1983250
H	-5.2735740	2.7238650	1.5579790
H	-5.8242690	2.6282330	-0.1286230
C	-3.2972590	0.1357100	0.1624380
N	-4.3805750	0.4432380	0.4634670
C	0.4468020	4.4459250	-1.4228530
C	1.1168460	3.1148950	-1.0458160
H	-0.0948360	4.3590750	-2.3691820
H	-0.2547880	4.7632580	-0.6461700
H	1.2125970	5.2188930	-1.5321680
C	1.8562670	3.2096530	0.3015680
C	2.0627450	2.6304140	-2.1604580
H	2.2407570	2.2286590	0.5897600
H	2.6871290	3.9152270	0.2072260
H	1.1839710	3.5664570	1.0872100
H	2.8560080	3.3697390	-2.3049850
H	2.5190860	1.6752130	-1.8896580
H	1.5242140	2.5092500	-3.1046720
C	-0.5549120	1.1599990	-0.6643300
N	0.0804230	2.1104180	-0.8928400
O	-1.5689400	-2.8385820	1.3115450
O	-2.2923890	-2.3666190	0.1547590
O	1.5260940	-0.2692060	0.6936400
C	1.5180520	-1.0645620	-0.2676380
C	2.7380180	-1.5185000	-0.9855380
C	4.0515000	-1.3084600	-0.7269040
C	4.8363960	-0.6539830	0.3299460
C	4.3297560	-0.1660070	1.5521080
C	5.1842380	0.4134830	2.4883630
C	6.5538800	0.5273090	2.2372680
C	7.0731580	0.0453500	1.0340300
C	6.2246650	-0.5423110	0.0999670
H	4.7042000	-1.7396150	-1.4878250
H	3.2660910	-0.2404260	1.7393820
H	4.7740610	0.7792400	3.4259930
H	7.2108950	0.9823850	2.9734670
H	8.1370030	0.1210950	0.8266330
H	6.6377530	-0.9250220	-0.8304930
N	0.3137100	-1.5634680	-0.6936490
O	0.3324580	-2.1985670	-1.9660370
C	-0.0604550	-3.5675300	-1.8355590

H	0.6878290	-4.1380930	-1.2673380
H	-0.1133040	-3.9569140	-2.8563730
H	-1.0382050	-3.6374870	-1.3507190
H	2.5219710	-2.0841820	-1.8843480
H	-0.6740890	-2.9452730	0.9379100

Table 56. Atom coordinates and absolute energy of IM4c-z (Energy=−1370. 405921a.u.)

Atom	X	Y	Z
Pd	-1.2124790	-0.1059820	0.3141670
O	0.0045320	-2.4011040	-0.5600870
O	-0.3682790	-1.8864150	0.7291130
C	-2.7878480	-1.3182500	0.1360060
C	-1.9734520	1.6967300	-0.1470370
C	-3.8469750	-3.6563680	-0.1344440
C	-2.5268070	4.1873930	-0.6878000
C	-1.8869780	4.4952060	-2.0542070
H	-2.0373750	5.5515780	-2.2944470
H	-0.8135720	4.2903760	-2.0343360
H	-2.3429370	3.8910250	-2.8431720
C	-1.8441370	4.9872780	0.4374250
H	-1.9351800	6.0573880	0.2298350
H	-2.3153250	4.7782560	1.4017660
H	-0.7858190	4.7238720	0.5058900
C	-4.0438720	4.4389720	-0.7162190
H	-4.2319410	5.4974440	-0.9167700
H	-4.5235650	3.8471690	-1.5007060
H	-4.5001240	4.1815090	0.2435010
C	-5.3766700	-3.7558540	-0.2089780
H	-5.7636960	-3.2121470	-1.0755560
H	-5.6672710	-4.8059060	-0.3032030
H	-5.8410140	-3.3498110	0.6942990
C	-3.1768070	-4.1736940	-1.4213650
H	-2.0956260	-4.0203030	-1.3723360
H	-3.3876240	-5.2416090	-1.5329690
H	-3.5666650	-3.6503310	-2.2993050
C	-3.2844340	-4.3755950	1.1058020
H	-3.7670290	-4.0121630	2.0177480
H	-3.4706200	-5.4502060	1.0187100
H	-2.2089330	-4.1982420	1.1839690
N	-3.4687680	-2.2558900	-0.0042690
N	-2.3042760	2.7838890	-0.4083490
N	0.6290900	0.8435970	0.5854800

O	0.6250360	2.0736410	1.2961620
C	0.7193100	1.8199770	2.6955630
H	-0.1045580	1.1785390	3.0336250
H	1.6735300	1.3424690	2.9484180
H	0.6523650	2.7967520	3.1842390
C	1.7765940	0.5379980	-0.0642360
O	1.8343410	-0.4682110	-0.8119030
H	0.7705190	-1.7984760	-0.7535850
C	2.9302670	1.4653540	0.1113510
C	4.2620900	1.2489040	0.0169680
H	2.6367650	2.4779640	0.3657500
H	4.8524680	2.1513740	0.1836580
C	5.1281810	0.0811170	-0.1999760
C	6.5178380	0.3042790	-0.0989600
C	7.4357280	-0.7298600	-0.2610230
C	6.9836090	-2.0229410	-0.5301980
C	5.6111570	-2.2620720	-0.6371420
C	4.6898070	-1.2293330	-0.4779800
H	6.8768710	1.3082610	0.1157880
H	8.4999510	-0.5273730	-0.1767050
H	7.6936950	-2.8354570	-0.6583630
H	5.2515600	-3.2649040	-0.8514490
H	3.6282330	-1.4117780	-0.5835700

Table 57. Atom coordinates and absolute energy of IM5a-z (Energy=-1962.821904a.u.)

Atom	X	Y	Z
Pd	1.5273400	-0.1169730	0.2541810
C	-0.8303240	-3.3967520	-3.2329360
C	-1.5319270	-2.7518930	-2.0239040
H	-0.4908850	-2.6362270	-3.9420070
H	0.0311460	-3.9910010	-2.9145310
H	-1.5349360	-4.0577320	-3.7450130
C	-1.9874350	-3.8101370	-1.0023290
C	-2.7134200	-1.8730350	-2.4714400
H	-2.4412130	-3.3326820	-0.1305720
H	-2.7274720	-4.4606910	-1.4781220
H	-1.1419100	-4.4250350	-0.6791660
H	-3.4206650	-2.4942200	-3.0288130
H	-3.2334310	-1.4530310	-1.6088040
H	-2.3747250	-1.0620250	-3.1219730
C	0.2095960	-1.2352840	-0.7952640
N	-0.5561570	-1.8989300	-1.3666680

C	4.8991450	-3.7168400	-1.7713200
C	5.1605950	-2.8237040	-0.5455650
H	4.0226130	-4.3507440	-1.6119100
H	4.7355760	-3.1114650	-2.6670180
H	5.7663350	-4.3608550	-1.9417050
C	6.3683090	-1.8984500	-0.7799720
C	5.3486600	-3.6679820	0.7280990
H	6.5327520	-1.2464230	0.0818350
H	7.2648300	-2.5062460	-0.9314440
H	6.2166440	-1.2768190	-1.6664020
H	6.2284650	-4.3069630	0.6111290
H	5.4981130	-3.0267810	1.6006660
H	4.4777750	-4.3043090	0.9069980
C	3.0760790	-1.2925720	-0.1607950
N	3.9932960	-1.9873490	-0.3499460
O	-0.6061500	1.6537810	-0.3774110
O	0.0197800	1.1192340	0.8201380
O	4.4011530	2.5253850	1.9720850
C	3.7949190	1.8095350	1.1663980
C	4.2580950	1.7571560	-0.2682960
C	3.7417970	2.4199730	-1.3185780
C	2.5569170	3.2927090	-1.3692150
C	2.0335790	3.9499310	-0.2377460
C	0.9005880	4.7569030	-0.3505970
C	0.2711110	4.9337710	-1.5880400
C	0.7948240	4.3066660	-2.7211340
C	1.9283180	3.5035460	-2.6104590
H	4.2544860	2.3081900	-2.2744700
H	2.5260150	3.8506190	0.7225950
H	0.5135770	5.2564830	0.5328390
H	-0.6101430	5.5636130	-1.6682370
H	0.3215540	4.4444520	-3.6891940
H	2.3313960	3.0173660	-3.4957420
N	2.7445810	1.0075030	1.4601390
O	2.2283290	1.1674850	2.7556350
C	2.9677660	0.3971610	3.6991400
H	2.9440590	-0.6717840	3.4431430
H	2.4660480	0.5491590	4.6587430
H	4.0018240	0.7506290	3.7623600
H	5.1894900	1.2138800	-0.4202110
H	-0.1711840	2.5227850	-0.4267650
O	-3.8960480	-1.6331910	0.9600440
C	-3.2494830	-0.5839080	1.0752570
C	-3.6616330	0.7685010	0.6228140

C	-4.8680290	1.2521270	0.2439590
C	-6.2370540	0.7273980	0.1537920
C	-6.6320480	-0.5993680	0.4220630
C	-7.9699550	-0.9718720	0.3096680
C	-8.9439640	-0.0458150	-0.0721110
C	-8.5695980	1.2712890	-0.3450890
C	-7.2344900	1.6482690	-0.2332370
H	-4.8265980	2.3011170	-0.0516020
H	-5.8755640	-1.3208570	0.7043730
H	-8.2544150	-1.9993140	0.5207890
H	-9.9842460	-0.3477570	-0.1576180
H	-9.3154240	2.0026260	-0.6437710
H	-6.9502440	2.6763990	-0.4445300
N	-2.0210440	-0.5529700	1.6883080
O	-1.4155820	-1.7953470	1.9248930
C	-1.7903840	-2.2866590	3.2139000
H	-1.5068220	-1.5795260	4.0017570
H	-1.2371240	-3.2212740	3.3390150
H	-2.8657650	-2.4852520	3.2541920
H	-2.8372380	1.4756800	0.5737460
H	-1.3002710	0.1562030	1.4448210

Table 58. Atom coordinates and absolute energy of IM5b-z (Energy=−1962. 810772a.u.)

Atom	X	Y	Z
Pd	-0.8797530	1.0213880	0.5749350
O	0.4442110	-0.4382380	1.0316090
C	0.6918280	2.2364370	0.3887650
C	-2.1961250	2.3930570	-0.0179750
C	2.7599450	3.8271250	0.2092800
C	-4.0949090	3.8292730	-1.0217530
C	-4.0147470	3.4682230	-2.5165510
H	-4.8816670	3.8883090	-3.0356420
H	-3.1078450	3.8803510	-2.9687010
H	-4.0102910	2.3826420	-2.6354540
C	-4.0241920	5.3469110	-0.7968930
H	-4.8829010	5.8257750	-1.2758080
H	-4.0463220	5.5874070	0.2699590
H	-3.1109930	5.7658750	-1.2294310
C	-5.3532950	3.2158750	-0.3807120
H	-6.2430520	3.6329660	-0.8619790
H	-5.3416540	2.1318560	-0.5144450
H	-5.3981020	3.4457860	0.6878940

C	3.6664260	3.5208580	1.4148470
H	3.9900750	2.4787800	1.3785480
H	4.5448320	4.1719110	1.3705140
H	3.1403490	3.7128090	2.3547910
C	3.4765680	3.5147180	-1.1168000
H	2.8146780	3.6974680	-1.9687890
H	4.3464620	4.1721970	-1.2085480
H	3.8113720	2.4756850	-1.1247130
C	2.2418370	5.2760490	0.2433300
H	1.7062950	5.4807840	1.1748330
H	3.0920350	5.9605440	0.1759790
H	1.5719540	5.4742850	-0.5984960
N	1.6025250	2.9537360	0.3010140
N	-2.9466010	3.2114760	-0.3767140
O	0.2113630	-0.8920490	2.3842240
H	-0.6204980	-1.3884240	2.2455820
C	4.1989460	-0.6500280	0.2568750
O	2.9967560	-2.6545360	0.7452390
C	2.8240800	-3.1455820	2.0806910
H	1.9465170	-2.6852790	2.5454970
H	2.6756690	-4.2232430	1.9735930
H	3.7148460	-2.9498110	2.6910670
N	3.0999410	-1.2593840	0.7726700
H	2.1851840	-0.7785850	0.8324730
O	4.2073050	0.5816480	0.0977170
N	-2.4808740	-0.2971450	0.8183560
C	-3.4588340	-0.4770810	-0.1088430
O	-3.5764480	0.3246530	-1.0583790
O	-2.4228040	-1.2802860	1.8448500
C	-2.9672660	-0.7456380	3.0563590
H	-4.0319170	-0.5170790	2.9330130
H	-2.8390880	-1.5248690	3.8130670
H	-2.4262580	0.1578970	3.3578400
C	-4.3899920	-1.6309570	0.0482370
C	-5.4002100	-1.7958210	-0.8236020
H	-4.2062890	-2.3202080	0.8629960
H	-5.4806060	-1.0518580	-1.6145060
C	6.4997370	-0.9551400	-0.5127160
C	5.3650990	-1.5137520	-0.0567450
H	6.4917300	0.1284720	-0.6214440
H	5.2501950	-2.5808690	0.0893030
C	-6.4360340	-3.9108750	0.1032990
C	-7.4152720	-4.8970290	0.0407450
C	-8.3889700	-4.8651180	-0.9632140

C	-8.3721090	-3.8360440	-1.9053980
C	-7.3904150	-2.8485870	-1.8418050
C	-6.4039950	-2.8636860	-0.8386350
H	-5.6862680	-3.9522490	0.8872560
H	-7.4208460	-5.6965260	0.7764050
H	-9.1515120	-5.6372990	-1.0089580
H	-9.1223280	-3.8024980	-2.6904280
H	-7.3789240	-2.0492920	-2.5784610
C	10.0531570	-1.4403370	-1.6520770
C	10.1969170	-2.8273310	-1.5999580
C	9.1186090	-3.6183650	-1.1894350
C	7.9096160	-3.0297750	-0.8331900
C	7.7469420	-1.6311300	-0.8780680
C	8.8411050	-0.8515500	-1.2956610
H	10.8839050	-0.8170370	-1.9706770
H	11.1391630	-3.2908410	-1.8777670
H	9.2230230	-4.6990040	-1.1491640
H	7.0816650	-3.6583310	-0.5205310
H	8.7313910	0.2291270	-1.3374080

Table 59. Atom coordinates and absolute energy of IM5c-z (Energy=−1962. 812106a.u.)

Atom	X	Y	Z
Pd	0.5966480	0.8955380	-0.0591230
O	-0.0277970	-1.4835700	-1.3589290
O	-0.2412410	-0.9540190	-0.0286570
C	-1.0704090	1.4807780	-1.0178180
C	1.5378530	2.6443520	-0.1831610
C	-3.3397550	1.7370660	-2.2817740
C	2.8850200	4.8589330	-0.5282550
C	2.6104720	5.7962730	0.6614300
H	3.1789290	6.7214960	0.5318790
H	1.5481240	6.0471110	0.7241160
H	2.9152250	5.3311860	1.6027180
C	2.4170040	5.4910270	-1.8515170
H	2.9826550	6.4089280	-2.0347620
H	2.5826350	4.8078750	-2.6887500
H	1.3535230	5.7416540	-1.8092580
C	4.3718540	4.4654820	-0.5961520
H	4.9771000	5.3631090	-0.7515630
H	4.6911690	3.9867200	0.3331560
H	4.5541850	3.7738610	-1.4227190
C	-3.6800950	0.3064730	-2.7380710

H	-3.7254090	-0.3643620	-1.8777550
H	-4.6514420	0.3144260	-3.2414910
H	-2.9258500	-0.0669580	-3.4359340
C	-4.3850750	2.2642920	-1.2828290
H	-4.1133100	3.2596120	-0.9190810
H	-5.3542420	2.3320730	-1.7854370
H	-4.4819710	1.5878230	-0.4307590
C	-3.1801270	2.6905880	-3.4784010
H	-2.4101610	2.3288280	-4.1654370
H	-4.1279180	2.7477920	-4.0209470
H	-2.9108630	3.6979130	-3.1470890
N	-2.0626560	1.6746270	-1.5935290
N	2.1181620	3.6464540	-0.3247110
N	2.2136360	0.0747470	0.9566760
O	2.2180810	0.2431470	2.3630660
C	2.7553660	-1.0779780	0.4848070
O	2.6236080	-1.3485350	-0.7335480
H	0.9446580	-1.6415680	-1.2989350
C	3.1671300	1.2327670	2.7338690
H	2.9302920	2.2032460	2.2774670
H	3.0991900	1.3203520	3.8220790
H	4.1853810	0.9384130	2.4492880
H	-1.7668680	-0.9174760	0.2324230
N	-2.0191390	0.2488680	2.2073780
C	-3.0255540	-0.2835890	1.5823540
O	-2.7754720	-0.8711490	0.4026240
O	-2.3810870	0.7920030	3.4567380
C	-1.2536180	1.4737590	3.9823210
H	-1.0274260	2.3822620	3.4065660
H	-1.5237010	1.7498290	5.0054180
H	-0.3692900	0.8275190	3.9841410
C	3.4883720	-1.9370660	1.4502910
C	4.4567070	-2.8637150	1.2620730
H	3.1819200	-1.7781250	2.4783660
H	4.7775430	-3.3346380	2.1924810
C	5.2301910	-3.3675580	0.1187850
C	6.2885130	-4.2513130	0.4205040
C	5.0087570	-3.0413260	-1.2347750
C	7.1013090	-4.7821420	-0.5770950
H	6.4728000	-4.5190340	1.4583610
C	5.8243090	-3.5757570	-2.2301410
H	4.1843310	-2.3839840	-1.4819500
C	6.8719100	-4.4438040	-1.9120660
H	7.9091720	-5.4593760	-0.3139240

H	5.6344950	-3.3154680	-3.2681510
H	7.4997520	-4.8568950	-2.6969150
C	-4.4127420	-0.2048200	2.0427860
C	-5.5471730	-0.8124620	1.6199130
H	-4.5277780	0.5065950	2.8534710
H	-6.4438630	-0.4492380	2.1238700
C	-5.8639030	-1.8668630	0.6443620
C	-7.2075250	-1.9630380	0.2262380
C	-4.9521240	-2.8211840	0.1513910
C	-7.6221010	-2.9427420	-0.6722420
H	-7.9322470	-1.2509830	0.6144340
C	-5.3708320	-3.8066500	-0.7399960
H	-3.9174460	-2.7787070	0.4617690
C	-6.7014550	-3.8712580	-1.1616070
H	-8.6625370	-2.9869960	-0.9823510
H	-4.6500170	-4.5330470	-1.1048310
H	-7.0189870	-4.6435630	-1.8566710

Table 60. Atom coordinates and absolute energy of TS5a-z (Energy=−1962. 784131a.u.)

Atom	X	Y	Z
Pd	0.9566560	-0.3649240	-0.0326130
C	-2.0111050	-3.7980460	-2.8561000
C	-2.5382510	-2.6351980	-1.9972330
H	-1.4442340	-3.4282610	-3.7154100
H	-1.3692410	-4.4598490	-2.2677130
H	-2.8590340	-4.3809840	-3.2261210
C	-3.3043980	-3.1487470	-0.7631310
C	-3.3972130	-1.6723900	-2.8350000
H	-3.5716080	-2.3302910	-0.0895840
H	-4.2140360	-3.6554180	-1.0990510
H	-2.6950800	-3.8642730	-0.2033160
H	-4.2765980	-2.2091650	-3.2017440
H	-3.7275560	-0.8264880	-2.2288500
H	-2.8351910	-1.2962400	-3.6948990
C	-0.5290750	-1.2776350	-1.0206450
N	-1.3871050	-1.8912330	-1.5116330
C	3.8234340	-4.7465130	-1.2478500
C	4.0496980	-3.6893100	-0.1542480
H	2.8697470	-5.2615870	-1.1033790
H	3.8287720	-4.2890870	-2.2409450
H	4.6267170	-5.4869870	-1.2036980
C	5.3763220	-2.9354650	-0.3658990

C	3.9856120	-4.3171470	1.2501570
H	5.4858080	-2.1197150	0.3541020
H	6.2094230	-3.6324000	-0.2378550
H	5.4297170	-2.5187630	-1.3756060
H	4.7812680	-5.0610100	1.3476310
H	4.1245270	-3.5561250	2.0220850
H	3.0245420	-4.8120600	1.4138600
C	2.1958870	-1.8478900	-0.2155650
N	2.9776620	-2.7127940	-0.2431920
O	-0.3625050	2.4852280	-1.3708200
O	0.3713470	1.9869960	-0.2187200
O	4.7425510	0.7711450	1.3363080
C	3.7445120	0.6914200	0.6130580
C	3.8879780	0.7869950	-0.8846630
C	3.6495200	1.8571710	-1.6631290
C	3.1372400	3.1832950	-1.2830880
C	3.3235830	3.7420270	-0.0062150
C	2.8024090	4.9977180	0.3000790
C	2.0919840	5.7260590	-0.6566730
C	1.9224850	5.1965060	-1.9396570
C	2.4508820	3.9423460	-2.2502080
H	3.8550080	1.7422670	-2.7276780
H	3.8942780	3.2007370	0.7399620
H	2.9553300	5.4109190	1.2928190
H	1.6879680	6.7040700	-0.4118250
H	1.3951220	5.7656770	-2.7007000
H	2.3251760	3.5359350	-3.2510550
N	2.4576010	0.5461790	1.0513580
O	2.2940520	0.5613250	2.4327040
C	2.7222280	-0.6417000	3.0758200
H	2.1126940	-1.4901150	2.7415330
H	2.5454930	-0.4746710	4.1408100
H	3.7870900	-0.8180760	2.9004340
H	4.3404940	-0.0854060	-1.3515490
H	0.1340830	3.3097830	-1.5134460
O	-3.0740420	-0.7439850	1.7299790
C	-2.4168110	0.1023130	1.0983260
C	-2.9765780	0.9538520	0.0062070
C	-4.2535380	1.2211140	-0.3613060
C	-5.5951760	0.8376850	0.1066740
C	-5.8785770	0.0072940	1.2106900
C	-7.1981570	-0.2696800	1.5636290
C	-8.2651230	0.2627640	0.8356270
C	-8.0023810	1.0870760	-0.2602770

C	-6.6859380	1.3694830	-0.6145700
H	-4.3158660	1.9119270	-1.2040640
H	-5.0491670	-0.4144630	1.7660020
H	-7.3943020	-0.9106800	2.4192690
H	-9.2899900	0.0394970	1.1197410
H	-8.8206230	1.5119030	-0.8354910
H	-6.4897790	2.0183120	-1.4653190
N	-1.0950020	0.4038170	1.3228460
O	-0.5895440	-0.3597950	2.4232560
C	-0.7554900	0.3745180	3.6280700
H	-0.2270500	1.3347300	3.5831050
H	-0.3178760	-0.2439310	4.4181430
H	-1.8177850	0.5364790	3.8466080
H	-2.2271170	1.4829950	-0.5756780
H	-0.3400260	1.7187260	0.4444640

Table 61. Atom coordinates and absolute energy of TS5b-z (Energy=−1962. 787736a.u.)

Atom	X	Y	Z
]Pd	-0.2183890	0.2268430	0.2806270
O	-0.5914200	-1.5159500	1.6934520
C	1.1411950	0.7056090	1.6616700
C	-0.2679490	2.0190070	-0.4777620
C	2.8648010	0.9156450	3.5762630
C	-0.5015270	4.3959820	-1.5410560
C	-1.6214810	4.2979910	-2.5926150
H	-1.7678580	5.2781350	-3.0550300
H	-1.3601550	3.5804860	-3.3749660
H	-2.5618040	3.9845750	-2.1319250
C	0.8388170	4.7886980	-2.1876350
H	0.7426740	5.7779990	-2.6435780
H	1.6367440	4.8268040	-1.4411180
H	1.1220920	4.0740550	-2.9648960
C	-0.8828320	5.3705620	-0.4120840
H	-1.0166030	6.3719650	-0.8306420
H	-1.8168600	5.0650010	0.0664120
H	-0.0976690	5.4138210	0.3475180
C	2.8909900	-0.5377040	4.0849490
H	3.0638720	-1.2157020	3.2462850
H	3.6963660	-0.6455020	4.8179090
H	1.9435370	-0.7980760	4.5651530
C	4.1895130	1.2743010	2.8804970
H	4.1563810	2.2904680	2.4752910

H	5.0017820	1.2227570	3.6116530
H	4.3912210	0.5690600	2.0719620
C	2.5248250	1.9093060	4.6973070
H	1.5629450	1.6663530	5.1573840
H	3.2986790	1.8614190	5.4685310
H	2.4811720	2.9341160	4.3164040
N	1.8149350	0.9865070	2.5696130
N	-0.3413670	3.0810210	-0.9509550
O	-1.9205990	-2.1034760	1.6244070
H	-2.4548080	-1.2969570	1.4085320
C	2.3851410	-1.9579450	-0.0671480
O	0.7432980	-2.9219850	-1.3777400
C	-0.2595330	-3.8598380	-1.0176080
H	-1.1539050	-3.3609930	-0.6272700
H	-0.5157960	-4.3949290	-1.9364160
H	0.1087610	-4.5754330	-0.2681490
N	1.0525890	-2.0951820	-0.2517260
H	-0.0294780	-2.0460370	1.0245380
O	2.8207760	-1.1355050	0.7816610
N	-1.6964230	-0.2583570	-1.0917430
C	-2.9721730	-0.3030950	-0.6442810
O	-3.1840350	0.0590210	0.5475200
O	-1.4088490	-1.0383170	-2.2196800
C	-0.4619560	-0.4016010	-3.0654700
H	0.4912860	-0.2624770	-2.5429480
H	-0.3114300	-1.0899770	-3.8989250
H	-0.8389610	0.5614770	-3.4359710
C	-4.0149040	-0.7340660	-1.5984000
C	-5.3515570	-0.9095970	-1.4521960
H	-3.6230600	-0.9541890	-2.5845280
H	-5.8259850	-1.2456150	-2.3753450
C	4.5866420	-2.6742120	-1.2155980
C	3.3020360	-2.8490440	-0.8370800
H	5.0242410	-3.5448880	-1.7060410
H	2.8521900	-3.7972070	-1.1127470
C	-7.6515350	-1.2051100	-0.6813040
C	-8.6771720	-1.1362820	0.2565570
C	-8.4177400	-0.6323920	1.5327280
C	-7.1280520	-0.2009550	1.8523550
C	-6.0976360	-0.2699060	0.9171850
C	-6.3398250	-0.7815210	-0.3741190
H	-7.8607790	-1.5983770	-1.6733240
H	-9.6756230	-1.4735480	-0.0072630
H	-9.2137980	-0.5746080	2.2700000

H	-6.9201960	0.1951280	2.8426930
H	-5.0983850	0.0664300	1.1618660
C	7.8112210	-0.7920850	-1.6367620
C	7.4809660	0.5007810	-1.2289170
C	6.1793230	0.7691650	-0.7952850
C	5.2151320	-0.2357740	-0.7599210
C	5.5311280	-1.5472910	-1.1682360
C	6.8458070	-1.7964240	-1.6111690
H	8.8173700	-1.0182280	-1.9791540
H	8.2274080	1.2901470	-1.2492510
H	5.9131620	1.7743330	-0.4773800
H	4.2170110	-0.0292160	-0.3955630
H	7.1086330	-2.7988200	-1.9410240

Table 62. Atom coordinates and absolute energy of TS5c-z (Energy=-1962.798412a.u.)

Atom	X	Y	Z
Pd	0.3942140	0.8848870	0.2476970
O	0.1968300	-1.4365680	-1.6349370
O	-0.2564330	-1.1992390	-0.2676240
C	-1.0160090	1.6398030	-0.9683800
C	1.6698510	2.3421240	0.0241960
C	-3.0987170	2.0290540	-2.4839380
C	3.5971450	4.0667170	-0.3445410
C	3.3540060	5.3292970	0.5012100
H	4.1767570	6.0332460	0.3476950
H	2.4202260	5.8192610	0.2118150
H	3.3036330	5.0817670	1.5649570
C	3.6285670	4.4038020	-1.8464300
H	4.4576940	5.0884860	-2.0465050
H	3.7709010	3.4996400	-2.4439700
H	2.6978290	4.8862090	-2.1576310
C	4.8862920	3.3448320	0.0888730
H	5.7432720	4.0046450	-0.0746180
H	4.8461380	3.0814740	1.1490660
H	5.0312280	2.4294060	-0.4901880
C	-3.3903680	0.6259080	-3.0474340
H	-3.5062020	-0.0878930	-2.2286620
H	-4.3125570	0.6632390	-3.6351370
H	-2.5751680	0.2913670	-3.6949510
C	-4.2355730	2.4955790	-1.5569690
H	-4.0055400	3.4677520	-1.1109710
H	-5.1547170	2.5921040	-2.1420540

H	-4.4037810	1.7669520	-0.7605890
C	-2.8308610	3.0497170	-3.6019620
H	-1.9975340	2.7280270	-4.2328270
H	-3.7228280	3.1390060	-4.2281470
H	-2.5986790	4.0359980	-3.1891290
N	-1.8949330	1.9198970	-1.6771250
N	2.4931420	3.1565380	-0.1205140
N	1.8172040	-0.0499540	1.3936030
O	1.3943800	-0.4201190	2.6765320
C	2.6028830	-0.9548570	0.7349350
O	2.7178970	-0.8518710	-0.5102300
H	1.1613370	-1.3606350	-1.4539570
C	1.6038100	0.6484680	3.5917430
H	1.0663180	1.5481510	3.2717440
H	1.1925970	0.3046500	4.5430310
H	2.6725840	0.8753790	3.7001400
H	-1.3037200	-1.0940830	-0.3169240
N	-1.7115040	0.4280740	1.5895450
C	-2.7823280	-0.2074960	1.1203700
O	-2.6903820	-0.7889680	-0.0273020
O	-1.8727810	0.9585550	2.9073790
C	-1.8138310	2.3703270	2.8550390
H	-2.6674140	2.7966100	2.3066470
H	-1.8381840	2.7193410	3.8920700
H	-0.8852230	2.7132120	2.3745330
C	3.3102570	-1.9550600	1.5660400
C	4.2738600	-2.8573790	1.2582840
H	2.9804000	-1.9613870	2.5978030
H	4.5617810	-3.4623520	2.1192200
C	5.0529480	-3.2342950	0.0721290
C	5.9678950	-4.2963880	0.2422390
C	4.9781970	-2.6269820	-1.1981270
C	6.7714250	-4.7408280	-0.8033960
H	6.0429620	-4.7774320	1.2145760
C	5.7860740	-3.0736300	-2.2416420
H	4.2759850	-1.8163720	-1.3434210
C	6.6833870	-4.1280190	-2.0548810
H	7.4638680	-5.5623450	-0.6424380
H	5.7110810	-2.5939940	-3.2140270
H	7.3071410	-4.4696660	-2.8763820
C	-4.0565690	-0.1900340	1.8750980
C	-5.2515070	-0.7859940	1.6467680
H	-4.0135520	0.4407150	2.7554180
H	-6.0115680	-0.4956100	2.3741950

C	-5.7980670	-1.7438180	0.6729150
C	-7.1976080	-1.9242340	0.6901120
C	-5.0462540	-2.5217090	-0.2305130
C	-7.8280800	-2.8210980	-0.1681170
H	-7.7951430	-1.3466720	1.3918230
C	-5.6791490	-3.4259710	-1.0810020
H	-3.9726250	-2.3918960	-0.2575410
C	-7.0679160	-3.5791650	-1.0606770
H	-8.9083250	-2.9338260	-0.1347740
H	-5.0790030	-4.0190310	-1.7659630
H	-7.5518380	-4.2864680	-1.7287560

Table 63. Atom coordinates and absolute energy of IM6a-z (Energy=−1811. 298544a.u.)

Atom	X	Y	Z
Pd	0.1186040	-1.0733930	-0.4374760
C	3.7627420	-3.1621340	3.1071380
C	3.8717180	-2.2197780	1.8980780
H	3.1922140	-2.7003230	3.9183550
H	3.2795640	-4.1029370	2.8285410
H	4.7668740	-3.3873400	3.4767990
C	4.6383910	-2.8673150	0.7294360
C	4.4989420	-0.8687960	2.2864900
H	4.6185660	-2.2108620	-0.1443380
H	5.6738420	-3.0382560	1.0397610
H	4.1919720	-3.8285240	0.4597860
H	5.5175470	-1.0404690	2.6463110
H	4.5390510	-0.2051430	1.4199780
H	3.9278000	-0.3839510	3.0836350
C	1.5581750	-1.6610050	0.8374150
N	2.5265800	-1.9443260	1.4163060
C	-3.7997030	-0.6035180	3.0942810
C	-3.6244650	-1.8136000	2.1592980
H	-2.9503840	-0.5116730	3.7771400
H	-3.8973730	0.3209520	2.5203510
H	-4.7083240	-0.7404960	3.6873360
C	-4.7881800	-1.9121820	1.1560240
C	-3.4635190	-3.1186970	2.9589280
H	-4.6419470	-2.7519700	0.4712350
H	-5.7199940	-2.0714850	1.7061350
H	-4.8822730	-0.9929000	0.5727440
H	-4.3703730	-3.2964600	3.5434980
H	-3.3100890	-3.9704070	2.2905960

H	-2.6154480	-3.0552750	3.6464070
C	-1.4624720	-1.4117010	0.7437110
N	-2.4043550	-1.6116910	1.3989790
O	-3.1849940	0.5230570	-2.5563990
C	-2.2119830	0.4886160	-1.7898820
C	-1.9761420	1.4573700	-0.6748950
C	-2.8374640	2.1926460	0.0643600
C	-4.3020010	2.3070060	0.1396010
C	-5.2130220	1.7751460	-0.7973160
C	-6.5859290	1.9283630	-0.6082490
C	-7.0874050	2.6124750	0.5022880
C	-6.1985840	3.1566950	1.4314690
C	-4.8259640	3.0083170	1.2473620
H	-2.3464940	2.8179070	0.8114920
H	-4.8195570	1.2704060	-1.6726960
H	-7.2713940	1.5182450	-1.3451560
H	-8.1591730	2.7301280	0.6364100
H	-6.5728580	3.7015880	2.2937950
H	-4.1392330	3.4417700	1.9710660
N	-1.1782500	-0.4007410	-1.9099710
O	-1.2780630	-1.2842710	-2.9919720
C	-2.2821640	-2.2839130	-2.8036590
H	-2.0649780	-2.8898130	-1.9120060
H	-2.2268330	-2.9192200	-3.6914530
H	-3.2742230	-1.8321210	-2.7293380
H	-0.9257310	1.5838530	-0.4231110
O	3.9095000	-0.1422650	-1.3305880
C	2.6991060	0.0990840	-1.4263910
C	2.0619880	1.4382990	-1.2861270
C	2.5156750	2.6026840	-0.7658220
C	3.7705310	3.0479850	-0.1429260
C	5.0079170	2.3776090	-0.2291730
C	6.1394280	2.9041180	0.3924780
C	6.0727100	4.1010610	1.1095960
C	4.8569380	4.7829730	1.1949320
C	3.7263020	4.2655590	0.5689040
H	1.7741320	3.4024510	-0.7894910
H	5.0567550	1.4523780	-0.7903430
H	7.0858700	2.3764750	0.3078040
H	6.9607570	4.5040480	1.5888130
H	4.7917520	5.7199240	1.7412150
H	2.7850930	4.8067490	0.6311400
N	1.7374400	-0.8444230	-1.7530470
O	2.3083580	-2.1332660	-1.9071270

C	2.0507550	-2.5834500	-3.2378670
H	0.9857120	-2.5026380	-3.4759540
H	2.3725160	-3.6288480	-3.2637260
H	2.6309090	-2.0039310	-3.9663330
H	1.0477350	1.4569900	-1.6765650

Table 64. Atom coordinates and absolute energy of IM6b-z (Energy=−1811. 300777a.u.)

Atom	X	Y	Z
Pd	0.0000260	0.3619420	-0.0000480
C	1.3210370	1.7294930	0.5979630
C	-1.3210520	1.7293590	-0.5982040
C	3.2926780	3.2593300	1.2847360
C	-3.2929410	3.2588760	-1.2848840
C	-4.1808430	2.2939520	-2.0922300
H	-5.1387400	2.7781350	-2.3050030
H	-3.7058290	2.0343360	-3.0428790
H	-4.3520840	1.3793520	-1.5198560
C	-2.9344190	4.5149310	-2.0936910
H	-3.8497960	5.0574510	-2.3460940
H	-2.2852940	5.1814320	-1.5183100
H	-2.4242770	4.2485140	-3.0236750
C	-3.9582650	3.6213200	0.0554460
H	-4.8970850	4.1483100	-0.1387660
H	-4.1704140	2.7144640	0.6260910
H	-3.3114190	4.2730420	0.6500200
C	4.1808930	2.2943760	2.0917110
H	4.3522910	1.3799730	1.5190690
H	5.1386890	2.7787280	2.3045500
H	3.7060160	2.0343630	3.0423200
C	3.9578760	3.6225030	-0.0554620
H	3.3108220	4.2742580	-0.6497750
H	4.8965390	4.1497020	0.1389350
H	4.1703010	2.7159400	-0.6264720
C	2.9337810	4.5149720	2.0940250
H	2.4237200	4.2480380	3.0239040
H	3.8489990	5.0576630	2.3466370
H	2.2844570	5.1815010	1.5189010
N	2.0649590	2.5468750	0.9709580
N	-2.0649840	2.5466730	-0.9713510
C	2.6304440	-1.0583190	0.4412580
O	0.7847790	-2.2741340	1.2460300
C	0.1049250	-2.0079710	2.4675280

H	-0.7365280	-1.3225370	2.3062490
H	-0.2768880	-2.9738910	2.8075300
H	0.7830890	-1.5860990	3.2217370
N	1.2990880	-1.0855950	0.7030260
O	3.1117460	-0.0695320	-0.1632650
N	-1.2989880	-1.0857080	-0.7030070
C	-2.6303420	-1.0584770	-0.4411760
O	-3.1116650	-0.0696220	0.1632140
O	-0.7846180	-2.2743010	-1.2458410
C	-0.1047510	-2.0082410	-2.4673520
H	0.7366940	-1.3227870	-2.3061160
H	0.2770720	-2.9741890	-2.8072640
H	-0.7829060	-1.5864390	-3.2216060
C	-3.4446510	-2.1919940	-0.9497780
C	-4.7435290	-2.5156980	-0.7470510
H	-2.8935350	-2.8611960	-1.5997510
H	-5.0476650	-3.3976250	-1.3128080
C	4.7436560	-2.5154730	0.7473540
C	3.4447910	-2.1917170	0.9500700
H	5.0478060	-3.3972930	1.3132710
H	2.8937040	-2.8607930	1.6002020
C	-7.1059850	-2.6371650	-0.1197720
C	-8.2326550	-2.2536250	0.6024600
C	-8.1390670	-1.2228470	1.5392720
C	-6.9110520	-0.5865350	1.7379600
C	-5.7832010	-0.9616580	1.0107250
C	-5.8591740	-2.0006700	0.0606810
H	-7.1845940	-3.4478830	-0.8403580
H	-9.1792140	-2.7611790	0.4384120
H	-9.0128790	-0.9206460	2.1101330
H	-6.8298330	0.2136550	2.4692070
H	-4.8351660	-0.4587810	1.1525490
C	8.2326920	-2.2538020	-0.6024680
C	8.1391120	-1.2231000	-1.5393660
C	6.9111320	-0.5867100	-1.7380110
C	5.7833070	-0.9616820	-1.0106550
C	5.8592720	-2.0006150	-0.0605270
C	7.1060510	-2.6371870	0.1198890
H	9.1792230	-2.7614170	-0.4384490
H	9.0129030	-0.9210180	-2.1103200
H	6.8299160	0.2134270	-2.4693170
H	4.8352980	-0.4587420	-1.1524440
H	7.1846560	-3.4478430	0.8405460

Table 65. Atom coordinates and absolute energy of IM6c-z(Energy=−1811. 298485a.u.)

Atom	X	Y	Z
Pd	0.0361180	0.6317040	0.9571820
C	-1.3729380	1.8859260	0.3316810
C	1.5219540	1.8376170	0.4067250
C	-3.4035310	3.0518340	-0.7817910
C	3.5612230	3.2081530	-0.3846680
C	3.5514910	4.7203870	-0.1153920
H	4.4808930	5.1621430	-0.4858790
H	2.7126260	5.2048330	-0.6236950
H	3.4750900	4.9265400	0.9560420
C	3.6139150	2.9032910	-1.8928740
H	4.5466670	3.2961290	-2.3084730
H	3.5754350	1.8245060	-2.0574620
H	2.7760300	3.3733020	-2.4161660
C	4.7148490	2.5056770	0.3547240
H	5.6695220	2.8791520	-0.0280460
H	4.6687820	2.7106120	1.4283850
H	4.6558010	1.4268370	0.1950170
C	-3.2424110	2.6723810	-2.2654370
H	-3.1293690	1.5905170	-2.3631610
H	-4.1309670	2.9923440	-2.8176440
H	-2.3670760	3.1626060	-2.7012830
C	-4.6163240	2.3325360	-0.1643260
H	-4.7154090	2.5773570	0.8972650
H	-5.5262980	2.6536470	-0.6797230
H	-4.5054870	1.2516080	-0.2742100
C	-3.4876750	4.5738360	-0.5911470
H	-2.6048460	5.0708590	-1.0035180
H	-4.3719200	4.9549120	-1.1095610
H	-3.5705330	4.8325300	0.4683140
N	-2.2202410	2.5656180	-0.0911590
N	2.3201450	2.6415330	0.1207040
N	1.4663050	-0.7767980	1.4709330
O	1.1701130	-1.7437390	2.4433840
C	2.5390000	-1.0292220	0.6716850
O	2.7867980	-0.2624710	-0.2874590
C	1.3947380	-1.2154620	3.7445200
H	0.8130950	-0.3000150	3.9020300
H	1.0544000	-1.9853780	4.4413300
H	2.4601690	-1.0034860	3.9100670
N	-1.5271460	-0.6080630	1.5256530

C	-2.4706710	-1.0167210	0.6373310
O	-2.4546990	-0.5423450	-0.5204840
O	-1.5980880	-1.1030640	2.8410230
C	-2.2570330	-0.1643130	3.6860120
H	-3.3028670	-0.0186180	3.3849490
H	-2.2210250	-0.5885170	4.6935220
H	-1.7396210	0.8044230	3.6763680
C	3.3972220	-2.1877060	1.0325110
C	4.5216830	-2.6669950	0.4513880
H	3.0717660	-2.7105430	1.9232750
H	4.9586780	-3.4995470	1.0049920
C	5.3178100	-2.3553720	-0.7457710
C	6.5961460	-2.9481590	-0.8202650
C	4.8947980	-1.5658320	-1.8338940
C	7.4318980	-2.7442440	-1.9149540
H	6.9343760	-3.5768000	0.0001610
C	5.7280480	-1.3756980	-2.9346020
H	3.9163620	-1.1066140	-1.7912290
C	6.9990640	-1.9540640	-2.9813730
H	8.4141020	-3.2080890	-1.9396810
H	5.3789880	-0.7704750	-3.7673030
H	7.6422350	-1.7971580	-3.8430210
C	-3.4701100	-2.0052410	1.1248240
C	-4.6180550	-2.4542800	0.5664950
H	-3.2381080	-2.4050230	2.1054550
H	-5.1590820	-3.1485850	1.2114950
C	-5.3441960	-2.2259980	-0.6925750
C	-6.6923280	-2.6419230	-0.7248590
C	-4.7954740	-1.6751160	-1.8682770
C	-7.4739130	-2.4899080	-1.8667440
H	-7.1285510	-3.0876980	0.1661090
C	-5.5782530	-1.5366710	-3.0136230
H	-3.7587150	-1.3637610	-1.8564430
C	-6.9174080	-1.9341880	-3.0206520
H	-8.5113340	-2.8128080	-1.8593880
H	-5.1339480	-1.1186690	-3.9132870
H	-7.5188380	-1.8217130	-3.9186570

Table 66. Atom coordinates and absolute energy of TS7-z (Energy=-1811.270262a.u.)

Atom	X	Y	Z
Pd	-0.1032530	0.6563840	-0.1945120
C	1.3457760	1.5960010	0.7356020

C	-1.4813110	1.9535250	-0.6484140
C	3.4228220	2.5748910	1.9214870
C	-2.1943210	4.3192430	-0.6427890
C	-3.4041660	4.6321460	0.2547540
H	-3.4625190	5.7096850	0.4383250
H	-4.3328020	4.3079590	-0.2226010
H	-3.3159100	4.1200340	1.2172890
C	-2.3460240	5.0116060	-2.0079640
H	-2.3785550	6.0975100	-1.8743410
H	-1.5033830	4.7683790	-2.6618970
H	-3.2672980	4.6915460	-2.5019410
C	-0.8847250	4.7451500	0.0405650
H	-0.8885280	5.8254640	0.2180030
H	-0.7633350	4.2390090	1.0026790
H	-0.0214880	4.5029840	-0.5864920
C	3.9346220	1.3531690	2.7070360
H	4.0176600	0.4918890	2.0401840
H	4.9161740	1.5834000	3.1325320
H	3.2518770	1.1062700	3.5254750
C	4.3728720	2.9148460	0.7586900
H	3.9955530	3.7642130	0.1816100
H	5.3556150	3.1782030	1.1610980
H	4.4749500	2.0520590	0.0973590
C	3.1980100	3.7873750	2.8376470
H	2.4936160	3.5469050	3.6390570
H	4.1486890	4.0816910	3.2913090
H	2.8065670	4.6390540	2.2735490
N	2.1473400	2.2004910	1.3320620
N	-2.2257120	2.8699890	-0.8999500
C	2.2779100	-1.3352660	-0.1217600
O	0.1319790	-2.3187130	-0.2349520
C	-0.5019140	-2.6542120	1.0007250
H	-1.1370250	-1.8334660	1.3519460
H	-1.1233840	-3.5284790	0.7865790
H	0.2415720	-2.9075920	1.7680980
N	0.9303610	-1.1576230	-0.0733570
O	3.0270260	-0.3315980	-0.0917770
N	-1.9283180	0.2720430	-1.2465700
C	-3.0366640	-0.2577740	-0.5625600
O	-2.9812290	-0.2487060	0.6684550
O	-1.9531760	0.2805900	-2.6476790
C	-1.1221700	-0.7673450	-3.1683610
H	-1.5062740	-1.7528010	-2.8849600
H	-1.1556680	-0.6426790	-4.2530930

H	-0.0942370	-0.6624660	-2.8053030
C	4.0390600	-3.2278120	-0.2500840
C	2.7810660	-2.7346410	-0.1655260
H	4.0668640	-4.3174600	-0.1976580
H	1.9964210	-3.4785070	-0.0975790
C	8.0796980	-1.8563400	-0.7191390
C	7.7872050	-3.1839000	-0.4013970
C	6.4620770	-3.5854450	-0.2556690
C	5.3933580	-2.6760160	-0.4048920
C	5.7070880	-1.3404290	-0.7277560
C	7.0338830	-0.9447330	-0.8848840
H	9.1111710	-1.5369350	-0.8409020
H	8.5886750	-3.9064020	-0.2742010
H	6.2418490	-4.6239170	-0.0195400
H	4.8948990	-0.6341260	-0.8403900
H	7.2541330	0.0886420	-1.1404940
C	-4.1537810	-0.7267920	-1.3992920
C	-5.2587690	-1.4467170	-1.0780050
H	-4.0516340	-0.4564490	-2.4436660
H	-5.8925800	-1.6416350	-1.9440220
C	-7.0575820	-3.3589160	2.3063550
C	-7.5729000	-3.5109450	1.0172270
C	-6.9590100	-2.8670750	-0.0520900
C	-5.8133310	-2.0611730	0.1313230
C	-5.3104750	-1.9137530	1.4409250
C	-5.9302780	-2.5589620	2.5086270
H	-7.5336580	-3.8564070	3.1467400
H	-8.4509290	-4.1272570	0.8468940
H	-7.3646860	-2.9885390	-1.0535210
H	-4.4435570	-1.2866940	1.6009270
H	-5.5298810	-2.4318510	3.5105860

Table 67. Atom coordinates and absolute energy of IM8-z (Energy=-1811.278066a.u.)

Atom	X	Y	Z
Pd	-0.1466600	0.7405650	-0.2488920
C	1.3026620	1.7208230	0.6172340
C	-1.6616700	1.9274050	-0.6852430
C	3.4704410	2.6353070	1.6954260
C	-2.0760460	4.3103860	-0.3846710
C	-3.1681160	4.6875170	0.6352900
H	-3.0619550	5.7358640	0.9329660
H	-4.1627090	4.5448510	0.2037980

H	-3.0909400	4.0639850	1.5313130
C	-2.2192950	5.1775120	-1.6504290
H	-2.0940600	6.2360980	-1.4002700
H	-1.4618550	4.9063150	-2.3925450
H	-3.2051780	5.0380330	-2.1023870
C	-0.6846850	4.5018060	0.2342720
H	-0.5443470	5.5533740	0.5059460
H	-0.5655820	3.8966610	1.1365590
H	0.1042950	4.2221610	-0.4692390
C	3.9643890	1.4226570	2.5058770
H	3.9876940	0.5358070	1.8685430
H	4.9698490	1.6278500	2.8860740
H	3.3043890	1.2336100	3.3577510
C	4.3882640	2.8985460	0.4874730
H	4.0264250	3.7478430	-0.0996840
H	5.3971220	3.1281560	0.8435070
H	4.4234710	2.0139360	-0.1517540
C	3.3241600	3.8858950	2.5757580
H	2.6434470	3.6985410	3.4111940
H	4.3016130	4.1600660	2.9828950
H	2.9411350	4.7316250	1.9972900
N	2.1625930	2.2902980	1.1643510
N	-2.3803830	2.9331490	-0.8057510
C	2.2438370	-1.3185660	-0.2881880
O	0.0552850	-2.2277030	-0.3608510
C	-0.4861110	-2.6103930	0.9018930
H	-1.0525710	-1.7870880	1.3533180
H	-1.1608250	-3.4476050	0.6990040
H	0.3056580	-2.9328820	1.5909030
N	0.9056130	-1.0923720	-0.1992420
O	3.0274400	-0.3425330	-0.2349960
N	-2.1001640	0.5796800	-1.2128630
C	-3.1799890	-0.0745560	-0.5001770
O	-3.0898320	-0.0846400	0.7174730
O	-2.1719620	0.5838080	-2.6237940
C	-1.3502130	-0.4600850	-3.1712610
H	-1.6955490	-1.4476060	-2.8492950
H	-1.4542610	-0.3535670	-4.2530680
H	-0.3047570	-0.3258130	-2.8742000
C	3.9226850	-3.2909440	-0.4602760
C	2.6891430	-2.7330520	-0.4272080
H	3.8878630	-4.3796450	-0.5289410
H	1.8663100	-3.4347800	-0.4959510
C	8.0553220	-2.1367300	-0.3549080

C	7.6637940	-3.4731220	-0.2536710
C	6.3119830	-3.8035840	-0.2927100
C	5.3129930	-2.8147140	-0.4197850
C	5.7262550	-1.4716490	-0.5256530
C	7.0807320	-1.1454640	-0.4947850
H	9.1088680	-1.8715760	-0.3301290
H	8.4097340	-4.2563310	-0.1498870
H	6.0149380	-4.8473890	-0.2209610
H	4.9628440	-0.7106810	-0.6275570
H	7.3794020	-0.1038790	-0.5827670
C	-4.2461640	-0.6224590	-1.3391060
C	-5.2633640	-1.4672650	-1.0206470
H	-4.1980200	-0.3007420	-2.3719050
H	-5.8944810	-1.6936590	-1.8805830
C	-6.7523750	-3.7035960	2.3086570
C	-7.2729400	-3.8665030	1.0227120
C	-6.7622810	-3.1129660	-0.0282160
C	-5.7152350	-2.1843850	0.1709210
C	-5.2074230	-2.0274180	1.4783250
C	-5.7246410	-2.7829200	2.5276410
H	-7.1490020	-4.2862890	3.1352370
H	-8.0749930	-4.5758460	0.8415150
H	-7.1708160	-3.2426320	-1.0272710
H	-4.4208850	-1.3072820	1.6562690
H	-5.3236490	-2.6470950	3.5279280

Table 68. Atom coordinates and absolute energy of IM9-z (Energy=-2061.748697a.u.)

Atom	X	Y	Z
Pd	-0.3775230	0.0541710	-0.0242240
C	-1.5016660	-1.5629370	-0.3922080
C	0.8759870	1.5829460	0.3299360
N	-2.1815340	-2.4806190	-0.6277700
C	-3.3337360	-3.3371560	-0.8431550
N	1.6640080	2.4187790	0.5165710
C	2.7534660	3.3390530	0.7748480
C	-4.2462390	-2.6235760	-1.8580010
C	-2.8417970	-4.6931650	-1.3721140
C	-4.0427390	-3.4873740	0.5155480
H	-4.3397200	-2.5064930	0.8928620
H	-4.9349400	-4.1080130	0.3900220
H	-3.3866050	-3.9672830	1.2475520
H	-3.7436200	-2.5206550	-2.8244730

H	-5.1564720	-3.2133180	-2.0031170
H	-4.5096060	-1.6306500	-1.4860610
H	-2.1698870	-5.1736500	-0.6552590
H	-3.6999160	-5.3506510	-1.5381720
H	-2.3100700	-4.5733770	-2.3203200
C	3.3816050	2.9338840	2.1209690
C	2.1749190	4.7629860	0.8204780
C	3.7695260	3.1786640	-0.3712140
H	1.4278920	4.8556940	1.6134150
H	2.9824830	5.4733530	1.0191090
H	1.7054650	5.0259200	-0.1313470
H	3.3106580	3.4152070	-1.3355230
H	4.6050360	3.8656170	-0.2081770
H	4.1547750	2.1566760	-0.3973070
H	3.7080750	1.8919510	2.0832190
H	4.2434400	3.5769340	2.3229450
H	2.6630200	3.0520680	2.9368110
C	1.1091480	-1.1207430	0.7999310
N	1.3321430	-1.5236150	1.9716040
N	2.1362610	-1.4394260	-0.1733430
O	1.7019590	-2.3191000	-1.1793230
C	1.5600000	-1.6445320	-2.4382900
H	0.8350560	-0.8278430	-2.3622930
H	1.1913030	-2.4076820	-3.1280580
H	2.5256680	-1.2633920	-2.7895220
C	3.4987950	-1.2309710	0.0103500
O	3.8803440	-0.3816170	0.8195850
C	0.5468820	-1.2729270	3.1898030
C	1.0572110	0.0464810	3.8026940
H	0.6139120	0.2015690	4.7922800
H	0.7890160	0.8967130	3.1692340
H	2.1459090	0.0223670	3.9059200
C	-0.9781100	-1.2172160	2.9899950
H	-1.3397740	-2.1294450	2.5058150
H	-1.2931960	-0.3645740	2.3819140
H	-1.4727600	-1.1344630	3.9639580
C	0.8865910	-2.4402660	4.1388970
H	0.3921640	-2.3108180	5.1075940
H	1.9668230	-2.4993140	4.2979840
H	0.5571890	-3.3917250	3.7088760
O	-1.4776240	2.5781640	-1.4405610
C	-1.0869600	2.3638000	-2.7875080
H	-1.9273010	2.0119590	-3.4016660
H	-0.2685550	1.6330080	-2.8523630

H	-0.7390800	3.3313600	-3.1629260
O	-3.6047200	0.1917610	0.0219940
N	-1.8819140	1.3429120	-0.8523880
C	-3.2072440	1.2140170	-0.5875730
C	4.3729760	-2.0727210	-0.8420950
C	5.6683940	-1.9127800	-1.2049260
H	3.8758080	-2.9497640	-1.2412490
H	6.0234150	-2.7065060	-1.8635510
C	7.7627150	0.9570150	0.1854230
C	8.8491550	0.9148160	-0.6913590
C	8.8793800	-0.0465400	-1.7040690
C	7.8290270	-0.9502880	-1.8317510
C	6.7126170	-0.9080070	-0.9689000
C	6.7030210	0.0610170	0.0548160
H	7.7430050	1.6909720	0.9865470
H	9.6703880	1.6174580	-0.5806970
H	9.7227550	-0.0966880	-2.3868170
H	7.8623150	-1.7022600	-2.6164410
H	5.8651910	0.0831700	0.7392310
C	-5.4642800	2.4169880	-1.0075940
C	-4.1183600	2.2861670	-1.0754030
H	-5.8255190	3.3109020	-1.5190840
H	-3.6033240	3.0884490	-1.5903470
C	-9.0173690	1.4611970	-0.2746220
C	-7.8805290	2.0859930	-0.7801120
C	-6.5828140	1.6634410	-0.4205560
C	-6.4683570	0.5927220	0.4889790
C	-7.6088300	-0.0230360	1.0013200
C	-8.8855620	0.3996720	0.6226650
H	-10.0031360	1.8058780	-0.5748660
H	-7.9915030	2.9191990	-1.4703230
H	-5.4758740	0.2624950	0.7684310
H	-7.4989170	-0.8429320	1.7066570
H	-9.7682680	-0.0889260	1.0263780

Table 69. Atom coordinates and absolute energy of TS9-z (Energy=-2061.716325a.u.)

Atom	X	Y	Z
Pd	-0.5228820	0.7558760	-0.3724980
C	-0.7646230	-1.1998080	-0.7055840
C	-0.2728370	2.7038020	-0.0087970
N	-0.9174220	-2.3347850	-0.9158960
C	-1.4713920	-3.6703130	-1.0454370

N	-0.1817020	3.8445720	0.2012480
C	-0.1544500	5.2734400	0.4375050
C	-2.8180820	-3.5291630	-1.7793070
C	-0.4773790	-4.5343970	-1.8367550
C	-1.6789720	-4.2124160	0.3806140
H	-2.3570010	-3.5606160	0.9360820
H	-2.1138950	-5.2146950	0.3247840
H	-0.7276150	-4.2764370	0.9165240
H	-2.6673200	-3.1461130	-2.7928810
H	-3.2963350	-4.5108090	-1.8476920
H	-3.4699270	-2.8424150	-1.2342320
H	0.4816210	-4.6068430	-1.3159400
H	-0.8859820	-5.5423120	-1.9520800
H	-0.3023170	-4.1162300	-2.8318850
C	-0.7643190	5.5255170	1.8286580
C	-0.9991030	5.9349240	-0.6668000
C	1.3116840	5.7361290	0.3793250
H	-2.0186260	5.5410400	-0.6603390
H	-1.0345690	7.0147700	-0.4971810
H	-0.5608500	5.7519380	-1.6516780
H	1.7491600	5.5242110	-0.5997580
H	1.3563080	6.8147410	0.5547470
H	1.9111450	5.2334340	1.1426650
H	-0.1844210	5.0204200	2.6057060
H	-0.7587660	6.5995940	2.0343290
H	-1.7960940	5.1670330	1.8719690
C	1.4567000	0.4430050	-0.0250700
N	2.1543590	-0.0256770	0.9829440
N	2.4303320	0.7359810	-0.9289800
O	2.1608260	0.3864960	-2.2737850
C	2.8478560	1.2904440	-3.1343210
H	2.5052030	2.3214060	-2.9832530
H	2.6125080	0.9651680	-4.1509410
H	3.9314130	1.2441840	-2.9762130
C	3.6512230	0.0719530	0.0257200
O	4.5135740	0.8353920	0.4477980
C	1.9511210	0.0484570	2.4367490
C	2.2117320	1.4983080	2.8980270
H	2.1714450	1.5683590	3.9907510
H	1.4563480	2.1743140	2.4835030
H	3.1958890	1.8259590	2.5537020
C	0.5295430	-0.4005080	2.8128450
H	0.3437030	-1.4255800	2.4781690
H	-0.2323140	0.2447980	2.3651900

H	0.4064620	-0.3672620	3.9008610
C	2.9873200	-0.8945600	3.0749420
H	2.9017420	-0.8667190	4.1657830
H	4.0008950	-0.5960850	2.7961830
H	2.8289810	-1.9248140	2.7420850
O	-2.9423500	2.3442750	-1.3980170
C	-2.7184410	2.2745330	-2.8017370
H	-3.3653940	1.5228750	-3.2732260
H	-1.6702380	2.0326770	-3.0220860
H	-2.9580660	3.2658830	-3.1985310
O	-3.3037000	-0.7371460	0.2604250
N	-2.5750540	1.1088140	-0.7930090
C	-3.5886210	0.3235850	-0.3422230
C	3.8524340	-1.3346700	-0.4558000
C	4.9580580	-2.1065390	-0.5312770
H	2.9370880	-1.7899260	-0.8222010
H	4.7568370	-3.0919540	-0.9546120
C	8.3400130	-0.7965570	0.6679120
C	9.1413960	-1.9132340	0.4177790
C	8.5654210	-3.0591120	-0.1335870
C	7.2044970	-3.0776770	-0.4269590
C	6.3795790	-1.9600010	-0.1797350
C	6.9771370	-0.8110290	0.3766830
H	8.7809120	0.0999780	1.0960120
H	10.2028400	-1.8908060	0.6494440
H	9.1742970	-3.9363330	-0.3349990
H	6.7636660	-3.9742190	-0.8570350
H	6.3573970	0.0563830	0.5685620
C	-6.1754570	0.2039260	-0.3273370
C	-4.9802890	0.7647750	-0.6284610
H	-7.0167220	0.7680490	-0.7335760
H	-5.0332980	1.6900460	-1.1900120
C	-8.5895410	-2.3521850	0.9782380
C	-8.0232300	-1.2699910	0.3103000
C	-6.6463360	-0.9765700	0.4121460
C	-5.8554830	-1.8068590	1.2321310
C	-6.4282270	-2.8831940	1.9072240
C	-7.7907470	-3.1664230	1.7833470
H	-9.6518740	-2.5557990	0.8757700
H	-8.6538510	-0.6343840	-0.3070920
H	-4.7981920	-1.5900060	1.3161410
H	-5.8024210	-3.5078060	2.5395440
H	-8.2267130	-4.0094040	2.3125700

Table 70. Atom coordinates and absolute energy of TS9'-z (Energy=−1811. 275694a.u.)

Atom	X	Y	Z
Pd	0.7829150	-0.3350680	-0.1188020
C	1.5898400	-2.1713360	-0.0565850
N	1.8134210	-3.3177070	-0.0307910
C	1.9451810	-4.7589990	-0.0727490
C	2.7950720	-5.1171900	-1.3056820
C	0.5240410	-5.3410420	-0.1900770
C	2.6344830	-5.2170840	1.2242470
H	0.0123770	-4.9280880	-1.0629170
H	0.5825390	-6.4291360	-0.2869320
H	-0.0660990	-5.1008990	0.6983910
H	2.0476500	-4.9269400	2.0997820
H	2.7316020	-6.3064730	1.2171370
H	3.6330190	-4.7804000	1.3126970
H	3.7858280	-4.6589640	-1.2431890
H	2.9167720	-6.2028070	-1.3589050
H	2.3092340	-4.7768370	-2.2240510
C	2.2308950	0.6806390	0.9504920
N	3.4869950	0.7168440	1.0170300
N	1.5007030	1.4753720	1.8901880
O	2.2178660	2.1954270	2.8454950
C	0.2754910	2.0594100	1.5420430
O	-0.2912580	2.8642140	2.2656230
C	4.5178030	0.1010880	0.1826310
C	4.9213660	-1.2500480	0.8063820
H	5.7657340	-1.6880550	0.2622020
H	4.0913440	-1.9593700	0.7853410
H	5.2211520	-1.1083680	1.8493040
C	4.1204520	-0.0662800	-1.2979690
H	3.8132410	0.8969440	-1.7179000
H	3.2958160	-0.7690410	-1.4275870
H	4.9758980	-0.4320980	-1.8770060
C	5.7262320	1.0600320	0.2569820
H	6.5790060	0.6596300	-0.3028340
H	6.0259220	1.2116260	1.2976320
H	5.4638800	2.0364260	-0.1614980
H	-1.2542020	0.6556690	0.3045110
O	-0.8481150	-2.2991560	-2.0395200
C	-0.3081800	-1.8335150	-3.2705670
H	0.6651410	-1.3506840	-3.1152030
H	-0.9868320	-1.1253880	-3.7632810

H	-0.1841720	-2.7205490	-3.8977540
O	-2.3124320	-0.0747550	0.2421880
N	-0.9552070	-1.2101850	-1.1358860
C	-2.1783110	-1.0009280	-0.6450050
C	2.3063720	1.4475330	4.0576220
H	2.8652000	0.5171800	3.9054870
H	2.8537260	2.0923600	4.7495300
H	1.3111480	1.2330140	4.4619000
C	-0.2328360	1.5351190	0.2438590
C	-0.3629170	2.2813600	-0.8970920
H	-0.7393950	1.7239910	-1.7569010
C	-0.1016990	3.6866760	-1.2156850
C	-0.1436520	4.0509170	-2.5786840
C	0.1801510	4.6903760	-0.2640820
C	0.1126090	5.3561270	-2.9860270
H	-0.3724610	3.2895710	-3.3204310
C	0.4289800	5.9964510	-0.6766120
H	0.1702590	4.4517870	0.7916550
C	0.4024020	6.3348660	-2.0325700
H	0.0821240	5.6115140	-4.0412840
H	0.6387300	6.7587080	0.0681070
H	0.5978770	7.3573590	-2.3432760
C	-3.3215370	-1.7955570	-1.1171270
C	-4.6384150	-1.7922120	-0.7896470
H	-3.0331650	-2.5195370	-1.8691150
H	-5.1970260	-2.5345560	-1.3615130
C	-5.5307620	-1.0707780	0.1254770
C	-6.8863100	-1.4684110	0.0998680
C	-5.1658440	-0.0357030	1.0107730
C	-7.8380810	-0.8672430	0.9172460
H	-7.1900560	-2.2643080	-0.5760540
C	-6.1217000	0.5638440	1.8276330
H	-4.1346940	0.2858800	1.0458550
C	-7.4571160	0.1556240	1.7880390
H	-8.8729040	-1.1949610	0.8749480
H	-5.8179870	1.3597540	2.5017940
H	-8.1942640	0.6306730	2.4294010

Table 71. Atom coordinates and absolute energy of IM10-z (Energy=-2061.757779a.u.)

Atom	X	Y	Z
Pd	-0.4663700	1.0783770	-0.3624150
C	0.0282430	-0.8224580	-0.7641880

C	-1.0453800	2.9511320	0.0078280
N	0.3086150	-1.9302850	-0.9809250
C	0.4689450	-3.3654960	-1.1085510
N	-1.5320450	3.9893260	0.2091540
C	-2.2685150	5.2225760	0.3817890
C	-0.9009390	-3.9371310	-1.5178560
C	1.5426320	-3.6324350	-2.1768490
C	0.9144370	-3.8963530	0.2672140
H	0.1463850	-3.7002450	1.0195860
H	1.0694330	-4.9771900	0.1990340
H	1.8475040	-3.4240270	0.5859630
H	-1.1781880	-3.5950850	-2.5192660
H	-0.8490410	-5.0299020	-1.5270740
H	-1.6755820	-3.6139150	-0.8185660
H	2.4969080	-3.1834070	-1.8891540
H	1.6814310	-4.7117530	-2.2859640
H	1.2387660	-3.2240060	-3.1450840
C	-3.1527690	5.0662050	1.6326740
C	-3.1275190	5.4167830	-0.8817730
C	-1.2568370	6.3677940	0.5565060
H	-3.7708750	4.5482330	-1.0426100
H	-3.7494800	6.3091020	-0.7656220
H	-2.4936450	5.5466340	-1.7633330
H	-0.6060550	6.4483150	-0.3182070
H	-1.7950570	7.3120660	0.6781900
H	-0.6339180	6.2066620	1.4405080
H	-2.5421510	4.8835500	2.5210930
H	-3.7255070	5.9850500	1.7880150
H	-3.8518380	4.2346840	1.5117010
C	1.4407520	1.4449270	0.3342790
N	2.0308300	0.5242210	1.2667590
N	2.2117210	2.4089020	-0.0055890
O	1.6491410	3.2360570	-0.9939250
C	2.5653120	4.2892060	-1.2701790
H	2.7450880	4.9088860	-0.3832580
H	2.0947570	4.8907690	-2.0519340
H	3.5227720	3.8988620	-1.6328310
C	2.9727580	-0.4005340	0.8389970
O	3.3975970	-1.2839670	1.5958100
C	1.5490510	0.5037160	2.7058230
C	2.7637980	0.6925210	3.6385800
H	2.4168620	0.7365160	4.6766280
H	3.2744580	1.6334470	3.4093650
H	3.4731130	-0.1272220	3.5408760

C	0.5869780	1.6782420	2.9543730
H	-0.3460050	1.5703930	2.3966710
H	1.0419720	2.6388470	2.6980680
H	0.3384440	1.6913600	4.0200550
C	0.8064000	-0.8121420	3.0061330
H	0.4547430	-0.8023040	4.0437570
H	1.4640300	-1.6705320	2.8717370
H	-0.0678780	-0.9183050	2.3558450
O	-3.1930400	1.6563190	-1.7301600
C	-2.7996240	1.6330400	-3.0970000
H	-3.0616960	0.6786680	-3.5726640
H	-1.7189650	1.7993270	-3.1977290
H	-3.3427750	2.4482120	-3.5850650
O	-2.5668310	-1.2172410	0.1975670
N	-2.4603260	0.6729610	-1.0064200
C	-3.1609380	-0.3907390	-0.5322530
C	3.3931700	-0.3162570	-0.5876100
C	4.5455190	-0.7078090	-1.1812910
H	2.6633510	0.1234200	-1.2572640
H	4.5437430	-0.5310260	-2.2575870
C	7.4248520	-2.1750820	0.8579820
C	8.4220580	-2.2123790	-0.1195900
C	8.1313710	-1.7736510	-1.4126610
C	6.8570120	-1.3015070	-1.7129730
C	5.8391130	-1.2468140	-0.7363220
C	6.1478970	-1.7027890	0.5615650
H	7.6409110	-2.5234680	1.8643750
H	9.4137550	-2.5846390	0.1222240
H	8.8947370	-1.7998100	-2.1852830
H	6.6393380	-0.9580400	-2.7216010
H	5.3724490	-1.6971340	1.3158820
C	-5.5092840	-1.4739170	-0.6982980
C	-4.5854600	-0.5147470	-0.9439930
H	-6.4614080	-1.2752940	-1.1934900
H	-4.9254560	0.3052590	-1.5660530
C	-6.9070240	-4.7174900	0.5629830
C	-6.7312930	-3.5119560	-0.1106600
C	-5.5684160	-2.7308560	0.0623500
C	-4.5867940	-3.2012390	0.9584280
C	-4.7706350	-4.4046680	1.6371750
C	-5.9229310	-5.1706420	1.4436580
H	-7.8111790	-5.2990240	0.4050040
H	-7.5059170	-3.1621920	-0.7893080
H	-3.6923170	-2.6069380	1.0982610

H	-4.0040970	-4.7473550	2.3274990
H	-6.0550230	-6.1082960	1.9767500

Table 72. Atom coordinates and absolute energy of IM11-z (Energy=−1811. 312405a.u.)

Atom	X	Y	Z
Pd	0.5162010	0.3100730	-0.0171930
C	1.2055510	2.1741520	-0.0567060
N	1.4892820	3.3002280	-0.1312930
C	1.7057240	4.7305420	-0.1579280
C	1.2051670	5.2526680	-1.5171550
C	3.2115760	4.9907640	0.0173540
C	0.8905180	5.3334500	1.0012160
H	-0.1623730	5.0549340	0.9131640
H	0.9771730	6.4235970	0.9779610
H	1.2645110	4.9744290	1.9639300
H	1.7542940	4.7871060	-2.3400460
H	1.3570750	6.3346630	-1.5666330
H	0.1400090	5.0430300	-1.6446800
H	3.5695050	4.5782450	0.9642790
H	3.3956670	6.0688720	0.0145230
H	3.7833350	4.5383420	-0.7974170
C	2.3639920	-0.4451140	-0.4252470
N	2.4292140	-1.3452480	-1.5270580
N	3.4287480	-0.2544970	0.2563330
O	3.2432880	0.6786470	1.3040770
C	4.4281660	0.7069860	2.0862880
H	5.2958540	1.0226040	1.4932300
H	4.2395130	1.4362100	2.8783610
H	4.6372160	-0.2720290	2.5333750
C	1.3276570	-2.1785370	-1.6186710
O	1.2799380	-3.2291130	-2.2472650
C	3.6824600	-1.6159400	-2.3399320
C	4.4574300	-2.7821110	-1.7031600
H	5.3747810	-2.9758920	-2.2697230
H	4.7315570	-2.5396480	-0.6732460
H	3.8533450	-3.6929590	-1.7111330
C	4.5582710	-0.3500990	-2.3989040
H	3.9804690	0.5078550	-2.7588670
H	4.9908990	-0.0972670	-1.4334830
H	5.3679650	-0.5321500	-3.1120660
C	3.2838220	-1.9462450	-3.7952460
H	4.1981590	-2.0393890	-4.3894000
H	2.7193470	-2.8720600	-3.8724400

H	2.6868270	-1.1336780	-4.2228500
H	-0.7267690	-1.3846130	-1.5780760
O	-1.4427960	2.3213400	1.1985720
C	-1.5092020	2.0462630	2.5917490
H	-2.4442570	1.5340770	2.8541950
H	-0.6579860	1.4324690	2.9149700
H	-1.4719290	3.0166930	3.0969850
N	-1.4065570	1.0932400	0.4671960
C	-2.5691320	0.7437850	-0.1493010
O	-2.5863910	-0.2849940	-0.8614340
C	-8.2035740	-0.6279810	-0.6057980
C	-7.7223250	-1.8634490	-1.0433500
C	-6.3453930	-2.0526360	-1.1855420
C	-5.4470820	-1.0281790	-0.8935460
C	-5.9152840	0.2234180	-0.4442320
C	-7.3099180	0.3985020	-0.3139140
H	-9.2718510	-0.4640160	-0.4939390
H	-8.4137760	-2.6688300	-1.2758380
H	-5.9644180	-3.0091350	-1.5335970
H	-4.3802370	-1.1659040	-1.0190230
H	-7.6918810	1.3579420	0.0274700
C	-3.7552700	1.6198650	0.0605590
C	-5.0790440	1.3789220	-0.0891710
H	-3.4993120	2.6164530	0.4025730
H	-5.6948670	2.2490800	0.1446060
C	2.1189140	-4.0905180	2.3742410
C	1.6936350	-3.8225610	3.6775440
C	0.6262570	-2.9472420	3.8924810
C	-0.0025390	-2.3396490	2.8093320
C	0.4343410	-2.5786420	1.4928280
C	1.4973970	-3.4768330	1.2888270
H	2.9326130	-4.7885390	2.2004100
H	2.1819520	-4.3041950	4.5198740
H	0.2802080	-2.7452910	4.9020070
H	-0.8367570	-1.6627340	2.9723560
H	1.8117080	-3.7268400	0.2824210
C	0.0796720	-1.7010740	-0.9164700
C	-0.2901360	-1.9141360	0.3965980
H	-1.3198680	-1.6381170	0.6102960

Table 73. Atom coordinates and absolute energy of TS11-z (Energy=-1811.284475a.u.)

Atom	X	Y	Z

Pd	0.8236820	-0.4543150	-0.2303270
C	2.2041210	-1.8899560	-0.2075210
N	2.9643540	-2.7728430	-0.1525220
C	3.9753060	-3.8027610	-0.0814540
C	3.3756720	-5.0071880	0.6662200
C	5.1812070	-3.2187890	0.6773200
C	4.3600830	-4.1844620	-1.5226250
H	3.4923300	-4.5655550	-2.0677510
H	5.1266700	-4.9643380	-1.4993230
H	4.7581970	-3.3196710	-2.0600520
H	3.0742240	-4.7248920	1.6784540
H	4.1236160	-5.8024100	0.7350980
H	2.5004360	-5.3952970	0.1384760
H	5.5570230	-2.3253460	0.1727460
H	5.9806990	-3.9640600	0.7219320
H	4.9013480	-2.9458840	1.6982750
C	2.0210390	0.9268780	0.6326460
N	1.3111800	1.6809310	1.6144190
N	3.2349350	1.2484470	0.3926670
O	3.8425130	0.4093550	-0.5760790
C	5.0905240	0.9849520	-0.9285750
H	5.7556600	1.0730890	-0.0599810
H	5.5329910	0.3060500	-1.6629920
H	4.9644060	1.9763300	-1.3808380
C	0.0327700	2.0478220	1.2057170
O	-0.6521540	2.8957980	1.7752980
C	1.9310590	2.2490760	2.8725200
C	2.3309710	3.7142270	2.6244590
H	2.7876020	4.1381950	3.5258180
H	3.0552390	3.7758380	1.8075930
H	1.4525230	4.3115300	2.3699650
C	3.1633290	1.4219120	3.2832170
H	2.9113010	0.3596540	3.3706110
H	3.9868970	1.5249140	2.5793880
H	3.4928130	1.7717150	4.2664680
C	0.9155910	2.1396220	4.0318640
H	1.4019510	2.4739030	4.9539330
H	0.0289010	2.7447630	3.8607370
H	0.6085630	1.0975080	4.1707280
H	-1.2711170	0.2188360	0.2701410
O	-0.4819360	-2.8753000	-1.7924650
C	-0.1525740	-2.4611780	-3.1129350
H	-1.0013550	-1.9638140	-3.6007290
H	0.7097440	-1.7821520	-3.1078160

H	0.1005710	-3.3748540	-3.6574110
N	-0.7323250	-1.7355500	-0.9925980
C	-1.9471740	-1.6740810	-0.4426930
O	-2.1914400	-0.6938510	0.3585420
C	-7.5677120	-2.0837920	1.1848000
C	-7.3730180	-0.8276170	1.7624770
C	-6.1303860	-0.2007410	1.6424710
C	-5.0834420	-0.8131660	0.9575210
C	-5.2601270	-2.0818440	0.3682970
C	-6.5254970	-2.6967760	0.4964550
H	-8.5288420	-2.5831640	1.2683540
H	-8.1822730	-0.3415500	2.3003270
H	-5.9713210	0.7771930	2.0881840
H	-4.1223490	-0.3257260	0.8752410
H	-6.6857150	-3.6734050	0.0458430
C	-2.9537200	-2.7029640	-0.7435790
C	-4.2574510	-2.8365680	-0.3932710
H	-2.5523630	-3.5012740	-1.3556110
H	-4.6903400	-3.7557910	-0.7903190
C	-0.8623500	5.6103540	-1.5370030
C	-0.9492010	5.7245340	-2.9271740
C	-1.0145770	4.5720210	-3.7135180
C	-0.9890930	3.3201720	-3.1072290
C	-0.8757180	3.1854220	-1.7066120
C	-0.8263060	4.3596670	-0.9258170
H	-0.8319960	6.5048510	-0.9213420
H	-0.9776870	6.7052830	-3.3936800
H	-1.0920540	4.6499580	-4.7941430
H	-1.0441410	2.4237190	-3.7198850
H	-0.7972670	4.2798010	0.1532110
C	-0.4586420	1.2686340	0.0184900
C	-0.8332560	1.8190020	-1.1780890
H	-1.1557080	1.0851650	-1.9189910

Table 74. Atom coordinates and absolute energy of TS11'-z (Energy=-1811.241247a.u.)

Atom	X	Y	Z
Pd	0.7832910	0.2522500	-0.2025510
C	2.1244380	1.8398330	-0.1068400
N	2.9354140	2.6783980	-0.0542590
C	3.9378050	3.7187560	0.0122590
C	4.2100310	4.0149850	1.4985340
C	3.3786860	4.9594380	-0.7074460

C	5.2056360	3.1952540	-0.6870070
H	5.5795060	2.2960660	-0.1901420
H	5.9838840	3.9629540	-0.6509070
H	5.0013930	2.9561310	-1.7340720
H	3.3017210	4.3625680	1.9980030
H	4.9717820	4.7956890	1.5797230
H	4.5698350	3.1201860	2.0131110
H	3.1673370	4.7375440	-1.7568450
H	4.1139130	5.7680620	-0.6633130
H	2.4547080	5.2995290	-0.2325130
C	2.2001090	-1.1176750	0.2371580
N	2.5807730	-1.9597220	-0.8183840
N	2.6713580	-1.2593390	1.4153590
O	2.1771970	-0.2581020	2.3016500
C	2.4780580	-0.6637930	3.6287200
H	3.5576200	-0.8003750	3.7695300
H	2.1231070	0.1456370	4.2721040
H	1.9607950	-1.5940940	3.8920720
C	1.5961710	-2.1597130	-1.7780270
O	1.6720250	-2.9614210	-2.7019910
C	3.8723100	-2.7666140	-0.8927140
C	3.5523900	-4.2285580	-0.5367880
H	4.4651860	-4.8320510	-0.5855840
H	3.1515230	-4.2941500	0.4789880
H	2.8248170	-4.6464150	-1.2352430
C	4.9414270	-2.2138080	0.0658030
H	5.1256970	-1.1497510	-0.1120720
H	4.6762830	-2.3428660	1.1121620
H	5.8715520	-2.7541900	-0.1359930
C	4.4592910	-2.6503220	-2.3181080
H	5.4169610	-3.1797550	-2.3414400
H	3.8053830	-3.0768840	-3.0740580
H	4.6494180	-1.6002720	-2.5653920
H	-0.1158430	-1.2464930	-2.6761940
O	-0.7750510	3.0478080	0.2882610
C	-0.7148660	3.0262160	1.7109110
H	-1.6840350	2.7514010	2.1471520
H	0.0538760	2.3262790	2.0613360
H	-0.4543790	4.0446000	2.0115020
N	-1.0012870	1.7280910	-0.1901650
C	-2.1847630	1.5893940	-0.7334310
O	-2.5186750	0.4262630	-1.2564400
C	-7.6875400	0.5880390	-0.9487220
C	-7.3551980	-0.5466770	-0.2065680

C	-6.0743650	-0.6650160	0.3404530
C	-5.1252650	0.3323270	0.1366840
C	-5.4369250	1.4741160	-0.6254780
C	-6.7412800	1.5916120	-1.1429900
H	-8.6833720	0.6950750	-1.3691520
H	-8.0913140	-1.3294220	-0.0468220
H	-5.8064200	-1.5377600	0.9287100
H	-4.1433430	0.2178830	0.5772950
H	-7.0062480	2.4783540	-1.7138220
C	-3.1626450	2.6817860	-0.8509900
C	-4.5103380	2.5906310	-0.8614380
H	-2.7197240	3.6660260	-0.9464680
H	-5.0228730	3.5331880	-1.0563530
C	-2.5372480	-2.1762330	2.5326830
C	-2.9455770	-3.4851680	2.2542240
C	-2.5124860	-4.0837690	1.0663780
C	-1.6999630	-3.3978850	0.1711960
C	-1.2844970	-2.0634000	0.4346440
C	-1.7228050	-1.4750360	1.6496540
H	-2.8491400	-1.6968860	3.4577140
H	-3.5728730	-4.0303820	2.9527970
H	-2.8075540	-5.1041530	0.8338020
H	-1.3721650	-3.8776880	-0.7460640
H	-1.4015010	-0.4669950	1.8924500
C	0.2676640	-1.4320280	-1.6657910
C	-0.5422430	-1.3537610	-0.5586420
H	-1.7907490	-0.2860340	-1.0582640

Table 75. Atom coordinates and absolute energy of IM12-z (Energy=-1811.304932a.u.)

Atom	X	Y	Z
Pd	-1.1131220	-0.2002280	0.2576750
C	-2.7549360	-1.4348670	0.1043260
N	-3.6987410	-2.1026460	-0.0626920
C	-4.9495330	-2.8030670	-0.2419000
C	-4.7002540	-4.0031470	-1.1726120
C	-5.9489030	-1.8116310	-0.8665750
C	-5.4300350	-3.2713300	1.1441000
H	-4.7010870	-3.9468220	1.6002420
H	-6.3797310	-3.8040210	1.0401470
H	-5.5785720	-2.4172810	1.8099820
H	-4.3263050	-3.6698220	-2.1443920
H	-5.6374860	-4.5452920	-1.3283000

H	-3.9697840	-4.6896510	-0.7357770
H	-6.0623230	-0.9308300	-0.2299030
H	-6.9229090	-2.2963080	-0.9816210
H	-5.6041690	-1.4832670	-1.8507610
C	-2.1225550	1.5204230	-0.0286910
N	-1.4214870	2.4062650	-0.8919870
N	-3.2247160	1.9166300	0.4875450
O	-3.8169200	0.9317770	1.3267400
C	-4.8855560	1.5486560	2.0242060
H	-5.6486230	1.9378900	1.3371780
H	-5.3224780	0.7668870	2.6525250
H	-4.5328440	2.3696340	2.6610280
C	-0.0445460	2.3848360	-0.6643020
O	0.7252100	3.2135130	-1.1499530
C	-2.0558050	3.4617440	-1.7664710
C	-2.0189920	4.8140990	-1.0315320
H	-2.4698800	5.5948660	-1.6542860
H	-2.5808520	4.7516840	-0.0952990
H	-0.9883010	5.1005920	-0.8107570
C	-3.5084080	3.0833560	-2.1133840
H	-3.5582380	2.0817440	-2.5534760
H	-4.1648650	3.1103320	-1.2466700
H	-3.8721480	3.7969070	-2.8593680
C	-1.2924900	3.5395470	-3.1087950
H	-1.8137410	4.2438420	-3.7652860
H	-0.2649050	3.8691630	-2.9808910
H	-1.2892990	2.5604380	-3.5999170
H	1.2428070	-0.4144190	-0.8764280
O	-0.1453990	-3.0521030	1.2968250
C	-0.3516110	-2.6175600	2.6392750
H	0.5891190	-2.2912550	3.1006750
H	-1.0809860	-1.8003620	2.6776800
H	-0.7385030	-3.4908110	3.1692620
N	0.2354290	-1.9545220	0.4955660
C	1.2924030	-2.1994810	-0.2291740
O	1.7047510	-1.2612130	-1.0809840
C	6.5647820	-2.5319460	-2.0288040
C	6.6818460	-1.2431700	-1.5042830
C	5.6842940	-0.7436850	-0.6623800
C	4.5672330	-1.5172220	-0.3607810
C	4.4242890	-2.8111710	-0.8949600
C	5.4550170	-3.3119470	-1.7130830
H	7.3409990	-2.9323000	-2.6744840
H	7.5506350	-0.6352740	-1.7398720

H	5.7748000	0.2497330	-0.2333650
H	3.8128120	-1.1177430	0.3049950
H	5.3724910	-4.3197640	-2.1125750
C	2.0153370	-3.4717260	-0.2358660
C	3.3005590	-3.7046460	-0.5842320
H	1.4094770	-4.3193350	0.0603430
H	3.5715980	-4.7602950	-0.6166370
C	4.1959300	3.8330650	1.0520990
C	4.9997890	3.3426530	2.0839980
C	4.6340940	2.1614070	2.7327570
C	3.4772740	1.4897200	2.3470970
C	2.6475610	1.9722310	1.3096490
C	3.0378070	3.1627380	0.6621850
H	4.4762090	4.7481200	0.5371130
H	5.9019780	3.8723960	2.3773060
H	5.2470270	1.7647210	3.5375000
H	3.1966490	0.5736660	2.8621930
H	2.4305250	3.5380680	-0.1501740
C	0.3501180	1.2433640	0.2213970
C	1.4580130	1.1513110	1.0070310
H	1.4835980	0.2334720	1.5972020

Table 76. Atom coordinates and absolute energy of IM13-z (Energy=-1469.344398a.u.)

Atom	X	Y	Z
Pd	0.1635940	0.1389500	-0.0514260
C	1.2933090	1.8609740	-0.0709090
N	2.0081380	2.7854240	-0.0790720
C	3.0635930	3.7643520	0.0659850
C	2.9274790	4.7999560	-1.0627220
C	4.4009070	3.0054300	-0.0250580
C	2.8977720	4.4263140	1.4463750
H	1.9297870	4.9293370	1.5240920
H	3.6878330	5.1687320	1.5921590
H	2.9668040	3.6789160	2.2406990
H	3.0052650	4.3202760	-2.0422030
H	3.7270120	5.5413220	-0.9758550
H	1.9663740	5.3187290	-1.0039550
H	4.4297330	2.2046230	0.7172840
H	5.2293160	3.6976260	0.1529170
H	4.5251540	2.5599980	-1.0159130
C	1.7877640	-1.0755680	0.2687550
N	1.7292480	-2.2129860	-0.5824530

N	2.7742500	-0.9655570	1.0773930
O	2.7084440	0.2417730	1.8428640
C	3.4864820	0.0451830	3.0117670
H	4.5243380	-0.2159670	2.7672060
H	3.4641190	0.9965140	3.5518620
H	3.0661930	-0.7423480	3.6503300
C	0.4270390	-2.7189720	-0.6661030
O	0.1466680	-3.8300120	-1.1061620
C	2.9152780	-3.0155640	-1.0530760
C	3.1707020	-4.1678160	-0.0643600
H	4.0249260	-4.7695640	-0.3950950
H	3.3912480	-3.7707550	0.9303430
H	2.2931620	-4.8159930	-0.0048240
C	4.1637210	-2.1200820	-1.1692190
H	3.9610460	-1.2495740	-1.8026870
H	4.5137780	-1.7676310	-0.2013770
H	4.9575210	-2.7047580	-1.6451370
C	2.6297310	-3.5604610	-2.4708360
H	3.5280990	-4.0688240	-2.8363260
H	1.7961110	-4.2580570	-2.4817080
H	2.4065060	-2.7355320	-3.1562210
C	-1.6078180	1.0185900	-0.6237530
C	-3.8750330	1.8871500	-1.5903660
C	-4.6493950	2.5632430	-0.4441650
H	-5.6219830	2.8997170	-0.8151070
H	-4.8099040	1.8630840	0.3794040
H	-4.1032000	3.4322500	-0.0662650
C	-3.6032270	2.8787580	-2.7357940
H	-3.0525860	3.7515810	-2.3736850
H	-3.0221560	2.4050520	-3.5317110
H	-4.5544030	3.2185440	-3.1555060
C	-4.6219910	0.6406550	-2.1003660
H	-4.7777540	-0.0756810	-1.2898990
H	-5.5959260	0.9409510	-2.4984640
H	-4.0571260	0.1488480	-2.8970380
N	-2.5981900	1.4508880	-1.0671140
C	-0.5777560	-1.7657500	-0.0830420
C	-1.7549720	-2.3011830	0.2992240
H	-1.9086170	-3.3507390	0.0370150
C	-2.8643580	-1.6716540	1.0239840
C	-2.6820370	-0.6046500	1.9252430
C	-4.1692210	-2.1802390	0.8619620
C	-3.7651800	-0.0471690	2.6042440
H	-1.6765870	-0.2379230	2.1055290

C	-5.2531680	-1.6183090	1.5342440
H	-4.3246830	-3.0238420	0.1938650
C	-5.0569950	-0.5439460	2.4076780
H	-3.5977850	0.7668240	3.3049820
H	-6.2499580	-2.0257980	1.3874450
H	-5.8977180	-0.1155500	2.9464070

Table 77. Atom coordinates and absolute energy of TS13-z (Energy=−1469. 329275a.u.)

Atom	X	Y	Z
	-1469.82119575 a.u.		
Pd	-0.6338280	0.4682030	-0.0550200
C	-2.6664370	0.5729950	-0.2902000
N	-3.8257890	0.5970480	-0.4670480
C	-5.2460100	0.5597020	-0.7195160
C	-5.5004190	1.2034100	-2.0954480
C	-5.9528470	1.3523410	0.3955560
C	-5.6925230	-0.9143070	-0.7128300
H	-5.1618770	-1.4817000	-1.4817820
H	-6.7670130	-0.9739380	-0.9109790
H	-5.4906940	-1.3757900	0.2575130
H	-5.1577270	2.2417170	-2.1070980
H	-6.5719850	1.1877410	-2.3154630
H	-4.9742800	0.6553930	-2.8815530
H	-5.7474670	0.9108920	1.3745790
H	-7.0338040	1.3383260	0.2275100
H	-5.6157940	2.3925450	0.4061780
C	-0.2895380	-1.6322720	-0.0536340
N	0.1400040	-1.9999280	1.2702640
N	-0.8136190	-2.5057550	-0.8447220
O	-1.1234290	-1.9122140	-2.0956510
C	-1.4975370	-2.9435710	-2.9919000
H	-2.3721110	-3.4967750	-2.6242550
H	-1.7470220	-2.4446720	-3.9322950
H	-0.6773020	-3.6529780	-3.1611560
C	1.3613800	-1.3249540	1.2863920
O	2.2374290	-1.3408320	2.1358860
C	-0.2882890	-3.1392950	2.1176520
C	0.4614050	-4.4110620	1.6711510
H	0.1535790	-5.2682520	2.2800170
H	0.2441720	-4.6310200	0.6227110
H	1.5414070	-4.2792150	1.7872040

C	-1.8078740	-3.3291940	1.9721740
H	-2.3370330	-2.4116350	2.2492590
H	-2.0806750	-3.5926000	0.9497880
H	-2.1323120	-4.1293200	2.6453770
C	0.0358660	-2.8055830	3.5862880
H	-0.2998750	-3.6313650	4.2221470
H	1.1041760	-2.6499660	3.7355070
H	-0.4900170	-1.8971490	3.8975790
C	0.0491390	2.4098150	0.2519430
C	1.1493180	4.7164390	0.8133040
C	2.1975150	5.0125870	-0.2754370
H	2.6950820	5.9619110	-0.0559600
H	2.9521930	4.2226270	-0.3106570
H	1.7252720	5.0866130	-1.2588820
C	0.0614050	5.8057930	0.8399320
H	-0.4310310	5.8867470	-0.1331090
H	-0.6961380	5.5791620	1.5952570
H	0.5149270	6.7716900	1.0811590
C	1.8177330	4.5721130	2.1934730
H	2.5698130	3.7790060	2.1778220
H	2.3066040	5.5128100	2.4638320
H	1.0765790	4.3315220	2.9604730
N	0.5180330	3.4575330	0.4933900
C	1.2224190	-0.6640040	-0.0595630
C	2.1054740	-0.4873000	-1.0791310
H	1.6507930	-0.2133790	-2.0302810
C	3.5610830	-0.6155990	-1.1454740
C	4.4033730	-0.8159350	-0.0296660
C	4.1653420	-0.5059050	-2.4172740
C	5.7820900	-0.9178830	-0.1964480
H	3.9669410	-0.8872350	0.9601510
C	5.5441430	-0.6080180	-2.5770300
H	3.5331960	-0.3451910	-3.2873830
C	6.3623020	-0.8166890	-1.4644510
H	6.4121110	-1.0737500	0.6754140
H	5.9804590	-0.5245800	-3.5688560
H	7.4394370	-0.8951810	-1.5830790

Table 78. Atom coordinates and absolute energy of $1c^{Me}$ (Energy=-631.6720995a.u.)

Atom	X	Y	Z
O	2.4046740	2.0924420	0.0105680
C	2.1778020	0.7488540	-0.0219470

C	0.8049960	0.2687030	-0.0473340
C	-0.3580510	0.9435730	0.1255540
C	-1.6387040	0.1866190	0.0569130
C	-1.7269850	-1.1510200	0.4863590
C	-2.9258560	-1.8548100	0.4069970
C	-4.0722060	-1.2398520	-0.1001750
C	-4.0072820	0.0897280	-0.5174210
C	-2.8087750	0.7962220	-0.4315060
H	-0.8536560	-1.6321370	0.9146190
H	-2.9676330	-2.8832960	0.7539070
H	-5.0076390	-1.7882190	-0.1599230
H	-4.8922240	0.5809810	-0.9117250
H	-2.7796530	1.8275600	-0.7669820
N	3.2432410	0.0166470	-0.0540880
O	2.9556740	-1.3602170	-0.0568210
C	4.1743910	-2.0711530	-0.2202490
H	4.6471840	-1.8408740	-1.1825300
H	3.9028960	-3.1287460	-0.1874110
H	4.8780190	-1.8436960	0.5890410
H	0.7588160	-0.7947330	-0.2461580
H	3.3705040	2.1965510	0.0309980
C	-0.4700660	2.4304540	0.3707020
H	0.4740230	2.8616200	0.6923910
H	-0.7720680	2.9522300	-0.5466250
H	-1.2396160	2.6345160	1.1216690

Table 79. Atom coordinates and absolute energy of IM6^{Me} (Energy=-1889.845343a.u.)

Atom	X	Y	Z
Pd	0.0707420	1.1765590	-0.1181760
C	1.4644120	2.5942360	0.0340600
C	-1.4567080	2.4326370	-0.2628470
C	3.4241230	4.2680410	0.1174960
C	-3.7816020	3.5797770	-0.0826530
C	-3.7832110	5.0670300	-0.4696920
H	-4.7854650	5.4780910	-0.3203560
H	-3.0823120	5.6328700	0.1503870
H	-3.5080060	5.2002140	-1.5198280
C	-4.1330740	3.3737240	1.4031720
H	-5.1721620	3.6718900	1.5721890
H	-4.0001460	2.3246540	1.6801910
H	-3.4879880	3.9845090	2.0412680

C	-4.7203590	2.7646500	-0.9912080
H	-5.7420050	3.1392410	-0.8788030
H	-4.4289730	2.8599690	-2.0408530
H	-4.7025750	1.7069230	-0.7166640
C	4.4533420	3.5052900	0.9718380
H	4.5729800	2.4913240	0.5835210
H	5.4137180	4.0285900	0.9340380
H	4.1292400	3.4521870	2.0153970
C	3.8696050	4.3205730	-1.3554830
H	3.1257330	4.8369620	-1.9693470
H	4.8160640	4.8650040	-1.4276100
H	4.0048390	3.3070350	-1.7387310
C	3.1506830	5.6721790	0.6765950
H	2.7976410	5.6198300	1.7105240
H	4.0737450	6.2584940	0.6569040
H	2.3983430	6.1933640	0.0774000
N	2.1869700	3.5041140	0.1588230
N	-2.4392880	3.0583070	-0.2698950
C	2.8161350	-0.1515970	-0.2443750
O	1.1681410	-1.5011370	0.7430360
C	0.7511020	-1.3518030	2.1008320
H	-0.1262330	-0.6987860	2.1742770
H	0.4846480	-2.3586050	2.4342850
H	1.5667020	-0.9587580	2.7222420
N	1.5356080	-0.2549530	0.2016910
O	3.1844940	0.8895510	-0.8386760
N	-1.3670890	-0.2932780	-0.3800790
C	-2.4325280	-0.3871450	0.4595400
O	-2.3993170	0.2364370	1.5458290
O	-1.5453990	-0.7783400	-1.6919240
C	-0.6165430	-1.8286430	-1.9700370
H	-0.7600390	-2.6732720	-1.2870410
H	-0.8262000	-2.1327530	-2.9992580
H	0.4145000	-1.4719890	-1.8871490
C	4.9589520	-1.4968990	-0.4916360
C	3.7283510	-1.2929520	0.0330310
H	3.3374880	-2.0249820	0.7271500
C	7.1774770	-5.0138780	0.6715070
C	5.7848920	-5.0613160	0.5758770
C	5.0665930	-3.9299690	0.1949340
C	5.7188500	-2.7170540	-0.0966810
C	7.1232820	-2.6940990	-0.0150130
C	7.8426600	-3.8242630	0.3722750
H	7.7376360	-5.8968030	0.9659110

H	5.2558310	-5.9866370	0.7869200
H	3.9876870	-3.9904370	0.0932330
H	7.6594440	-1.7777180	-0.2396950
H	8.9260560	-3.7740290	0.4394660
C	-3.5685770	-1.2469250	0.0303970
C	-4.5988130	-1.6760100	0.7976580
H	-3.5375590	-1.5419200	-1.0111510
C	-7.6344070	-4.1975490	-0.9567580
C	-7.9576920	-3.3109610	0.0710740
C	-6.9720440	-2.5070510	0.6430030
C	-5.6400600	-2.5541030	0.1917810
C	-5.3309260	-3.4654680	-0.8357020
C	-6.3133510	-4.2733490	-1.4037290
H	-8.3999070	-4.8297770	-1.3974800
H	-8.9805750	-3.2443520	0.4316250
H	-7.2453500	-1.8229780	1.4397750
H	-4.3032020	-3.5595150	-1.1710970
H	-6.0437560	-4.9736450	-2.1895370
C	5.6414740	-0.5610980	-1.4620200
H	4.9256160	0.1329890	-1.8967370
H	6.4065750	0.0382110	-0.9503580
H	6.1531370	-1.1290450	-2.2462360
C	-4.7771410	-1.3198860	2.2556500
H	-3.8643830	-0.8872940	2.6594830
H	-5.5756700	-0.5760280	2.3795010
H	-5.0753690	-2.2029080	2.8311080

Table 80. Atom coordinates and absolute energy of TS7^{Me} (Energy=-1889.817611a.u.)

Atom	X	Y	Z
Pd	0.0534790	1.2170300	-0.0312790
C	1.3965550	2.6133130	0.2659380
C	-1.6511700	2.0947960	-0.3627960
C	3.3713820	4.2340840	0.6144530
C	-2.9006390	4.2158080	-0.6087490
C	-1.6447910	5.0360730	-0.2723870
H	-1.8780140	6.1054860	-0.2953830
H	-1.2723090	4.7858730	0.7252460
H	-0.8469710	4.8425460	-0.9953490
C	-4.0119840	4.4751400	0.4231600
H	-4.2921200	5.5332470	0.4115800
H	-4.8977260	3.8762810	0.1946980

H	-3.6734180	4.2166900	1.4306810
C	-3.4001480	4.5404120	-2.0272480
H	-3.6745040	5.5980530	-2.0929080
H	-2.6213310	4.3382330	-2.7685040
H	-4.2763070	3.9356120	-2.2758150
C	4.1767580	3.5121110	1.7104500
H	4.3224930	2.4667590	1.4297450
H	5.1495460	3.9998440	1.8259260
H	3.6519280	3.5547340	2.6694690
C	4.0977610	4.1560490	-0.7411300
H	3.5164530	4.6554020	-1.5221030
H	5.0681240	4.6556460	-0.6601030
H	4.2466360	3.1112810	-1.0211590
C	3.0550760	5.6851430	1.0056370
H	2.5093170	5.7258190	1.9527630
H	3.9886230	6.2430830	1.1217700
H	2.4533960	6.1768190	0.2356260
N	2.1178460	3.5110710	0.4649270
N	-2.6273730	2.7703410	-0.5778510
C	2.8086140	-0.2461440	-0.0721230
O	0.9152360	-1.5951500	0.3527700
C	0.6267220	-1.8360510	1.7306190
H	-0.0791780	-1.0941660	2.1201310
H	0.1700140	-2.8297070	1.7679880
H	1.5452660	-1.8293780	2.3324690
N	1.4738240	-0.2989920	0.1939600
O	3.3469330	0.8631650	-0.2929470
N	-1.8053000	0.2565070	-0.4909990
C	-2.5980080	-0.2758280	0.5399140
O	-2.3007600	0.0394340	1.6939360
O	-2.1316640	-0.0814510	-1.8119400
C	-1.1763950	-1.0116900	-2.3402640
H	-1.1651900	-1.9405040	-1.7611100
H	-1.5025230	-1.2010950	-3.3657270
H	-0.1705900	-0.5776340	-2.3384310
C	4.8809500	-1.7235100	-0.2764450
C	3.5547880	-1.5361570	-0.0794670
H	2.9330350	-2.4094340	0.0676480
C	6.4798670	-5.7339390	-0.1272290
C	5.4009970	-5.3758870	0.6842150
C	4.8869920	-4.0818630	0.6405310
C	5.4311660	-3.1084620	-0.2186230
C	6.5304940	-3.4823290	-1.0132200
C	7.0423680	-4.7790510	-0.9750360

H	6.8827790	-6.7421070	-0.0915910
H	4.9651690	-6.1037260	1.3632480
H	4.0687710	-3.8099440	1.2995940
H	6.9812380	-2.7567670	-1.6823300
H	7.8838460	-5.0424840	-1.6101140
C	-3.7262190	-1.1312800	0.1312490
C	-4.5078910	-1.8709990	0.9574810
H	-3.9275960	-1.1394260	-0.9320750
C	-7.6905900	-4.2475870	-0.7204420
C	-7.8190300	-3.6914120	0.5530550
C	-6.7823380	-2.9347580	1.0973860
C	-5.5985950	-2.6983110	0.3743310
C	-5.4824270	-3.2765820	-0.9038100
C	-6.5142650	-4.0401620	-1.4442190
H	-8.4946490	-4.8442420	-1.1413570
H	-8.7283660	-3.8470590	1.1266600
H	-6.9025380	-2.5071500	2.0872970
H	-4.5620110	-3.1504930	-1.4646660
H	-6.3949940	-4.4836980	-2.4286840
C	5.8663460	-0.6198740	-0.5809230
H	6.1650850	-0.6516260	-1.6371330
H	5.4166010	0.3517750	-0.3935600
H	6.7799480	-0.7441740	0.0109990
C	-4.3582690	-1.9010460	2.4593160
H	-3.3823250	-1.5308800	2.7652550
H	-5.1063710	-1.2489570	2.9290550
H	-4.5246960	-2.9124570	2.8425200

Table 81. Atom coordinates and absolute energy of IM8^{Me} (Energy=-1889.824904a.u.)

Atom	X	Y	Z
Pd	-0.0512750	1.2520210	0.0013910
C	-1.3650000	2.6721570	-0.2552370
C	1.7445020	1.9884070	0.3588820
C	-3.4321600	4.1932260	-0.5522640
C	2.6318160	4.2534420	0.5065510
C	1.2500920	4.8447330	0.1948650
H	1.3120910	5.9380810	0.1821880
H	0.8869780	4.5120870	-0.7811110
H	0.5136560	4.5536360	0.9484250
C	3.6468850	4.6822850	-0.5709100
H	3.7300440	5.7737250	-0.6000270

H	4.6335450	4.2610680	-0.3588130
H	3.3311670	4.3329610	-1.5588010
C	3.1102560	4.7236990	1.8937680
H	3.1886210	5.8156020	1.9169810
H	2.4060970	4.4117340	2.6714590
H	4.0892400	4.2964370	2.1276230
C	-4.2140080	3.4607410	-1.6584190
H	-4.3135700	2.4047250	-1.3978370
H	-5.2072120	3.9096190	-1.7571110
H	-3.6983990	3.5462720	-2.6196780
C	-4.1466750	4.0560980	0.8051900
H	-3.5822580	4.5635430	1.5933860
H	-5.1375770	4.5160330	0.7390380
H	-4.2496840	2.9999110	1.0621350
C	-3.1795190	5.6644000	-0.9144170
H	-2.6419000	5.7479470	-1.8633780
H	-4.1369310	6.1837890	-1.0136190
H	-2.5943120	6.1650490	-0.1375950
N	-2.1492870	3.5212120	-0.4239770
N	2.6830080	2.7828000	0.5396480
C	-2.8079210	-0.2937030	0.0551300
O	-0.8672370	-1.5671880	-0.4165810
C	-0.6321210	-1.7997590	-1.8032070
H	0.0026200	-1.0159370	-2.2336540
H	-0.1153650	-2.7628140	-1.8640120
H	-1.5755960	-1.8530750	-2.3628370
N	-1.4796890	-0.2871540	-0.2413710
O	-3.3868150	0.7932580	0.2843260
N	1.9452460	0.4962150	0.4632920
C	2.7230050	-0.1241330	-0.5949690
O	2.4338060	0.2006720	-1.7355680
O	2.2534770	0.1147050	1.7893210
C	1.2933090	-0.8378840	2.2742280
H	1.2966400	-1.7506770	1.6706720
H	1.6117240	-1.0535470	3.2964110
H	0.2865250	-0.4068980	2.2731010
C	-4.8160940	-1.8525740	0.2962210
C	-3.4997620	-1.6146620	0.0888950
H	-2.8432700	-2.4643720	-0.0479470
C	-6.2543110	-5.9264790	0.2435740
C	-5.1911140	-5.5449340	-0.5778680
C	-4.7292980	-4.2307100	-0.5659820
C	-5.3109420	-3.2592480	0.2705650
C	-6.3941320	-3.6579280	1.0752970

C	-6.8539960	-4.9745700	1.0689050
H	-6.6166700	-6.9505110	0.2326840
H	-4.7270920	-6.2708410	-1.2401840
H	-3.9231040	-3.9420400	-1.2327060
H	-6.8731580	-2.9348690	1.7272290
H	-7.6841050	-5.2559300	1.7112720
C	3.7649720	-1.0541520	-0.1541960
C	4.5593150	-1.8080200	-0.9609110
H	3.8909760	-1.1208150	0.9174040
C	7.5938600	-4.2895240	0.8239860
C	6.9701800	-4.6811350	-0.3616260
C	5.9980930	-3.8701020	-0.9444780
C	5.6106710	-2.6579610	-0.3435090
C	6.2579470	-2.2733110	0.8464640
C	7.2373990	-3.0786270	1.4219840
H	8.3577240	-4.9172930	1.2733540
H	7.2414440	-5.6197680	-0.8360360
H	5.5220650	-4.1929680	-1.8642300
H	6.0142630	-1.3195290	1.3030830
H	7.7310080	-2.7548970	2.3336910
C	4.4288220	-1.8634060	-2.4624660
H	3.8324040	-1.0367110	-2.8395360
H	5.4170380	-1.8583450	-2.9323450
H	3.9370020	-2.7978440	-2.7631440
C	-5.8431550	-0.7820940	0.5819140
H	-6.1335070	-0.7996370	1.6408320
H	-5.4319200	0.2015260	0.3692030
H	-6.7548700	-0.9561430	-0.0004360

Table 82. Atom coordinates and absolute energy of IM9^{Me} (Energy=-2140.291965a.u.)

Atom	X	Y	Z
Pd	0.3894690	0.1657190	0.3524820
C	0.7208990	2.1172920	0.0552900
C	-0.0670960	-1.7633790	0.6782860
N	0.9565580	3.2448630	-0.1296090
C	1.6868380	4.4897330	-0.2945310
N	-0.3977050	-2.8648930	0.8547310
C	-0.9648240	-4.1780150	1.0855130
C	2.7086640	4.2661170	-1.4246020
C	0.6862060	5.6025870	-0.6404670
C	2.4052140	4.7667180	1.0391510

H	3.0630620	3.9306510	1.2856490
H	2.9995230	5.6808220	0.9458610
H	1.6832990	4.9046630	1.8494280
H	2.2014640	4.0558340	-2.3710760
H	3.3130000	5.1697800	-1.5498030
H	3.3565220	3.4240210	-1.1700520
H	-0.0546350	5.7251950	0.1547640
H	1.2221980	6.5481270	-0.7633020
H	0.1601610	5.3805470	-1.5734550
C	-1.7156200	-4.1236080	2.4285580
C	0.1864400	-5.1967350	1.1155920
C	-1.9412860	-4.4597930	-0.0718070
H	0.8887970	-4.9678410	1.9216160
H	-0.2218740	-6.1973060	1.2842140
H	0.7335840	-5.1978890	0.1689700
H	-1.4175250	-4.4619570	-1.0321840
H	-2.3988380	-5.4425400	0.0755880
H	-2.7258500	-3.6998560	-0.0906550
H	-2.4824330	-3.3464510	2.3966530
H	-2.1883210	-5.0927840	2.6139670
H	-1.0262480	-3.9119640	3.2507280
C	-1.4603840	0.5545710	1.1817810
N	-1.8528150	0.7945370	2.3535770
N	-2.5146510	0.4119950	0.1900120
O	-2.5869460	1.5059410	-0.6912990
C	-2.1553020	1.1362210	-2.0091140
H	-1.1268260	0.7621870	-1.9939840
H	-2.2093520	2.0577120	-2.5941420
H	-2.8232160	0.3835460	-2.4436860
C	-3.6176260	-0.4237860	0.3394020
O	-3.5252430	-1.4189160	1.0646890
C	-1.0496390	0.8978770	3.5820870
C	-0.9353110	-0.5203950	4.1755190
H	-0.4813290	-0.4781590	5.1715130
H	-0.3124690	-1.1568280	3.5405910
H	-1.9244470	-0.9795480	4.2599740
C	0.3477230	1.5180320	3.4070310
H	0.2796450	2.5089380	2.9477540
H	1.0042610	0.9024740	2.7860700
H	0.8233720	1.6333910	4.3871230
C	-1.8777430	1.7841540	4.5347020
H	-1.3871240	1.8719980	5.5100050
H	-2.8756150	1.3602500	4.6776220
H	-1.9957950	2.7892860	4.1169860

O	2.4406000	-1.6330730	-1.0859110
C	1.9758860	-1.6146700	-2.4254360
H	2.5847840	-0.9529240	-3.0573180
H	0.9279200	-1.2870460	-2.4776370
H	2.0536520	-2.6434120	-2.7914730
O	3.3936320	1.4154380	0.3811390
N	2.2915300	-0.3335840	-0.5124040
C	3.4486480	0.3140220	-0.2182980
C	-4.8139730	-0.0333130	-0.4444200
C	-5.9395820	-0.7648830	-0.6310470
H	-4.7631870	0.9543840	-0.8841660
C	-8.4028940	1.7641370	-2.0578000
C	-9.2153260	0.9515860	-2.8517790
C	-8.9661550	-0.4203540	-2.9077730
C	-7.9141560	-0.9741150	-2.1792180
C	-7.0723740	-0.1678620	-1.3914140
C	-7.3468280	1.2118080	-1.3366710
H	-8.5994480	2.8304090	-1.9896720
H	-10.0398360	1.3821510	-3.4126250
H	-9.5929260	-1.0635550	-3.5191130
H	-7.7357950	-2.0428380	-2.2380040
H	-6.7448760	1.8495730	-0.6972810
C	5.9887820	0.0993150	-0.3896750
C	4.7282920	-0.3159690	-0.6563380
H	4.6045770	-1.2279700	-1.2257220
C	9.4312820	-1.4803690	-0.7966190
C	8.3595400	-0.7582550	-0.2719460
C	7.1368310	-0.6625580	-0.9614080
C	7.0462150	-1.2948500	-2.2161540
C	8.1172900	-2.0119880	-2.7442460
C	9.3162680	-2.1130120	-2.0349680
H	10.3590010	-1.5476870	-0.2347320
H	8.4701560	-0.2770580	0.6940790
H	6.1312240	-1.1985140	-2.7918200
H	8.0198040	-2.4832200	-3.7186380
H	10.1530690	-2.6697160	-2.4472310
C	6.3310620	1.2816630	0.4863630
H	5.4352090	1.8565360	0.7080660
H	6.7665110	0.9439500	1.4360320
H	7.0829660	1.9160650	0.0027470
C	-6.1222280	-2.1802350	-0.1368150
H	-6.0223450	-2.8921660	-0.9670850
H	-5.3751550	-2.4235500	0.6147070
H	-7.1270460	-2.3144300	0.2765250

Table 83. Atom coordinates and absolute energy of TS9^{Me} (Energy=−2140.261381a.u.)

Atom	X	Y	Z
Pd	-0.3426800	0.6747290	-0.1773360
C	0.1954180	-1.2479980	-0.1220090
C	-0.8397380	2.6095600	-0.2261820
N	0.5392740	-2.3608060	-0.1137340
C	0.5846990	-3.8030570	0.0417450
N	-1.1765320	3.7230020	-0.2601170
C	-1.6869720	5.0769560	-0.3216200
C	-0.6921020	-4.3634210	-0.6127500
C	1.8546820	-4.3298590	-0.6442070
C	0.5979020	-4.0914910	1.5542690
H	-0.2956640	-3.6749050	2.0250760
H	0.6147120	-5.1735090	1.7144180
H	1.4842810	-3.6581150	2.0262150
H	-0.6871450	-4.1750390	-1.6904340
H	-0.7369120	-5.4446660	-0.4503770
H	-1.5727400	-3.8869320	-0.1755680
H	2.7562720	-3.8977950	-0.2012700
H	1.9005070	-5.4170290	-0.5323740
H	1.8450580	-4.0931360	-1.7119840
C	-2.8150570	5.0927210	-1.3694250
C	-0.5279120	6.0038580	-0.7271910
C	-2.2237620	5.4351150	1.0763120
H	-0.1267210	5.7218980	-1.7042000
H	-0.8928420	7.0332420	-0.7846420
H	0.2820950	5.9608930	0.0054790
H	-1.4280300	5.3835740	1.8241950
H	-2.6185860	6.4548800	1.0595900
H	-3.0268030	4.7544050	1.3709250
H	-3.5935520	4.3716850	-1.1077440
H	-3.2560330	6.0927240	-1.4119050
H	-2.4270410	4.8418470	-2.3603800
C	1.6129070	1.1782640	0.0753410
N	2.4077810	1.2444580	1.1158130
N	2.4408020	1.5472190	-0.9412680
O	2.3350550	0.7878040	-2.1330180
C	2.6490350	1.6221090	-3.2438870
H	1.9462220	2.4603540	-3.3235550
H	2.5650200	0.9820590	-4.1261140

H	3.6699510	2.0145860	-3.1714530
C	3.8062950	1.5795220	0.0567070
O	4.3730890	2.6527730	0.2225110
C	2.1634280	1.5894350	2.5221890
C	1.8722770	3.1021030	2.6145770
H	1.7855990	3.4156870	3.6608900
H	0.9334630	3.3429480	2.1051610
H	2.6792590	3.6644730	2.1377490
C	0.9963090	0.7675380	3.0942080
H	1.2014860	-0.3044950	3.0176240
H	0.0598000	0.9706000	2.5658870
H	0.8508910	1.0144460	4.1516350
C	3.4603250	1.2642640	3.2860740
H	3.3513540	1.5255820	4.3434750
H	4.2990640	1.8281560	2.8700630
H	3.6930170	0.1973660	3.2155000
O	-3.2271050	1.0737710	-1.1448170
C	-3.1304990	0.8674780	-2.5493440
H	-3.5056910	-0.1238390	-2.8355620
H	-2.0928810	0.9696220	-2.8941120
H	-3.7497390	1.6409160	-3.0146490
O	-2.3156600	-1.6862170	0.8401130
N	-2.3798210	0.1487380	-0.4655840
C	-3.0028810	-0.8807260	0.1707320
C	4.4646760	0.2404850	-0.0928680
C	5.7877320	-0.0239480	-0.0878510
H	3.7723080	-0.5814390	-0.2377370
C	5.9690160	-3.5804280	-1.4410710
C	7.0932970	-4.0825830	-0.7810920
C	7.7995790	-3.2531040	0.0908120
C	7.3840160	-1.9387600	0.3053970
C	6.2421950	-1.4230390	-0.3329900
C	5.5522550	-2.2682480	-1.2232390
H	5.4251430	-4.2072310	-2.1429680
H	7.4216330	-5.1034610	-0.9546380
H	8.6789780	-3.6287370	0.6070230
H	7.9453700	-1.3110860	0.9899840
H	4.7006480	-1.8746670	-1.7698780
C	-5.2951260	-1.9277130	0.5634080
C	-4.4814140	-0.9919250	0.0208950
H	-4.9304830	-0.2206490	-0.5910800
C	-8.9193210	-2.9270220	-0.0337050
C	-7.5487390	-3.0010130	0.2135510
C	-6.7627600	-1.8385890	0.3154890

C	-7.4140690	-0.5968770	0.1910800
C	-8.7842930	-0.5214750	-0.0494440
C	-9.5448560	-1.6869090	-0.1680110
H	-9.4991690	-3.8418940	-0.1205220
H	-7.0811480	-3.9753420	0.3120960
H	-6.8407690	0.3165910	0.3137370
H	-9.2622630	0.4509720	-0.1318560
H	-10.6137290	-1.6283870	-0.3526600
C	-4.8216230	-3.0919100	1.4021870
H	-4.8412430	-4.0225920	0.8188200
H	-3.7987920	-2.9277600	1.7335800
H	-5.4856110	-3.2420260	2.2603310
C	6.8571880	1.0115520	0.1737970
H	6.4316410	2.0132360	0.1535090
H	7.3134330	0.8575010	1.1605880
H	7.6634370	0.9284590	-0.5638190

Table 84. Atom coordinates and absolute energy of IM10^{Me} (Energy=-2140.297842a.u.)

Atom	X	Y	Z
Pd	0.0028860	0.8933940	0.1218370
C	0.4632480	-1.0470540	0.3111660
C	-0.4369150	2.8331570	-0.1137990
N	0.8367000	-2.1392160	0.4724090
C	0.9232720	-3.5433140	0.8125610
N	-0.8074200	3.9285540	-0.2547400
C	-1.4086600	5.2239770	-0.4616990
C	0.1719820	-4.3081500	-0.2714270
C	2.3944350	-3.9338550	0.8745500
C	0.2401070	-3.7046240	2.1674210
H	-0.7812950	-3.3084810	2.1245670
H	0.2151410	-4.7679190	2.4337510
H	0.7970840	-3.1650360	2.9419060
H	0.6409770	-4.1619770	-1.2507100
H	0.1857110	-5.3782610	-0.0346800
H	-0.8675920	-3.9651640	-0.3208670
H	2.9226110	-3.3248030	1.6191300
H	2.4737120	-4.9908070	1.1544930
H	2.8809900	-3.7897050	-0.0985990
C	-1.9031160	5.7248090	0.8910130
C	-2.5676290	5.0284540	-1.4344370
C	-0.3461920	6.1518620	-1.0382990

H	-3.2805920	4.2940810	-1.0425460
H	-3.0816250	5.9845930	-1.5853590
H	-2.2005070	4.6718040	-2.4032600
H	0.0242070	5.7722570	-1.9967070
H	-0.7796600	7.1451790	-1.2005040
H	0.5008580	6.2480780	-0.3503020
H	-1.0736190	5.8138910	1.6008220
H	-2.3633670	6.7113900	0.7660060
H	-2.6491180	5.0404430	1.3080820
C	1.9371200	1.3477090	0.6487610
N	2.4877800	0.6878080	1.7838010
N	2.7381230	2.1394610	0.0439120
O	2.2030130	2.6441910	-1.1368030
C	3.0919810	3.6153310	-1.6443080
H	3.1537830	4.4921800	-0.9841980
H	2.6905190	3.9166140	-2.6159980
H	4.0999490	3.2011530	-1.7754310
C	3.3553270	-0.3798320	1.5994940
O	3.7453710	-1.0689880	2.5424500
C	1.9435780	0.9928040	3.1539760
C	3.1123340	1.3176480	4.0846040
H	2.7209960	1.5957120	5.0712620
H	3.6800520	2.1686140	3.6887230
H	3.7833680	0.4663700	4.1997730
C	1.0514900	2.2310800	3.0954830
H	0.1124020	2.0420520	2.5632820
H	1.5621890	3.0787320	2.6219550
H	0.7969040	2.5142240	4.1237100
C	1.1185280	-0.1824190	3.6745380
H	0.7281660	0.0575050	4.6717300
H	1.7306340	-1.0854010	3.7507020
H	0.2609650	-0.3810750	3.0165270
O	-2.8480540	1.3578830	-0.9366830
C	-2.6706110	1.1982180	-2.3241370
H	-3.0056630	0.2046340	-2.6621380
H	-1.6124030	1.3267440	-2.6046830
H	-3.2754980	1.9706980	-2.8134140
O	-2.0203570	-1.4892950	0.9162400
N	-2.0365740	0.4327130	-0.2521440
C	-2.6638630	-0.6664430	0.2396870
C	3.7385660	-0.6853290	0.2033840
C	4.8338190	-1.3759920	-0.1715450
H	3.0546720	-0.3638170	-0.5778630
C	4.8030200	-1.0053150	-3.9423680

C	5.4026420	-2.1953400	-4.3452780
C	5.8325110	-3.1046150	-3.3846670
C	5.6618890	-2.8275240	-2.0334560
C	5.0417770	-1.6435890	-1.6124860
C	4.6265560	-0.7313790	-2.5927840
H	4.4788830	-0.2794080	-4.6848840
H	5.5427790	-2.4078490	-5.4026930
H	6.3045050	-4.0366470	-3.6880050
H	5.9996190	-3.5503180	-1.2930830
H	4.1834050	0.2146890	-2.2849660
C	-4.8382180	-1.9467560	0.1132510
C	-4.1039710	-0.8306100	-0.0703450
H	-4.5944370	0.0464650	-0.4834120
C	-8.5525590	-2.6789210	0.0631040
C	-7.2103360	-2.6891970	0.4226460
C	-6.2639900	-1.9410870	-0.2900610
C	-6.7096830	-1.2070930	-1.3975980
C	-8.0490890	-1.2019400	-1.7633260
C	-8.9792600	-1.9347630	-1.0316990
H	-9.2689560	-3.2577930	0.6421260
H	-6.8935550	-3.2746490	1.2834890
H	-5.9843260	-0.6568670	-1.9943880
H	-8.3668990	-0.6314820	-2.6336300
H	-10.0281000	-1.9333370	-1.3194940
C	-4.3257990	-3.2185050	0.7233120
H	-3.2365510	-3.2560550	0.6883050
H	-4.6073970	-3.2767210	1.7839850
H	-4.7622850	-4.0917470	0.2243060
C	5.8678000	-1.9155180	0.7700160
H	5.8115930	-1.4387390	1.7484150
H	5.7093680	-2.9904440	0.9389430
H	6.8720330	-1.8006140	0.3455490

Table 85. Atom coordinates and absolute energy of IM11^{Me} (Energy=-1889.853938a.u.)

Atom	X	Y	Z
Pd	-1.0938270	0.0925130	-0.1992500
C	-0.9331860	2.0403170	-0.4527510
N	-0.7059740	3.1767220	-0.5687550
C	-0.2990950	4.5511820	-0.7623730
C	1.2327960	4.6007760	-0.6126390
C	-0.9945310	5.4093170	0.3089540

C	-0.7338520	4.9720100	-2.1780520
H	-0.2535840	4.3441070	-2.9331320
H	-0.4428470	6.0117720	-2.3522540
H	-1.8178860	4.8888270	-2.2927930
H	1.5324540	4.3094450	0.3974660
H	1.5843060	5.6193110	-0.8021300
H	1.7100080	3.9193750	-1.3212650
H	-2.0820380	5.3460570	0.2151210
H	-0.6946500	6.4539650	0.1867480
H	-0.7108030	5.0822450	1.3128230
C	-3.0820090	0.1648650	0.1816490
N	-3.4294730	-0.5465920	1.3664760
N	-4.0260530	0.6818330	-0.5095190
O	-3.5404410	1.3758700	-1.6453160
C	-4.6549350	1.8734220	-2.3698090
H	-5.2388710	2.5875920	-1.7752700
H	-4.2357320	2.3803570	-3.2429000
H	-5.3155730	1.0627450	-2.7007500
C	-2.7540240	-1.7478130	1.5167690
O	-3.0634290	-2.6335060	2.3025400
C	-4.5881180	-0.1879440	2.2792810
C	-5.8137280	-1.0331430	1.8907510
H	-6.6611370	-0.7839600	2.5387460
H	-6.1021220	-0.8311910	0.8552350
H	-5.5963750	-2.0978370	2.0041140
C	-4.9135700	1.3127080	2.1667180
H	-4.0210720	1.9224390	2.3419550
H	-5.3284630	1.5774620	1.1963330
H	-5.6451910	1.5573500	2.9427310
C	-4.1776780	-0.4459130	3.7459550
H	-4.9893590	-0.1063050	4.3970260
H	-3.9853370	-1.4976280	3.9430390
H	-3.2800550	0.1286880	3.9976630
H	-0.6012080	-1.9752330	1.2444990
O	1.6318300	0.7147390	-1.5128630
C	1.4673350	0.0500790	-2.7583290
H	1.9612270	-0.9291460	-2.7603630
H	0.4037740	-0.0880960	-2.9953620
H	1.9252400	0.6999930	-3.5104850
N	1.0127650	-0.0602720	-0.4854700
C	1.8045580	-0.3313820	0.5864700
O	1.2739370	-0.8493800	1.6001270
C	7.9993720	-0.1965810	1.5000490
C	8.3102000	0.7867860	0.5602190

C	7.2745020	1.4702210	-0.0811040
C	5.9459710	1.1668510	0.2082380
C	5.6119130	0.1677210	1.1423970
C	6.6689590	-0.4954050	1.7928220
H	8.7945710	-0.7342620	2.0093110
H	9.3462400	1.0253390	0.3371190
H	7.5022800	2.2519260	-0.8008610
H	5.1521190	1.7284480	-0.2738810
H	6.4492640	-1.2655520	2.5248390
C	3.2619890	-0.0584110	0.4740700
C	4.1935300	-0.1730840	1.4502600
H	3.5832550	0.2623210	-0.5085160
C	1.9296420	-3.9270060	-1.1604140
C	1.8493740	-4.3590270	-2.4864330
C	0.6630940	-4.1723820	-3.1972990
C	-0.4317000	-3.5669940	-2.5839080
C	-0.3695960	-3.1268130	-1.2467040
C	0.8387580	-3.3180620	-0.5468700
H	2.8487890	-4.0610440	-0.5979500
H	2.7026660	-4.8361560	-2.9600060
H	0.5859170	-4.5011890	-4.2296650
H	-1.3403300	-3.4356410	-3.1598500
H	0.9420880	-2.9744520	0.4756470
C	-1.5195640	-1.9534730	0.6591470
C	-1.5628440	-2.5232370	-0.6018710
C	-2.8871350	-2.6915980	-1.3163810
H	-2.8987820	-2.1625900	-2.2738180
H	-3.0587510	-3.7536560	-1.5224540
H	-3.7209450	-2.3160310	-0.7258810
C	3.9010680	-0.6476790	2.8547600
H	2.8302590	-0.6439700	3.0452960
H	4.2541910	-1.6782040	2.9947710
H	4.4294750	-0.0286700	3.5881470

Table 86. Atom coordinates and absolute energy of TS11^{Me} (Energy=-1889.830499a.u.)

Atom	X	Y	Z
Pd	1.0554600	0.1868070	0.1004840
C	1.6130410	2.0888700	0.1660320
N	1.9041450	3.2178370	0.1503110
C	2.3097610	4.6047670	0.1383130
C	1.4042050	5.3538240	-0.8558640

C	3.7843960	4.6565780	-0.3013620
C	2.1394400	5.1567640	1.5655060
H	1.0962120	5.0895090	1.8855730
H	2.4430750	6.2073380	1.5875440
H	2.7589230	4.5996030	2.2732870
H	1.5096360	4.9419750	-1.8630550
H	1.6864010	6.4103910	-0.8805170
H	0.3550300	5.2774540	-0.5586350
H	4.4116300	4.0795480	0.3829000
H	4.1276640	5.6951960	-0.3041120
H	3.9037040	4.2478700	-1.3083160
C	2.9371330	-0.4660250	-0.2257230
N	2.9472800	-1.3769470	-1.3205010
N	4.0334920	-0.2243060	0.3850630
O	3.8704660	0.7277640	1.4252320
C	5.0912730	0.8020500	2.1442180
H	5.9213960	1.1223680	1.5014550
H	4.9274560	1.5448350	2.9298360
H	5.3497220	-0.1606920	2.6022280
C	1.9103460	-2.3057010	-1.2635040
O	1.8331750	-3.2932920	-1.9869670
C	4.0503740	-1.4901310	-2.3488610
C	4.9440220	-2.6925160	-1.9953280
H	5.7535320	-2.7892170	-2.7274130
H	5.3890050	-2.5554510	-1.0054640
H	4.3612380	-3.6160740	-2.0015310
C	4.8896420	-0.2011440	-2.3861200
H	4.2570480	0.6769090	-2.5538480
H	5.4547430	-0.0481160	-1.4684730
H	5.5884050	-0.2777530	-3.2249510
C	3.4185670	-1.6604530	-3.7479850
H	4.2186430	-1.6822600	-4.4951250
H	2.8387820	-2.5773460	-3.8246710
H	2.7656710	-0.8110790	-3.9757410
H	-0.2402780	-1.5042210	-0.5758380
O	-1.5102690	1.9526600	0.5911010
C	-1.5628110	2.0000140	2.0110030
H	-2.2683920	1.2619730	2.4128250
H	-0.5718520	1.8190180	2.4477700
H	-1.8970810	3.0105770	2.2642810
N	-1.0341210	0.6831860	0.1738600
C	-1.9309210	-0.0836870	-0.4555690
O	-1.5457000	-1.2085550	-0.9326710
C	-7.9065350	0.5620600	-2.1554490

C	-8.2564410	1.5610600	-1.2460400
C	-7.3483520	1.9293110	-0.2509000
C	-6.1020740	1.3115830	-0.1729470
C	-5.7264320	0.3112300	-1.0889860
C	-6.6617800	-0.0607050	-2.0721490
H	-8.6043440	0.2647250	-2.9333490
H	-9.2291610	2.0408310	-1.3055840
H	-7.6159530	2.6921740	0.4750990
H	-5.4188680	1.5846800	0.6248860
H	-6.4065720	-0.8322220	-2.7911960
C	-3.3268610	0.3743680	-0.6031820
C	-4.3919190	-0.3491980	-1.0231510
H	-3.4751830	1.4147900	-0.3455010
C	-1.0968920	-1.3772060	3.8118260
C	-2.1768170	-2.2461620	3.9667140
C	-2.3326250	-3.3180630	3.0838140
C	-1.4059210	-3.5259830	2.0647090
C	-0.3248700	-2.6443770	1.8852550
C	-0.1819700	-1.5688150	2.7743200
H	-0.9605880	-0.5488500	4.5016200
H	-2.8903370	-2.0943810	4.7717020
H	-3.1747840	-3.9955810	3.1922020
H	-1.5370010	-4.3607320	1.3823480
H	0.6642730	-0.8984570	2.6587600
C	0.8852980	-1.9904500	-0.1966400
C	0.6717490	-2.8980630	0.8055900
C	1.3792420	-4.2276800	0.9199050
H	0.6461550	-5.0409660	0.9751130
H	2.0449520	-4.4243140	0.0821900
H	1.9415660	-4.2610050	1.8617200
C	-4.3351140	-1.7960750	-1.4542710
H	-4.3100690	-1.8706860	-2.5493200
H	-3.4361370	-2.2812190	-1.0825200
H	-5.2272740	-2.3314920	-1.1141660

Table 87. Atom coordinates and absolute energy of IM12^{Me} (Energy=-1889.84961a.u.)

Atom	X	Y	Z
Pd	1.0649550	0.0810750	0.1791350
C	1.3582330	2.1118970	0.2228670
N	1.5853560	3.2560730	0.1566660
C	1.9925580	4.6397440	0.0818130

C	0.7639690	5.5198780	0.3720110
C	2.5293580	4.8946120	-1.3391720
C	3.0951940	4.8585870	1.1341860
H	2.7120620	4.6720010	2.1411670
H	3.4511680	5.8917120	1.0820060
H	3.9354840	4.1836580	0.9542970
H	-0.0261830	5.3390080	-0.3616510
H	1.0503220	6.5744900	0.3232290
H	0.3657340	5.3141810	1.3693180
H	3.3847610	4.2478030	-1.5510090
H	2.8488380	5.9371630	-1.4269840
H	1.7546400	4.7037010	-2.0867050
C	2.9906540	-0.3401920	-0.2434780
N	3.0780170	-1.2377870	-1.3423200
N	4.0625630	0.0592350	0.3295350
O	3.7913080	0.9576940	1.4023550
C	5.0040170	1.1645170	2.1061600
H	5.7796170	1.5979770	1.4607270
H	4.7650350	1.8640550	2.9123030
H	5.3869570	0.2307300	2.5370830
C	2.0851960	-2.2215860	-1.2861030
O	2.0309640	-3.1752260	-2.0604730
C	4.1997120	-1.3102060	-2.3493570
C	5.1170900	-2.4940310	-1.9914390
H	5.9381930	-2.5685470	-2.7132640
H	5.5464470	-2.3519470	-0.9952200
H	4.5561050	-3.4308850	-2.0081540
C	5.0121350	-0.0032530	-2.3697740
H	4.3638400	0.8619100	-2.5432640
H	5.5590240	0.1605360	-1.4436690
H	5.7228480	-0.0635670	-3.2002470
C	3.5977440	-1.4837550	-3.7624330
H	4.4116300	-1.4839600	-4.4950620
H	3.0368180	-2.4105050	-3.8551450
H	2.9333010	-0.6445690	-3.9955130
H	-0.7290540	-1.5111010	-0.8694490
O	-1.6430080	1.5271520	1.0065300
C	-1.3115110	1.4882960	2.3941110
H	-1.8043190	0.6507600	2.8995180
H	-0.2279150	1.4060810	2.5328400
H	-1.6699880	2.4379220	2.7992620
N	-1.1492150	0.3656370	0.3697050
C	-2.0484160	-0.2229190	-0.3753850
O	-1.6672240	-1.2844310	-1.0882990

C	-8.1937630	0.0916660	-1.3063960
C	-8.3719630	1.4184200	-0.9114040
C	-7.2533910	2.2152510	-0.6583720
C	-5.9705770	1.6878960	-0.7887070
C	-5.7725540	0.3493540	-1.1758710
C	-6.9100790	-0.4332730	-1.4469480
H	-9.0559690	-0.5377700	-1.5074690
H	-9.3718700	1.8303750	-0.8110170
H	-7.3794750	3.2548470	-0.3694330
H	-5.1099700	2.3276730	-0.6209610
H	-6.7913650	-1.4682200	-1.7509670
C	-3.4421590	0.1959410	-0.4552560
C	-4.4076910	-0.2306780	-1.3077520
H	-3.6977460	0.9383970	0.2879470
C	-0.2992550	-1.6927220	4.0444340
C	-1.5583660	-2.2605540	4.2496530
C	-2.1278680	-3.0488090	3.2465240
C	-1.4386970	-3.2754490	2.0554880
C	-0.1793730	-2.6936670	1.8262330
C	0.3800690	-1.9011820	2.8430290
H	0.1606010	-1.0910570	4.8241690
H	-2.0872120	-2.0998580	5.1851530
H	-3.1076420	-3.4947630	3.3950810
H	-1.8912130	-3.8960890	1.2877400
H	1.3616270	-1.4653120	2.6860890
C	1.1399070	-1.9608980	-0.1471460
C	0.5834020	-2.9718330	0.5711530
C	0.6993990	-4.4496600	0.2378970
H	-0.2762470	-4.8500600	-0.0666100
H	1.3942830	-4.6271190	-0.5794000
H	1.0032840	-5.0116130	1.1285590
C	-4.2229600	-1.2733850	-2.3868290
H	-3.1881890	-1.3421460	-2.7132620
H	-4.5066860	-2.2667740	-2.0159790
H	-4.8629570	-1.0502550	-3.2446610

Table 88. Atom coordinates and absolute energy of IM13^{Me} (Energy=-1508.620328a.u.)

Atom	X	Y	Z
Pd	0.1417240	0.1616620	-0.1336230
C	1.1900070	1.9291420	-0.1611840
N	1.8815060	2.8716940	-0.1568150

C	2.9101520	3.8740450	0.0172770
C	2.8108110	4.8823670	-1.1396170
C	4.2637860	3.1389520	0.0086670
C	2.6654760	4.5621080	1.3729290
H	1.6860720	5.0483940	1.3925380
H	3.4342890	5.3221210	1.5403370
H	2.7088970	3.8326360	2.1854850
H	2.9448990	4.3832290	-2.1031870
H	3.5915860	5.6406720	-1.0308670
H	1.8387650	5.3838430	-1.1393820
H	4.2701620	2.3561650	0.7705450
H	5.0703300	3.8503170	0.2100630
H	4.4439490	2.6735450	-0.9642780
C	1.8090970	-0.9491770	0.2925590
N	1.8592270	-2.0748210	-0.5730960
N	2.7376960	-0.7892110	1.1591910
O	2.5485780	0.4061860	1.9251320
C	3.3053740	0.2700880	3.1161430
H	4.3697060	0.1055840	2.9026790
H	3.1809860	1.2107460	3.6610730
H	2.9394570	-0.5578120	3.7369370
C	0.5887430	-2.6390080	-0.7566910
O	0.4049390	-3.7036490	-1.3441190
C	3.1034210	-2.7769190	-1.0548410
C	3.3356800	-4.0368690	-0.1999090
H	4.2330090	-4.5655690	-0.5409050
H	3.4758920	-3.7616020	0.8496060
H	2.4834740	-4.7152430	-0.2801070
C	4.3304260	-1.8506340	-0.9696950
H	4.1549600	-0.9141470	-1.5095290
H	4.5981350	-1.6082320	0.0564470
H	5.1711880	-2.3629010	-1.4485510
C	2.9310070	-3.1464440	-2.5462410
H	3.8612440	-3.5985390	-2.9062790
H	2.1123930	-3.8445880	-2.7014610
H	2.7415100	-2.2449750	-3.1391600
C	-1.6533630	0.9487180	-0.7663840
C	-3.9357170	1.8241690	-1.6911100
C	-4.6368170	2.5802320	-0.5473250
H	-5.6134980	2.9329510	-0.8916870
H	-4.7814020	1.9257900	0.3159030
H	-4.0461050	3.4461030	-0.2347480
C	-3.6747760	2.7519750	-2.8914380
H	-3.0737360	3.6157210	-2.5936950

H	-3.1487020	2.2186640	-3.6879130
H	-4.6288120	3.1128130	-3.2864570
C	-4.7489210	0.5870750	-2.1137330
H	-4.8925970	-0.0843820	-1.2639030
H	-5.7280300	0.9054650	-2.4839280
H	-4.2368120	0.0396990	-2.9098060
N	-2.6564270	1.3644040	-1.1974380
C	-0.4805360	-1.8057410	-0.1163530
C	-1.6059340	-2.3557280	0.4049990
C	-2.5920060	-1.5437970	1.1737670
C	-2.1865910	-0.5522670	2.0869730
C	-3.9743580	-1.7880600	1.0501700
C	-3.1202340	0.1840810	2.8173150
H	-1.1252960	-0.3800560	2.2353150
C	-4.9097880	-1.0471210	1.7729880
H	-4.3214150	-2.5622510	0.3727780
C	-4.4875200	-0.0536120	2.6611960
H	-2.7755990	0.9349080	3.5236190
H	-5.9699970	-1.2543410	1.6514660
H	-5.2140200	0.5111590	3.2391800
C	-1.9729870	-3.8287260	0.2836270
H	-2.6931240	-3.9866150	-0.5301460
H	-1.1058890	-4.4405230	0.0463970
H	-2.4438940	-4.1830600	1.2067280

Table 89. Atom coordinates and absolute energy of TS13^{Me} (Energy=-1508.598806a.u.)

Atom	X	Y	Z
Pd	0.0949700	0.5302970	-0.1409200
C	1.7656340	1.5436280	0.4714920
N	2.7374360	2.0871990	0.8406500
C	3.9621300	2.6851630	1.3146750
C	3.6281510	3.5405230	2.5509590
C	4.5368020	3.5583440	0.1837180
C	4.9352120	1.5483980	1.6798130
H	4.5102720	0.9129170	2.4610890
H	5.8759890	1.9720490	2.0440570
H	5.1465040	0.9254690	0.8066740
H	2.9167330	4.3307490	2.2955790
H	4.5418310	4.0047940	2.9337320
H	3.1928030	2.9238220	3.3418240
H	4.7467350	2.9544630	-0.7032070

H	5.4692920	4.0235230	0.5168290
H	3.8331120	4.3483540	-0.0927220
C	0.8660200	-1.4735590	-0.3128270
N	0.9665040	-1.7128530	-1.7256630
N	1.6411750	-2.0867520	0.5144690
O	1.3946750	-1.6750310	1.8473500
C	2.0172650	-2.6013850	2.7192030
H	3.0959930	-2.6713030	2.5258730
H	1.8467370	-2.2188540	3.7289090
H	1.5754680	-3.6022550	2.6306210
C	-0.3965430	-1.6995730	-2.0246660
O	-0.9591270	-1.9316880	-3.0814410
C	2.0921180	-2.2714610	-2.5112040
C	2.0993820	-3.8064370	-2.3600320
H	2.9336090	-4.2409880	-2.9218200
H	2.2033110	-4.0835930	-1.3078510
H	1.1684840	-4.2333050	-2.7459810
C	3.4122590	-1.6721140	-1.9952660
H	3.3896780	-0.5800130	-2.0682620
H	3.5946600	-1.9476040	-0.9560010
H	4.2374020	-2.0416080	-2.6128650
C	1.9062960	-1.8739480	-3.9877190
H	2.7445460	-2.2702970	-4.5701710
H	0.9715690	-2.2603620	-4.3933170
H	1.8991230	-0.7843130	-4.0937340
C	-1.4067330	1.8970720	-0.5533350
C	-3.3824060	3.4357670	-1.3103680
C	-4.6040470	2.5209320	-1.5181420
H	-5.4589530	3.1191730	-1.8473790
H	-4.3947900	1.7628300	-2.2773890
H	-4.8707990	2.0141210	-0.5868980
C	-3.6572850	4.4793310	-0.2120760
H	-3.9165270	3.9904960	0.7309180
H	-2.7792650	5.1099270	-0.0471030
H	-4.4925580	5.1180630	-0.5140160
C	-2.9774580	4.1194940	-2.6295750
H	-2.7511000	3.3749730	-3.3974740
H	-3.7999710	4.7475860	-2.9844230
H	-2.0952280	4.7494060	-2.4859120
N	-2.2777600	2.6117180	-0.8791670
C	-0.8841860	-1.3728230	-0.6332990
C	-1.9775500	-1.9306880	-0.0286420
C	-2.3044970	-1.7957660	1.4090640
C	-1.7384610	-0.8059900	2.2397750

C	-3.2300940	-2.6787360	2.0085480
C	-2.0727730	-0.7094520	3.5872330
H	-1.0254830	-0.1018750	1.8212220
C	-3.5623250	-2.5842200	3.3586650
H	-3.6904730	-3.4615810	1.4172580
C	-2.9879830	-1.5965940	4.1591800
H	-1.6165910	0.0688030	4.1936410
H	-4.2742450	-3.2865530	3.7842260
H	-3.2509060	-1.5168450	5.2104250
C	-2.9211880	-2.7827790	-0.8608860
H	-2.7055200	-2.6896180	-1.9233930
H	-2.8395170	-3.8443300	-0.5892760
H	-3.9628420	-2.4900700	-0.6863940

Table 90. Atom coordinates and absolute energy of 2a^{Me} (Energy=-880.9496411a.u.)

Atom	X	Y	Z
C	-0.8454170	0.3951570	-0.0469100
N	-2.1049730	-0.2475110	0.1078350
N	-0.6791870	1.6514160	-0.2137140
O	0.6729820	1.9758410	-0.4210940
C	0.7807400	3.3827490	-0.5892520
H	0.4264890	3.9204180	0.2983200
H	1.8453930	3.5749120	-0.7380010
H	0.2159070	3.7234370	-1.4650420
C	-1.5322750	-1.5332910	0.0473310
O	-2.0150040	-2.6435250	0.0640180
C	-3.4814690	0.2874810	0.0783480
C	-3.7532190	0.8778300	-1.3195260
H	-4.7590760	1.3084870	-1.3542540
H	-3.0314560	1.6636530	-1.5549870
H	-3.6870730	0.0995610	-2.0859360
C	-3.6040470	1.3798250	1.1573670
H	-3.4082400	0.9629510	2.1500350
H	-2.8979680	2.1926070	0.9749880
H	-4.6189560	1.7896400	1.1514030
C	-4.4609410	-0.8581520	0.3773830
H	-5.4799250	-0.4597580	0.3648950
H	-4.3866220	-1.6575270	-0.3616760
H	-4.2732400	-1.2934580	1.3624080
C	-0.1490430	-0.9253980	-0.0337110
C	1.0786120	-1.4828310	-0.0555080
C	2.3511820	-0.7289770	0.0502590

C	2.5095910	0.2794520	1.0150900
C	3.4552490	-1.0661460	-0.7520630
C	3.7298420	0.9346270	1.1666870
H	1.6749100	0.5321280	1.6586790
C	4.6687070	-0.3961430	-0.6140530
H	3.3592680	-1.8432280	-1.5038060
C	4.8118020	0.6039260	0.3497250
H	3.8359690	1.7021230	1.9278590
H	5.5046340	-0.6592190	-1.2555820
H	5.7621710	1.1164210	0.4672910
C	1.1839930	-2.9897260	-0.1483760
H	0.2025600	-3.4631200	-0.1139140
H	1.6736110	-3.2796150	-1.0859000
H	1.8071130	-3.3785610	0.6642330