Decarboxylative-Coupling of Allyl Acetate catalysed by group 10 organometallics, $[(phen)M(CH_3)]^+$

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Supporting Information

***Complete citation for reference 55*:** *Gaussian 09*, revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B. Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr. J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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Table S1: $[(phen)M(CH_3)]^+$ generated *via* CID of the acetate complexes $[(phen)M(O_2CCH_3)]^+$; M = Ni, Pd, Pt and its products of ion-molecule reactions with allyl acetate identified *via* High Resolution FT-MS.

Isotope selected	Experimental High resolution *m/z* value	Theoretical exact *m/z* of isobaric species	error (ppm)	empirical formula	ion assignment
^{58}Ni	253.02693	253.02702	0.36ppm	$NiN_2C_{13}H_{11}$	$[(phen)Ni(CH_3)]^+$
	255.00622	255.00629	0.27ppm	$NiN_2C_{12}H_{10}O$	$[(phen)Ni(OH)]^+$
	271.03741	271.03759	0.66ppm	$NiN_2C_{13}H_{13}O$	$[(phen)Ni(CH_3)(H_2O)]^+$
	297.01650	297.01685	1.18ppm	$NiN_2C_{14}H_{11}O_2$	$[(phen)Ni(O_2CCH_3)]^+$
	353.07938	353.07945	0.20ppm	$NiN_2C_{18}H_{19}O_2$	$[(phen)Ni(CH_3)(C_3H_5CO_2CH_3)]^+$
^{106}Pd	300.99503	300.99516	0.43ppm	$PdN_2C_{13}H_{11}$	$[(phen)Pd(CH_3)]^+$
	319.00568	319.00572	0.13ppm	$PdN_2C_{13}H_{13}O$	$[(phen)Pd(CH_3)(H_2O)]^+$
	344.98482	344.98499	0.49ppm	$PdN_2C_{14}H_{11}O_2$	$[(phen)Pd(O_2CCH_3)]^+$
	401.04721	401.04759	0.95ppm	$PdN_2C_{18}H_{19}O_2$	$[(phen)Pd(CH_3)(C_3H_5CO_2CH_3)]^+$
^{195}Pt	390.05677	390.05645	0.82ppm	$PtN_2C_{13}H_{11}$	$[(phen)Pt(CH_3)]^+$
	408.06757	408.06701	1.37ppm	$PtN_2C_{13}H_{13}O$	$[(phen)Pt(CH_3)(H_2O)]^+$
	434.04688	434.04628	1.38ppm	$PtN_2C_{14}H_{11}O_2$	$[(phen)Pt(O_2CCH_3)]^+$
	474.07860	474.07758	2.15ppm	$PtN_2C_{17}H_{15}O_2$	$[(phen)Pt(O_2CCH_3C_3H_4)]^+$
	490.11018	490.10888	2.65ppm	$PtN_2C_{18}H_{19}O_2$	$[(phen)Pt(CH_3)(C_3H_5CO_2CH_3)]^+$

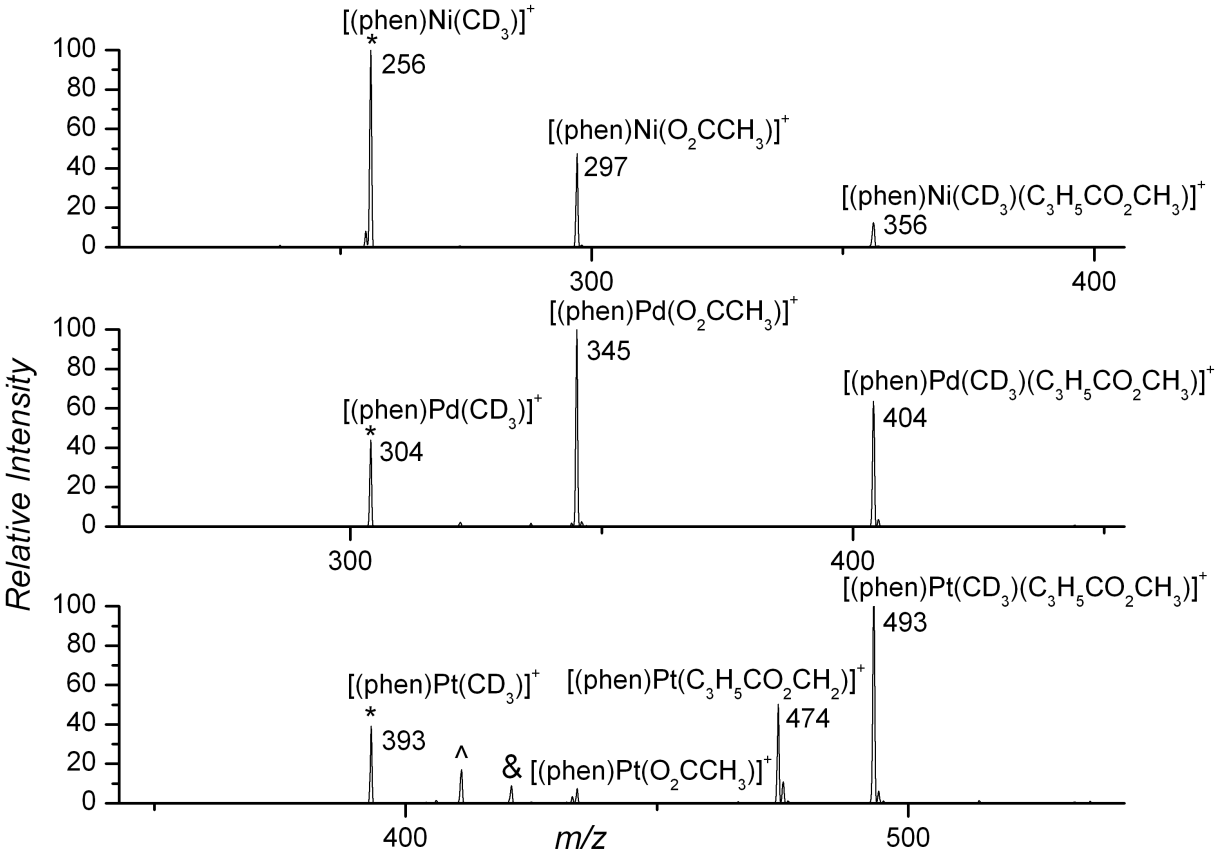


Figure S1: LTQ-FT-ICR MS^3 spectra of ion-molecule reactions of mass selected $[(phen)M(CD_3)]^+$ with allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.

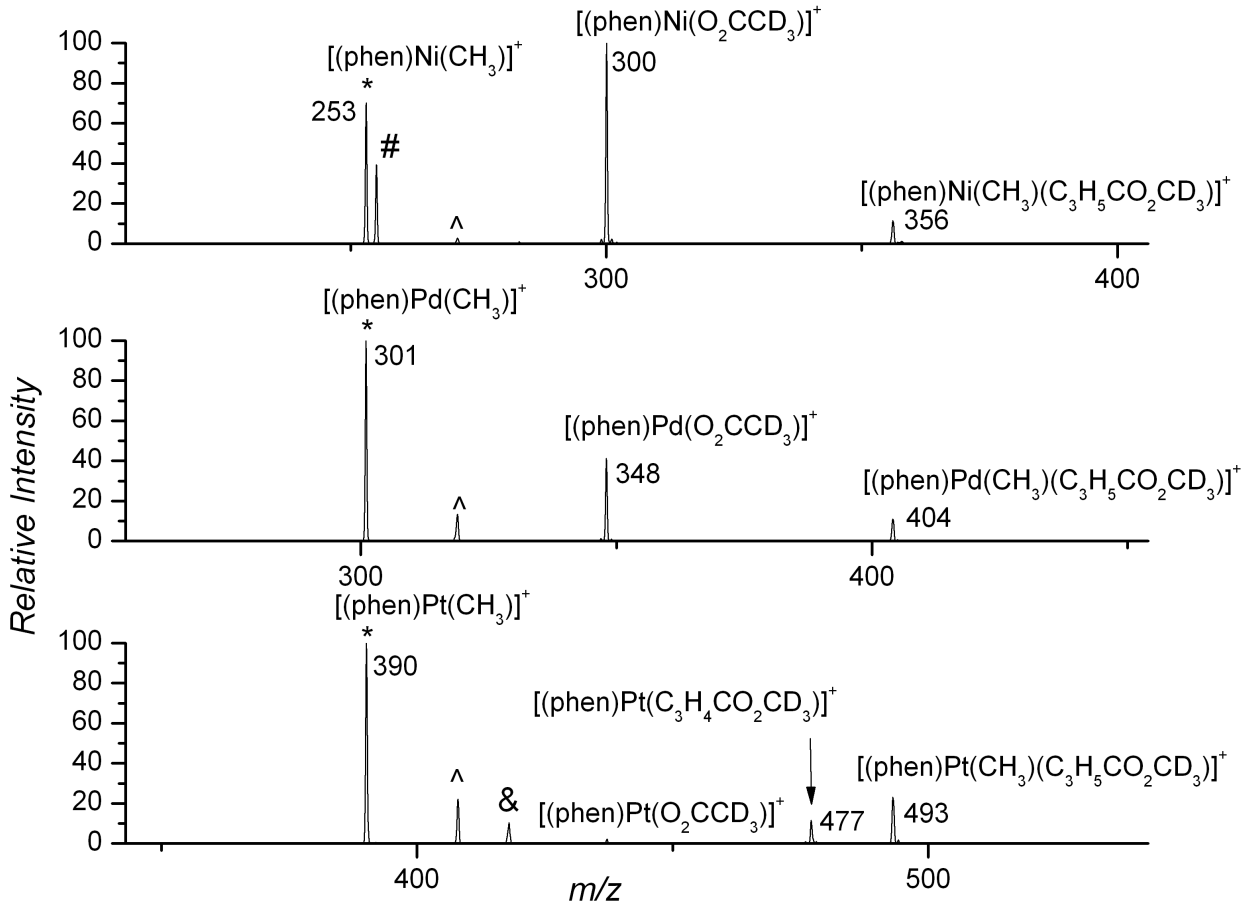


Figure S2: LTQ-FT-ICR MS^3 spectra of ion-molecule reactions of mass selected $[(phen)M(CH_3)]^+$ with D3-allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.

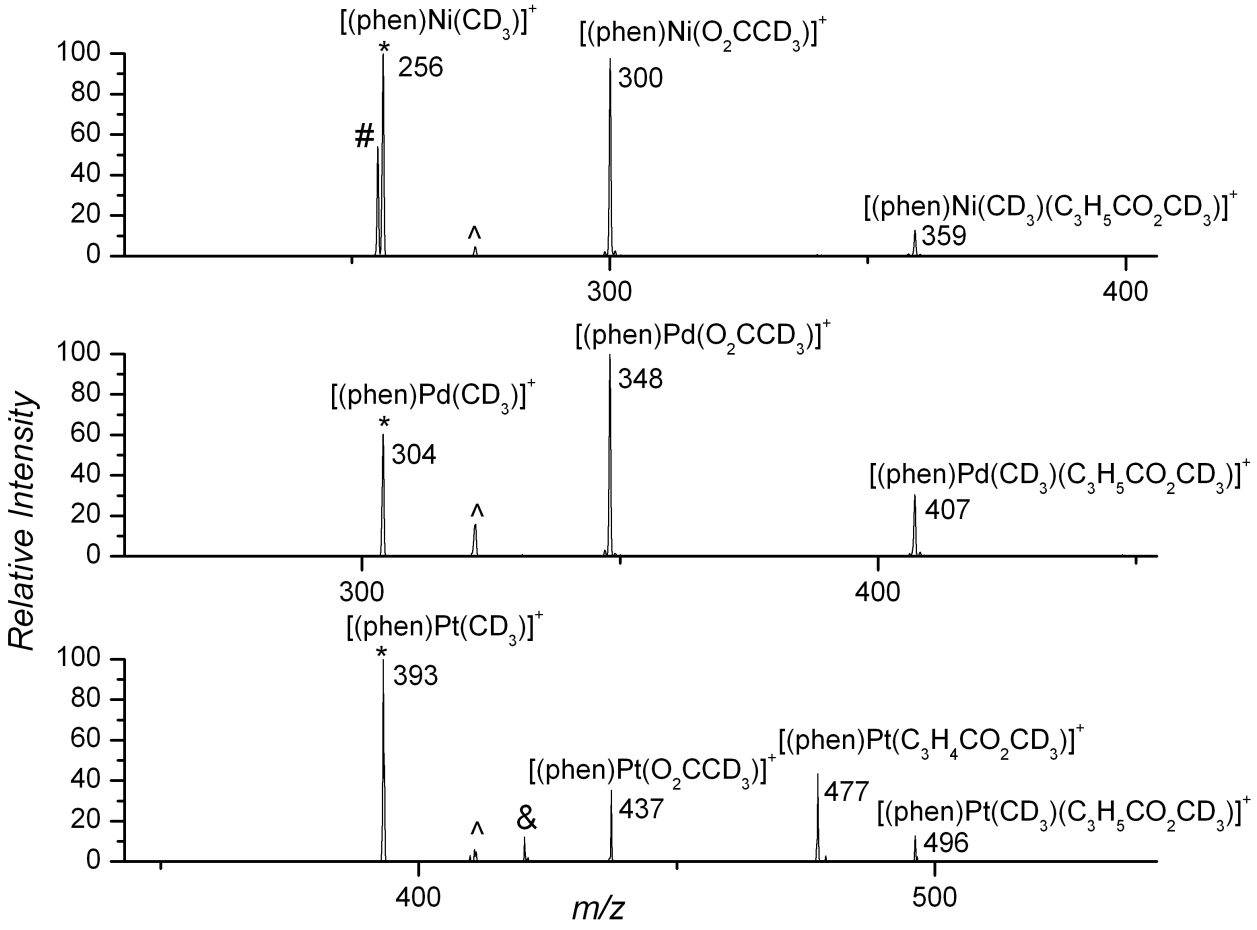


Figure S3: LTQ-FT-ICR MS^3 spectra of ion-molecule reactions of mass selected $[(phen)M(CD_3)]^+$ with D3-allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.

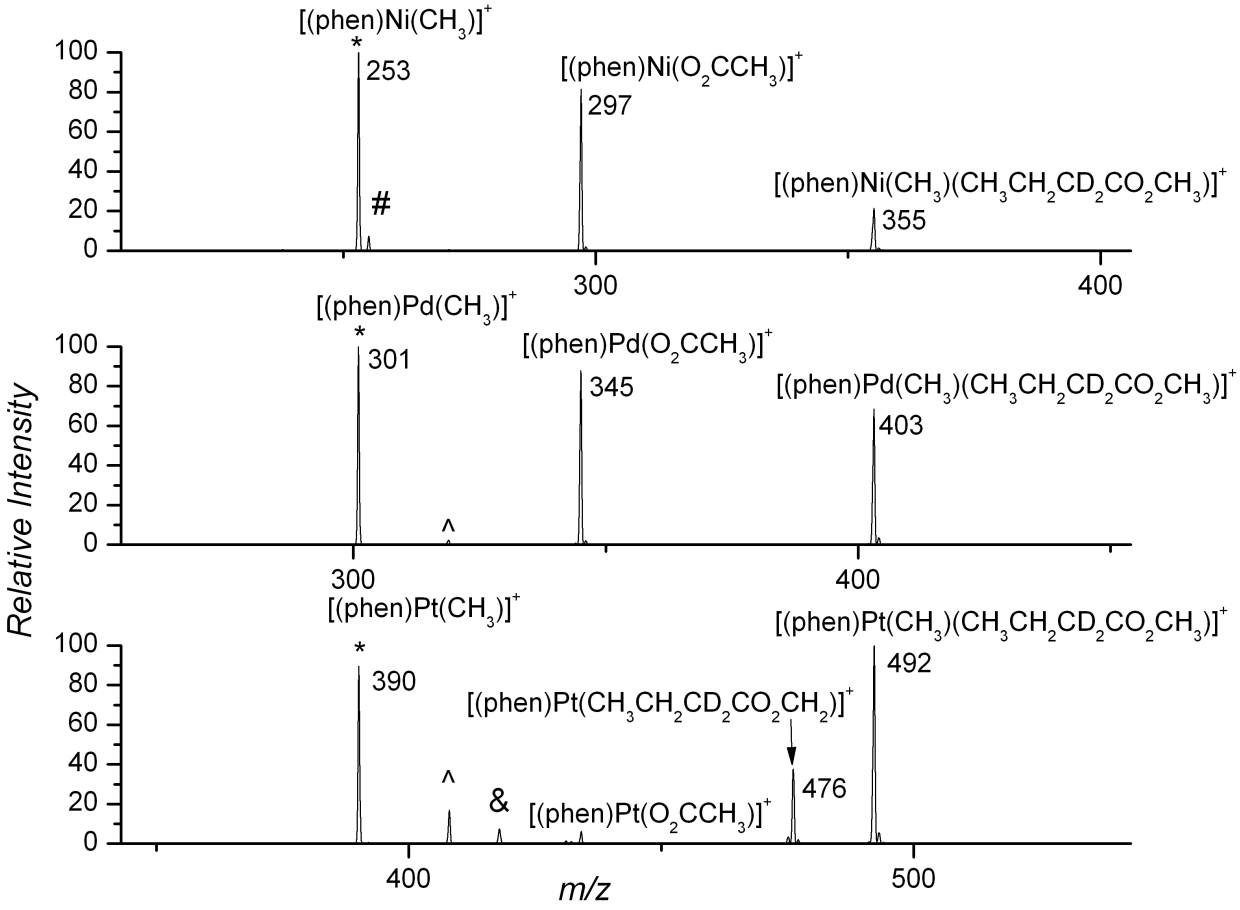


Figure S4: LTQ-FT-ICR MS^3 spectra of ion-molecule reactions of mass selected $[(phen)M(CH_3)]^+$ with D2-allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.

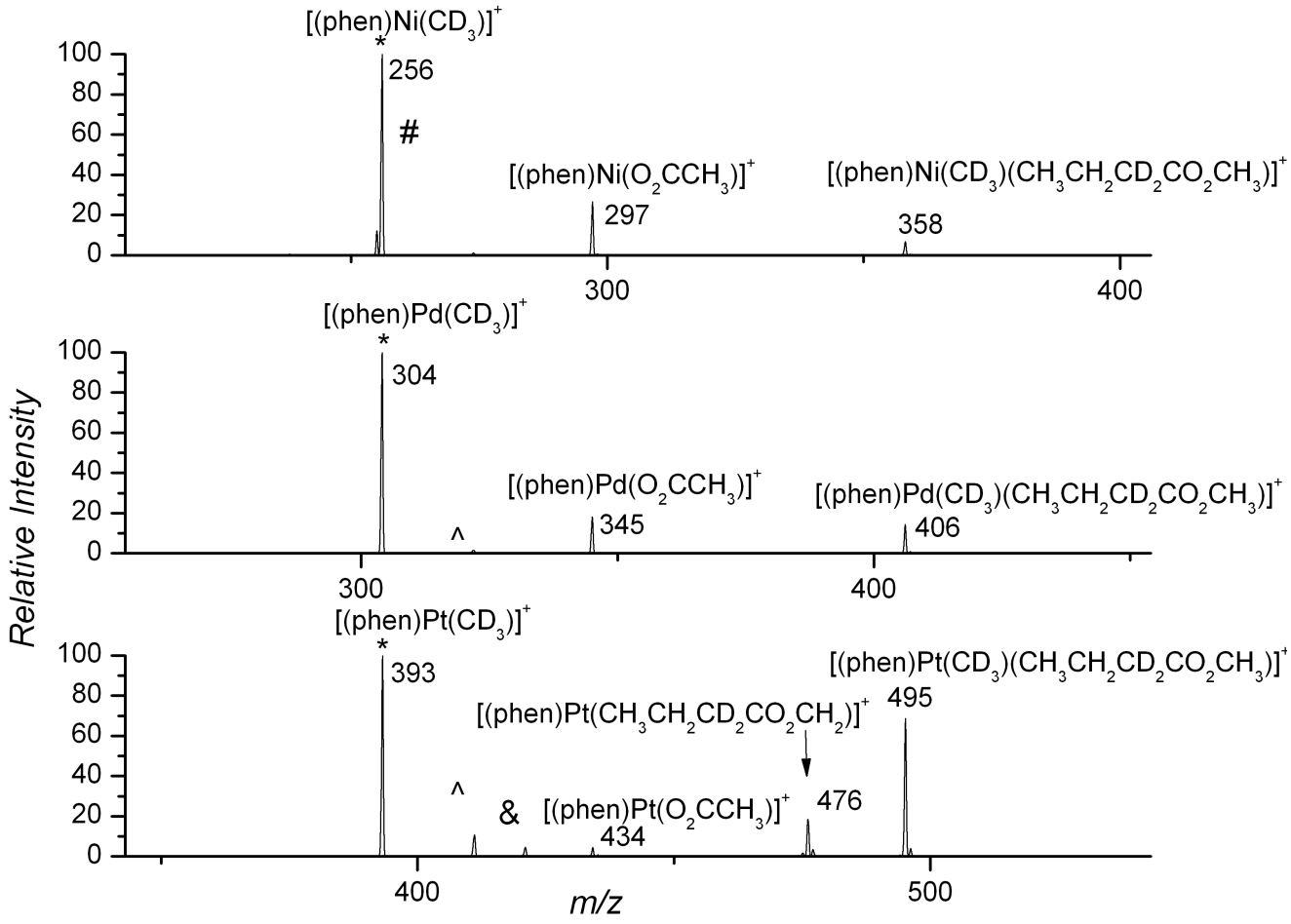


Figure S5: LTQ-FT-ICR MS^3 spectra of ion-molecule reactions of mass selected $[(phen)M(CD_3)]^+$ with D2-allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.

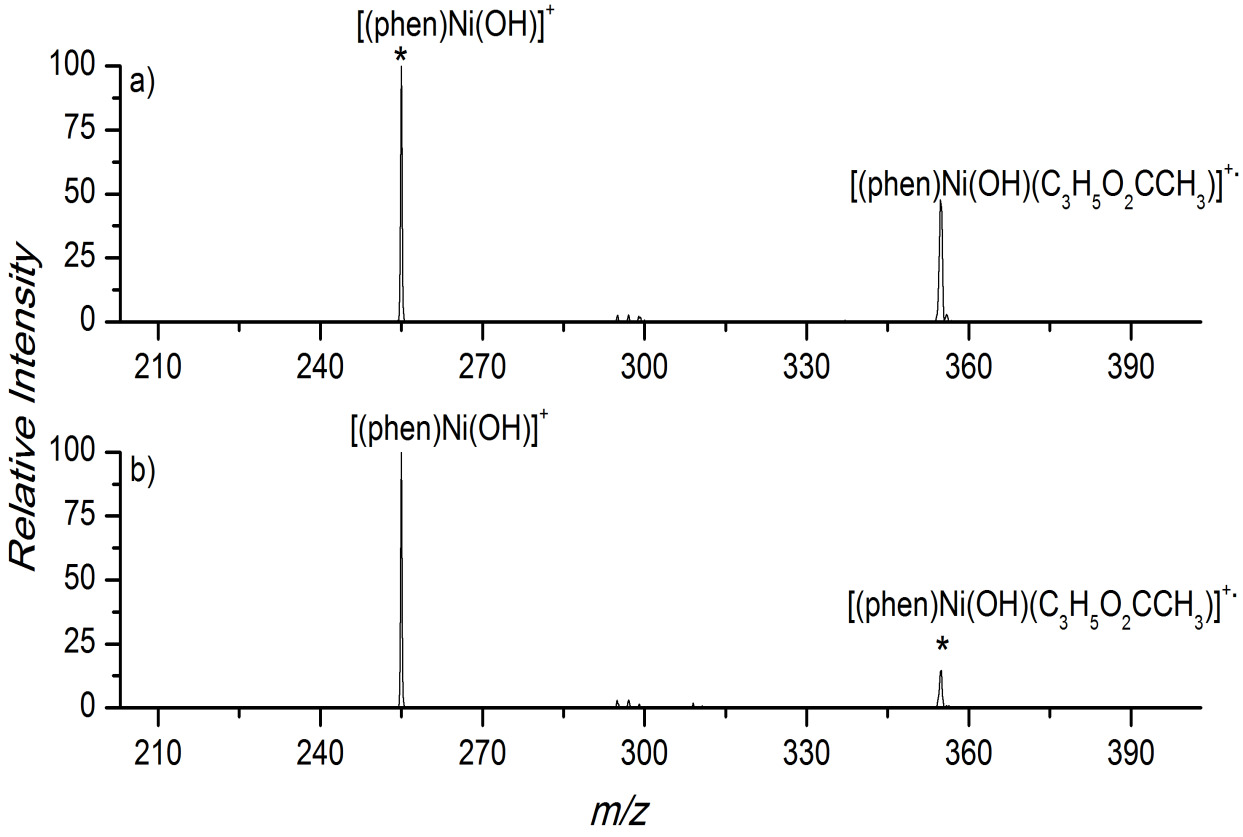


Figure S6: LTQ-FT-ICR MS^n spectra of ion-molecule reactions of mass selected $[(phen)Ni(OH)]^+$ with allyl acetate in the linear ion trap and subsequent CID of the adduct $[(phen)Ni(OH)(CH_3CO_2C_3H_5)]^+$. (a) IMR of $[(phen)Ni(OH)]^+$ with allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; (b) CID of $[(phen)Ni(OH)(CH_3CO_2C_3H_5)]^+$ at a normalized collision energy of 25 (arbitrary units).

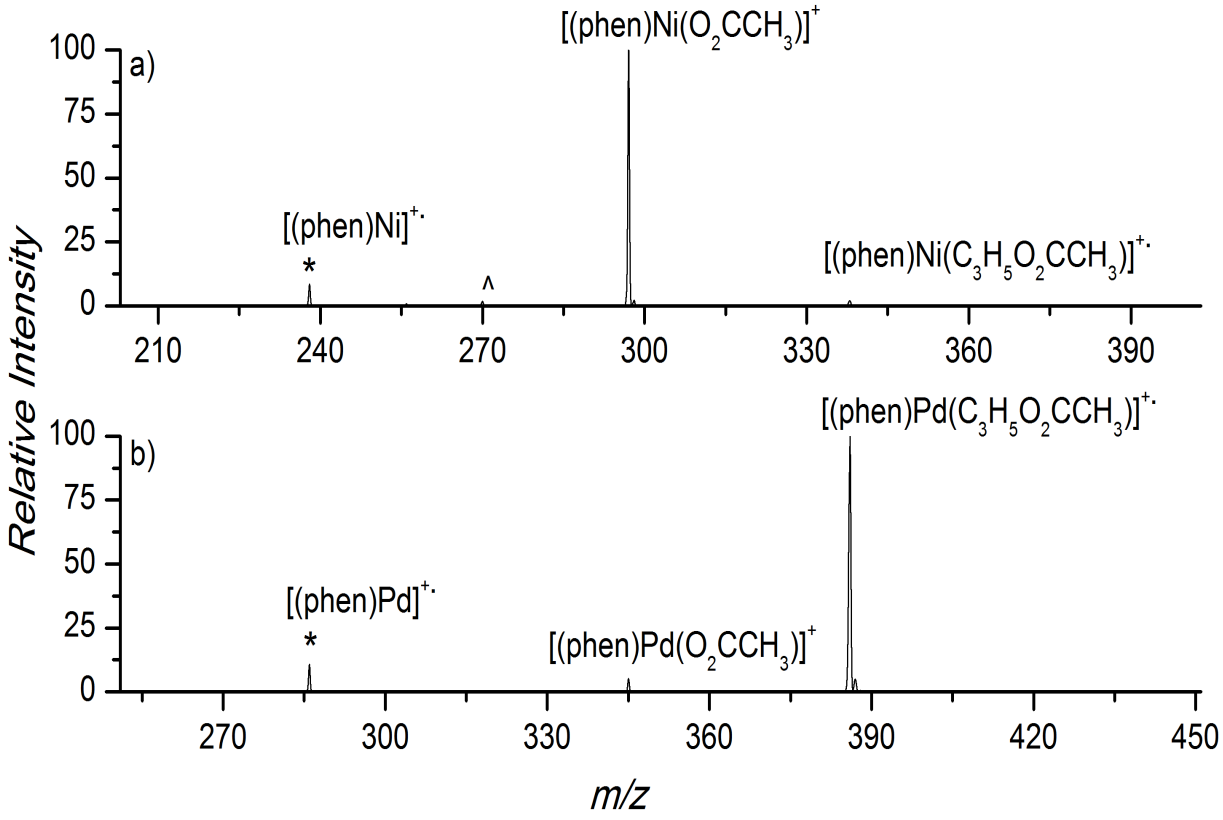


Figure S7: LTQ-FT-ICR MS^n spectra of ion-molecule reactions of mass selected $[(phen)M]^{+\bullet}$ with allyl acetate in the linear ion trap: (a) IMR of $[(phen)Ni]^{+\bullet}$ with allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni, Pd & Pt.; (b) IMR of $[(phen)Pd]^{+\bullet}$ with allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 30ms in the linear ion trap; M = Ni & Pd.

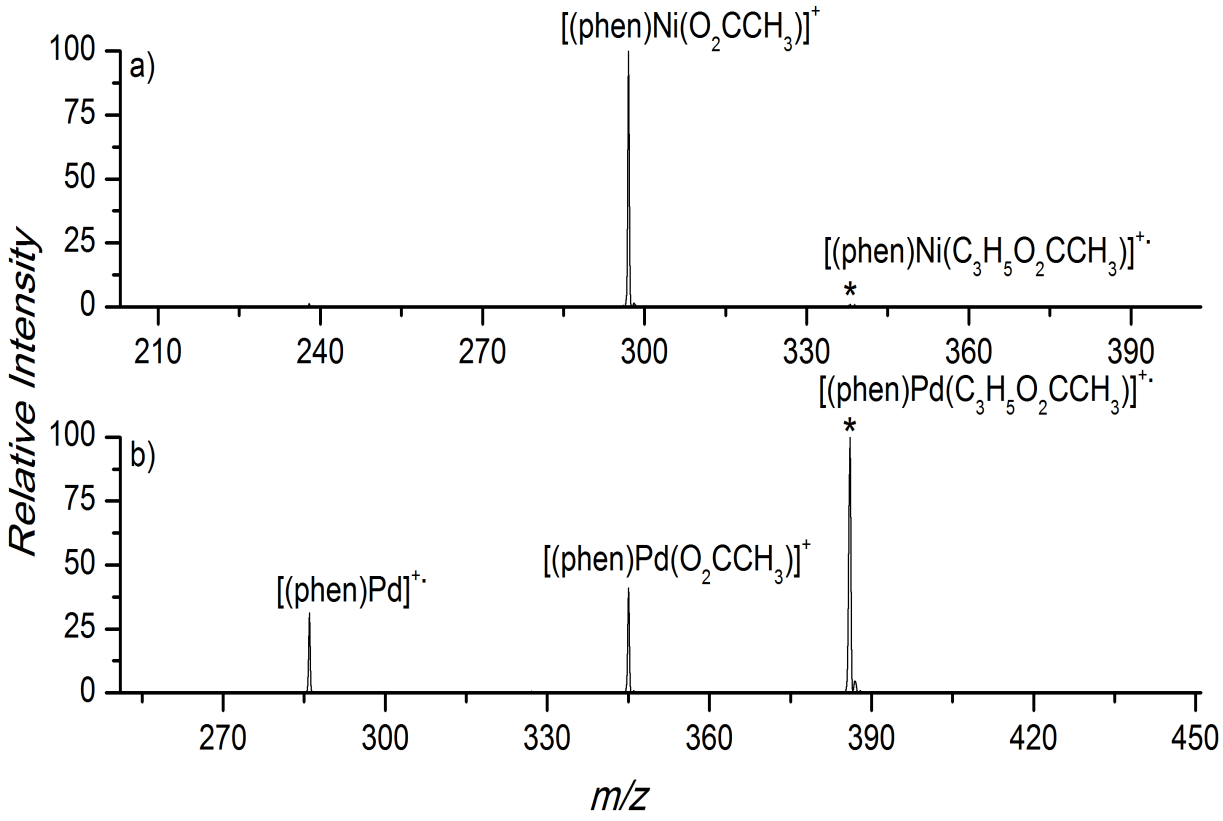


Figure S8: LTQ-FT-ICR MS^n spectra of CID reactions of $[(phen)M(CH_3CO_2C_3H_5)]^{+\bullet}$ at a normalized collision energy of 25 (arbitrary units). (a) CID of $[(phen)Ni(CH_3CO_2C_3H_5)]^{+\bullet}$ (b) CID of $[(phen)Pd(CH_3CO_2C_3H_5)]^{+\bullet}$

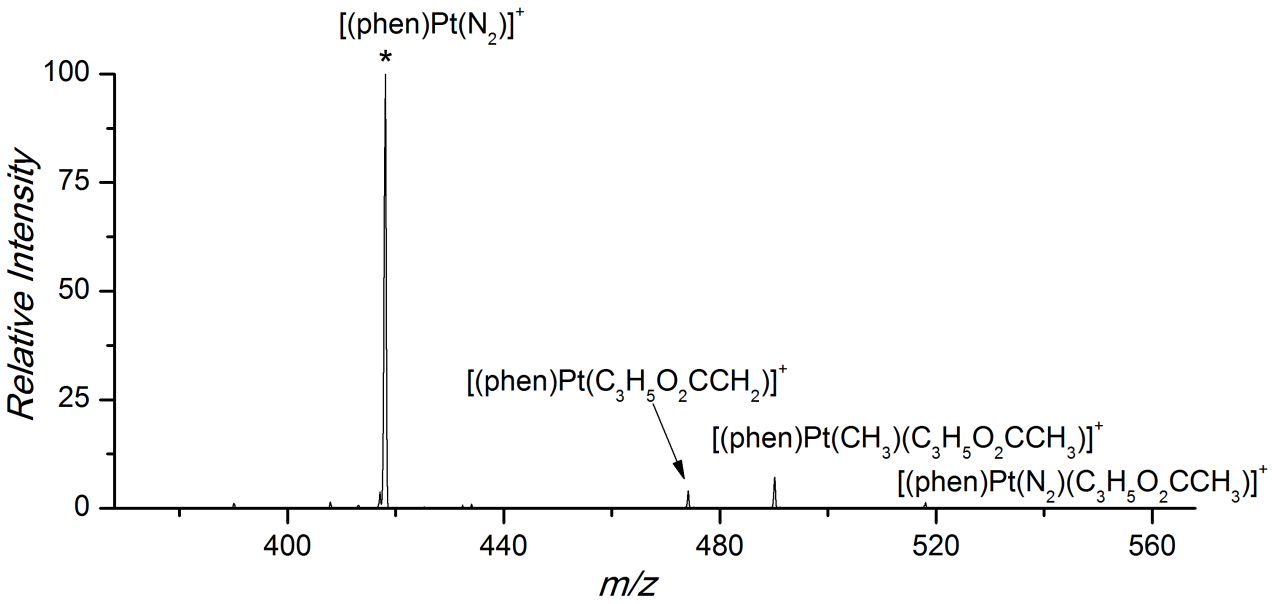


Figure S9: LTQ-FT-ICR MS^n spectra of ion-molecule reactions of mass selected $[(phen)Pt(N_2)]^+$ with allyl acetate with allyl acetate (~5 * 10^9 molecules/cm^3) for a period of 1000ms in the linear ion trap.

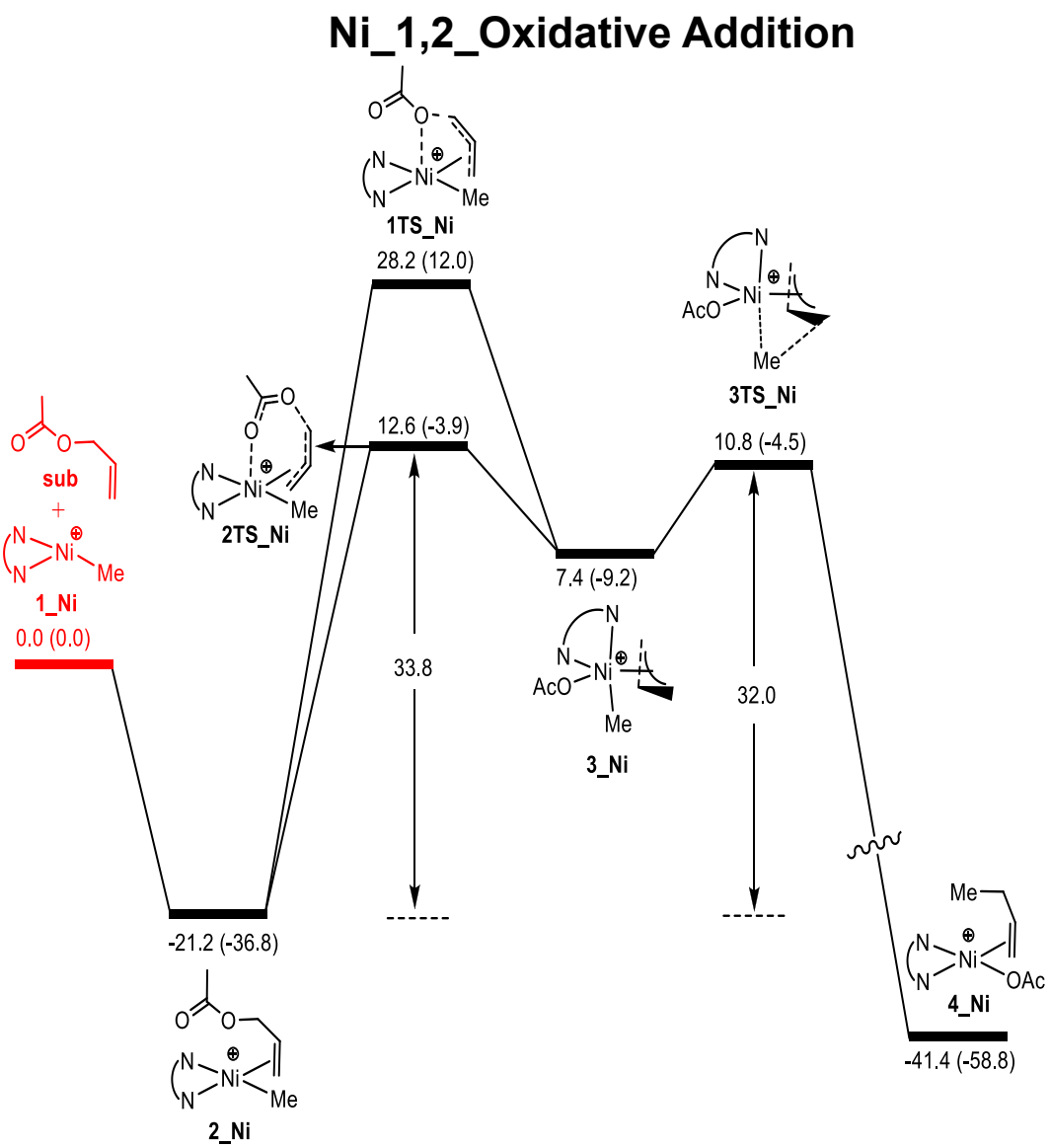


Figure S10: Calculated potential energy diagram for the reaction of $[(phen)Ni(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

Ni_3,4_Oxidative Addition

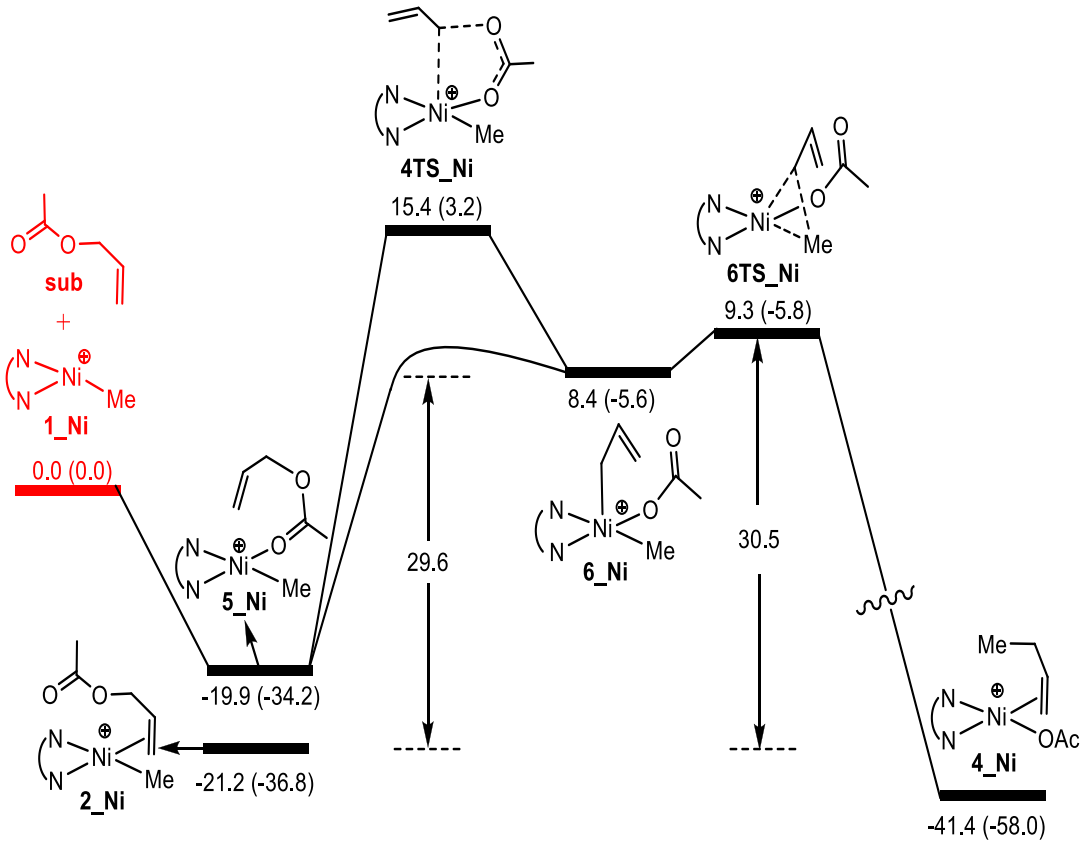


Figure S11: Calculated potential energy diagram for the reaction of $[(phen)Ni(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

Ni_5,6_Oxidative Addition

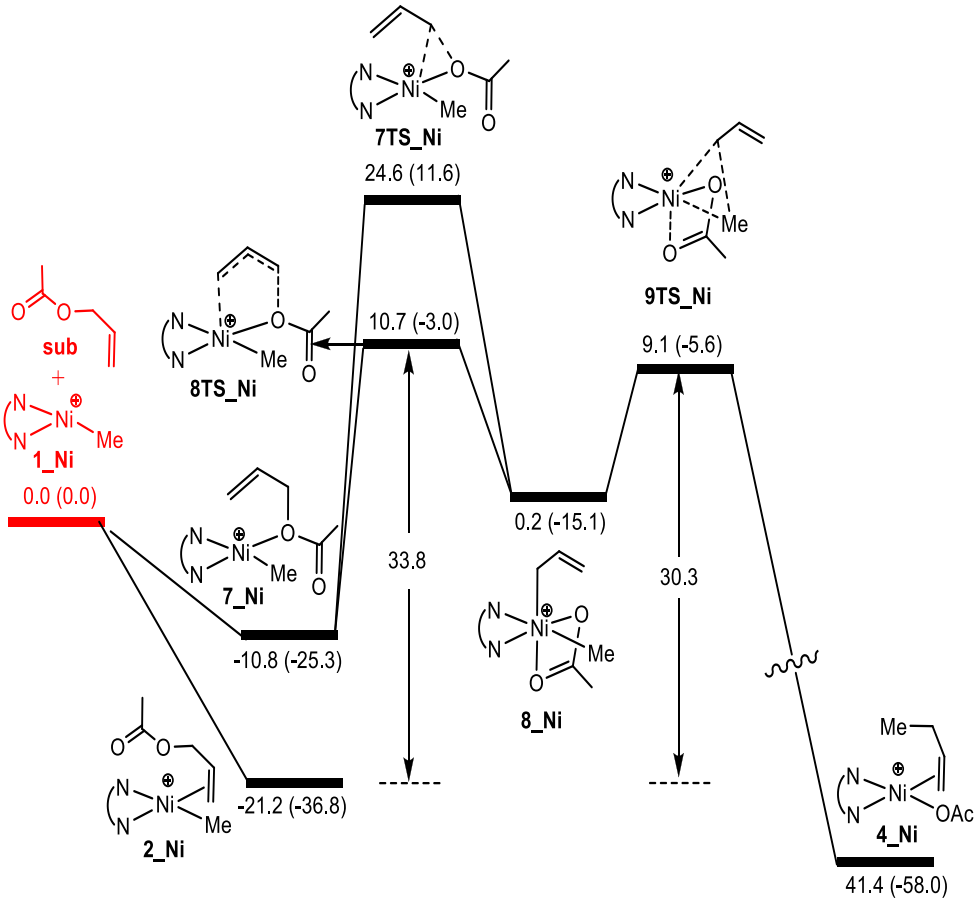


Figure S12: Calculated potential energy diagram for the reaction of $[(phen)Ni(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

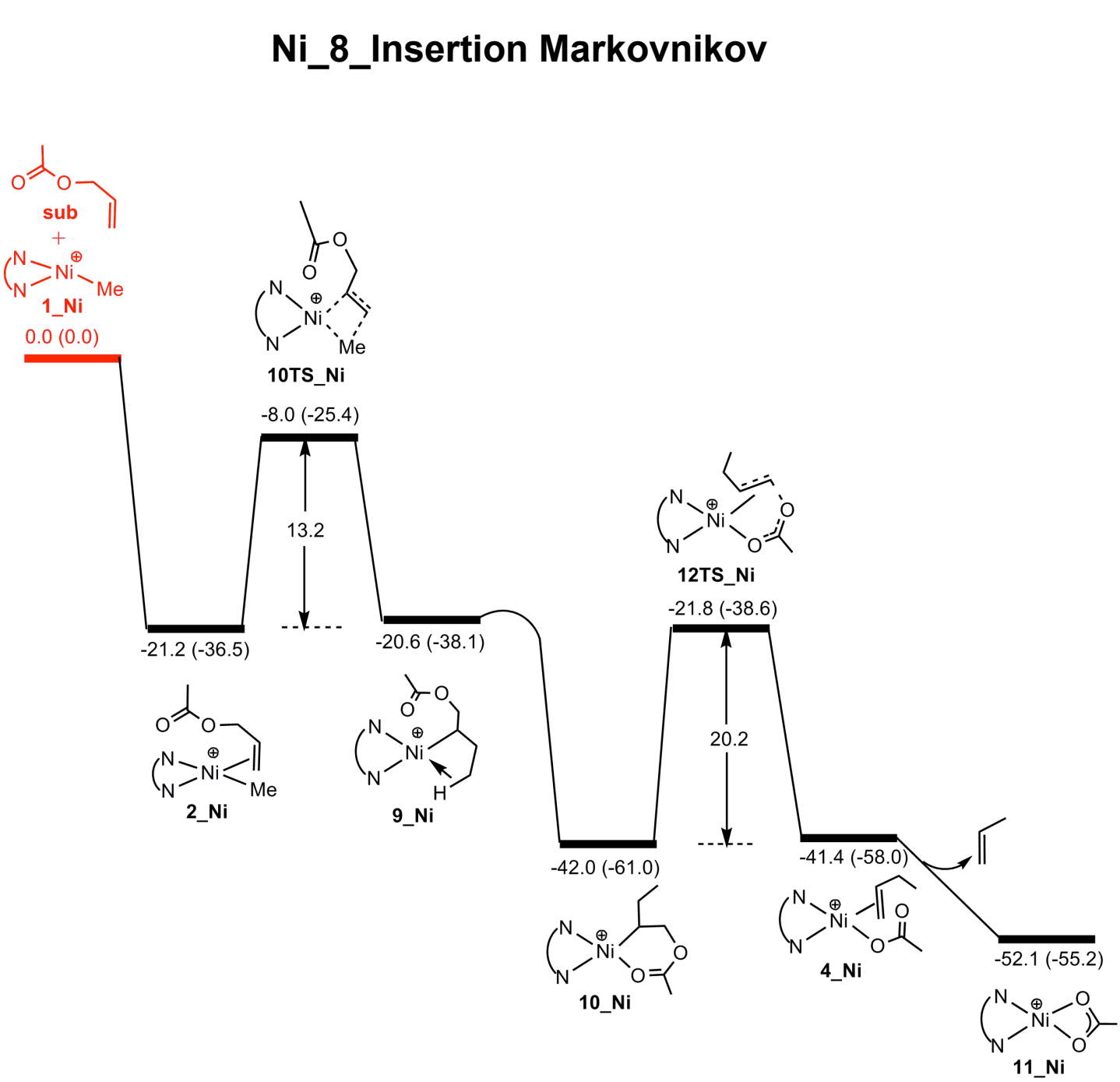


Figure S13: Calculated potential energy diagram for the reaction of $[(phen)Ni(CH_3)]^+$ and allyl acetate proceeding *via* the Markovinikov insertion pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

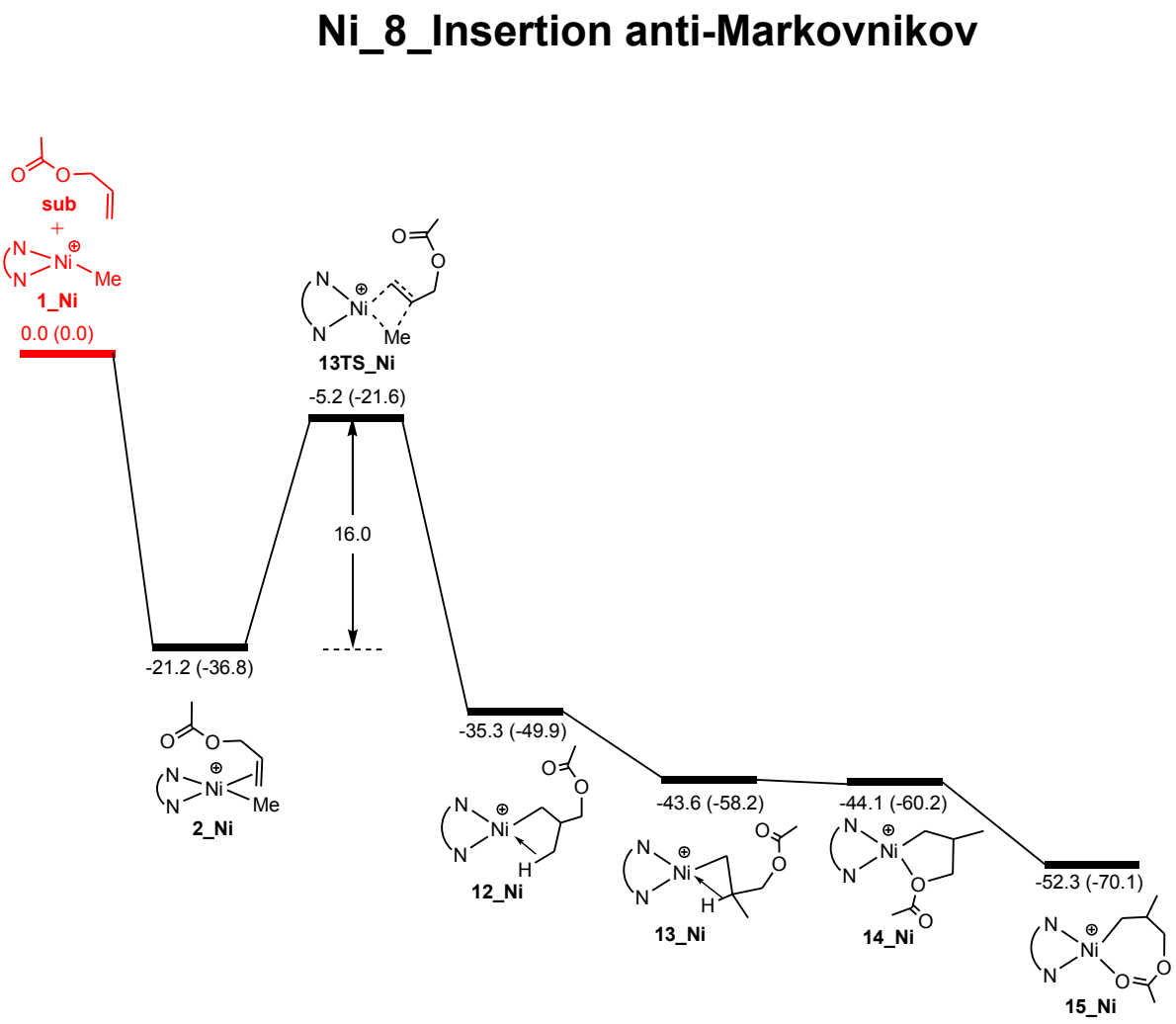


Figure S14: Calculated potential energy diagram for the reaction of $[(phen)Ni(CH_3)]^+$ and allyl acetate proceeding *via* the anti-Markovinikov insertion pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

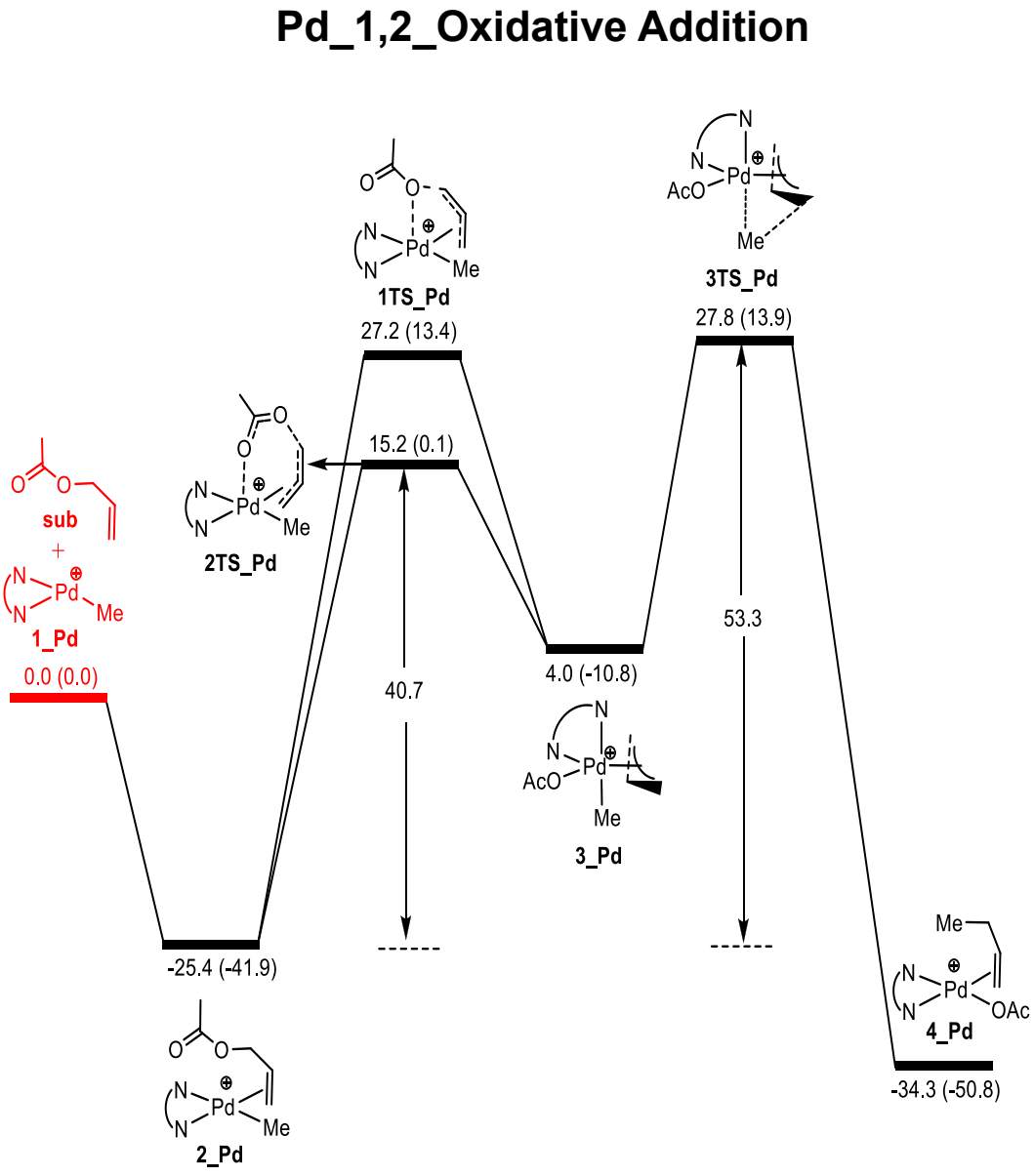


Figure S15: Calculated potential energy diagram for the reaction of $[(phen)Pd(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

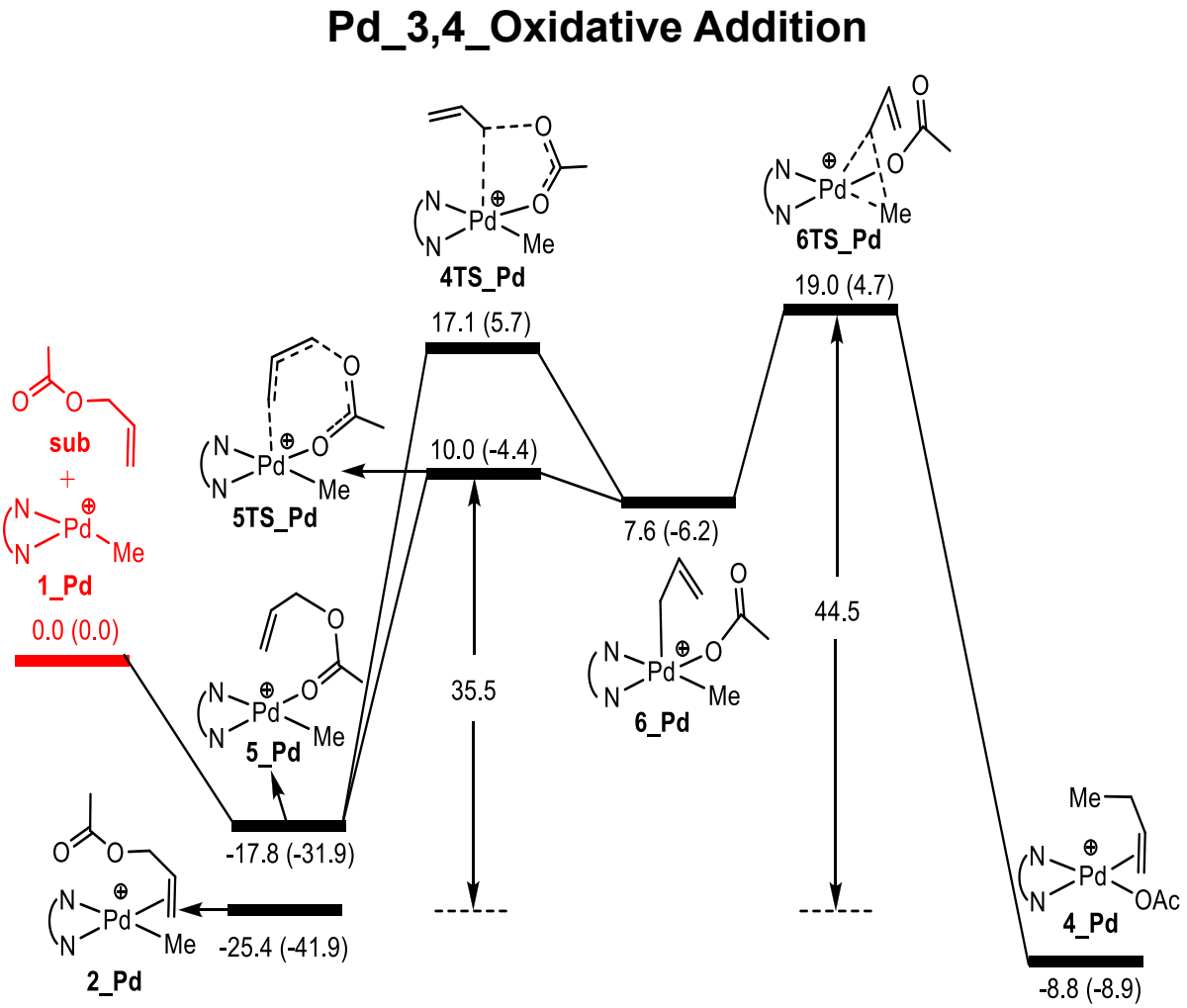


Figure S16: Calculated potential energy diagram for the reaction of $[(phen)Pd(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

Pd_8_Insertion anti-Markovnikov

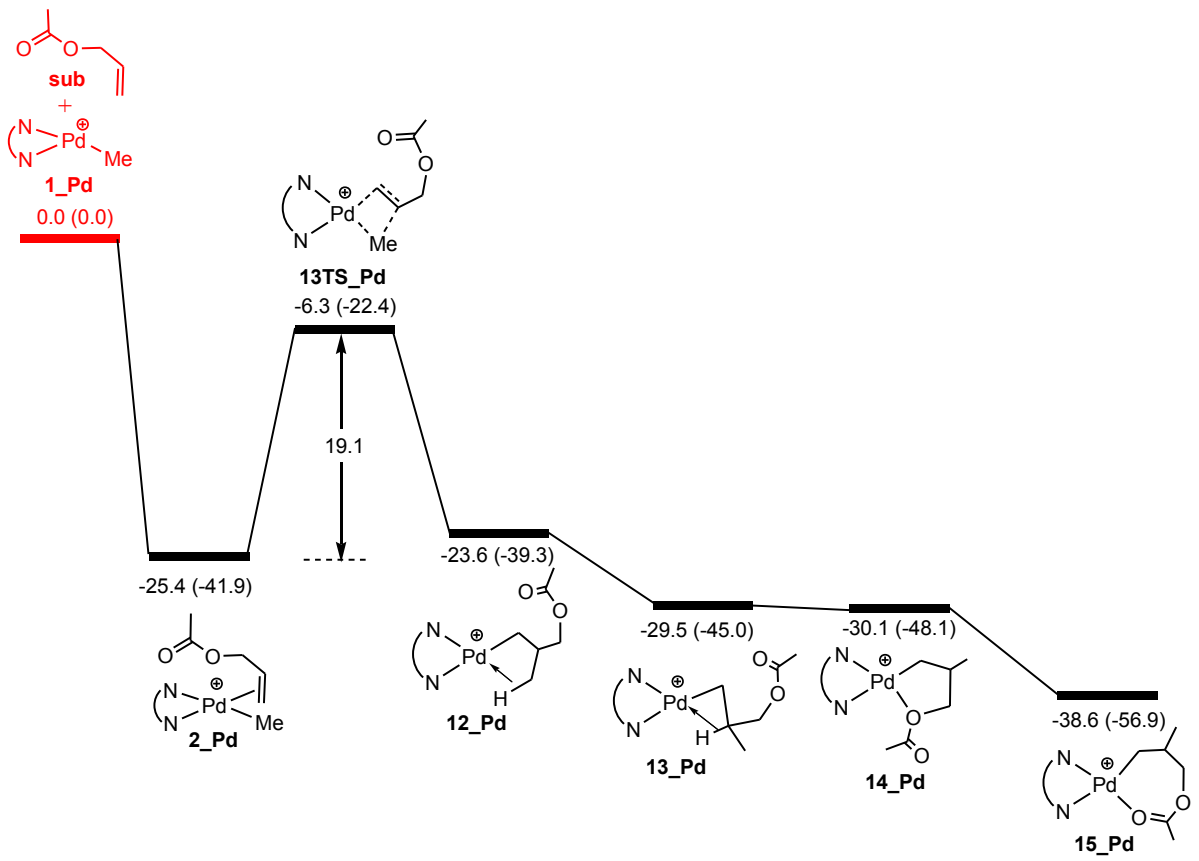


Figure S17: Calculated potential energy diagram for the reaction of $[(phen)Pd(CH_3)]^+$ and allyl acetate proceeding *via* the anti-markovinikov insertion pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

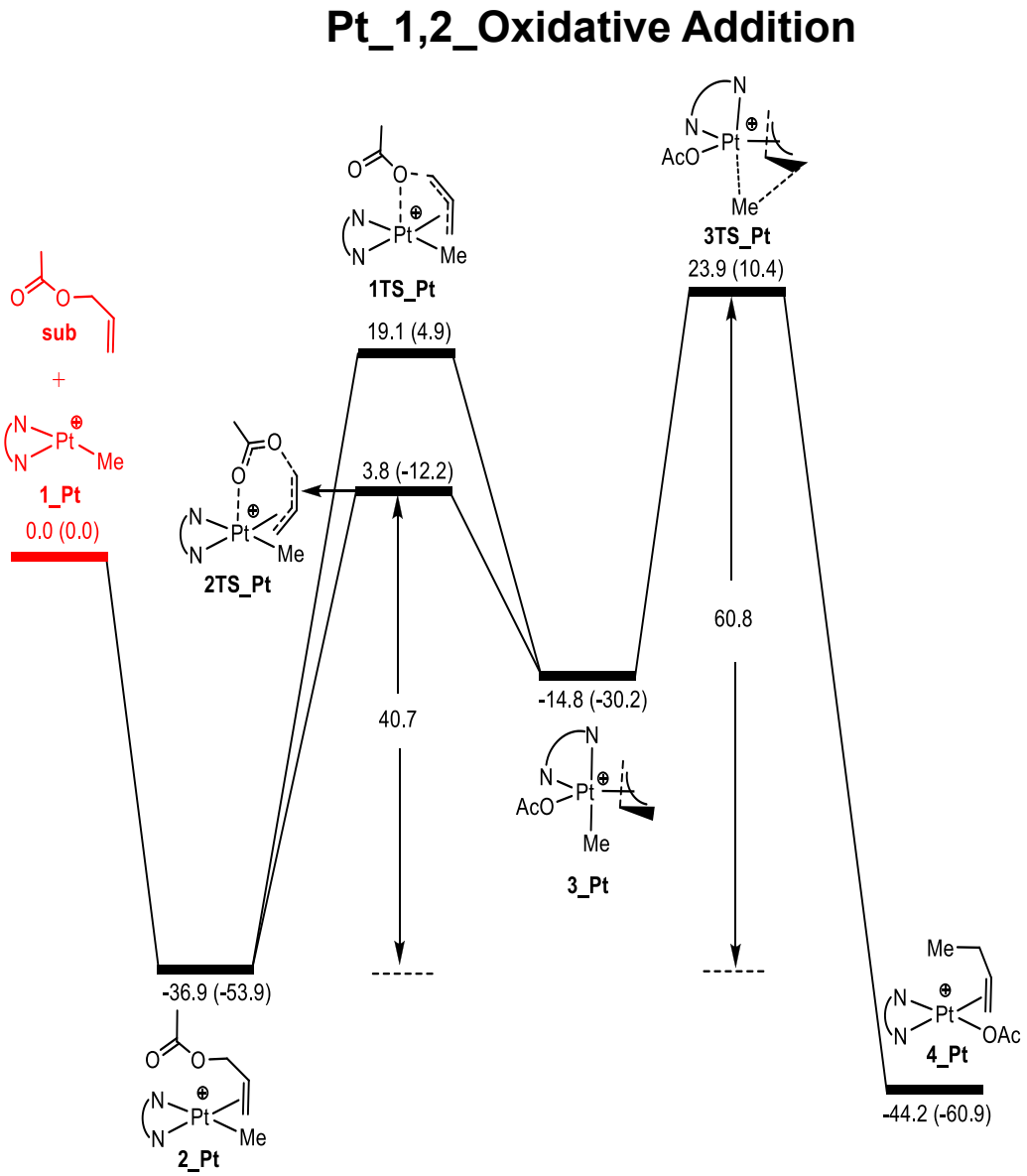


Figure S18: Calculated potential energy diagram for the reaction of $[(phen)Pt(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

Pt_3,4_Oxidative Addition

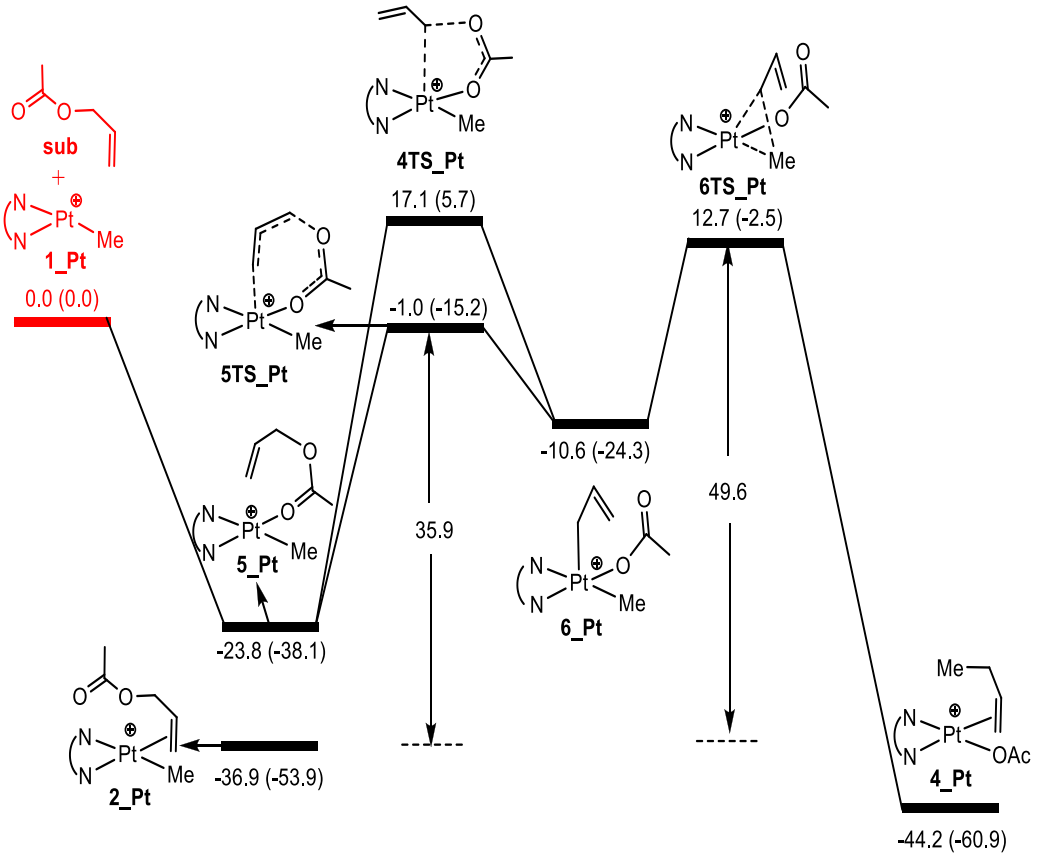


Figure S19: Calculated potential energy diagram for the reaction of $[(phen)Pt(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

Pt_5,6_Oxidative Addition

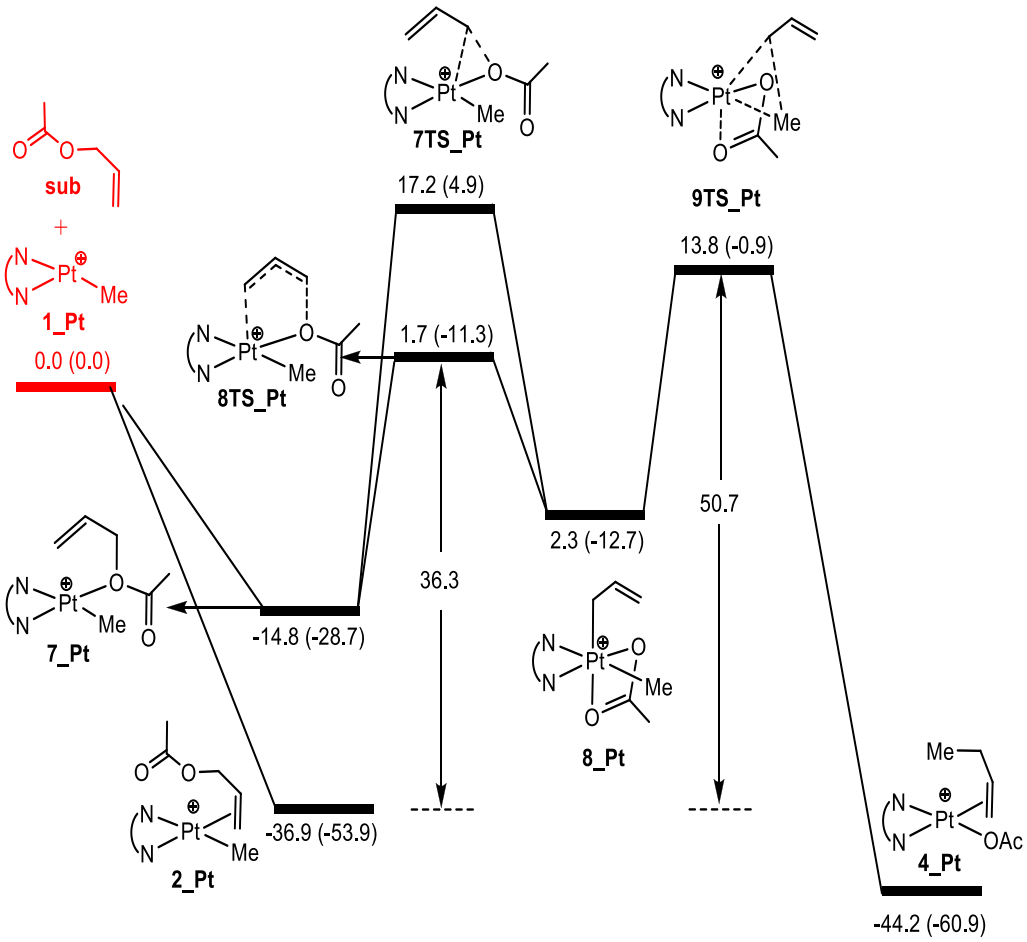


Figure S20: Calculated potential energy diagram for the reaction of $[(phen)Pt(CH_3)]^+$ and allyl acetate proceeding *via* the oxidative addition / reductive elimination pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

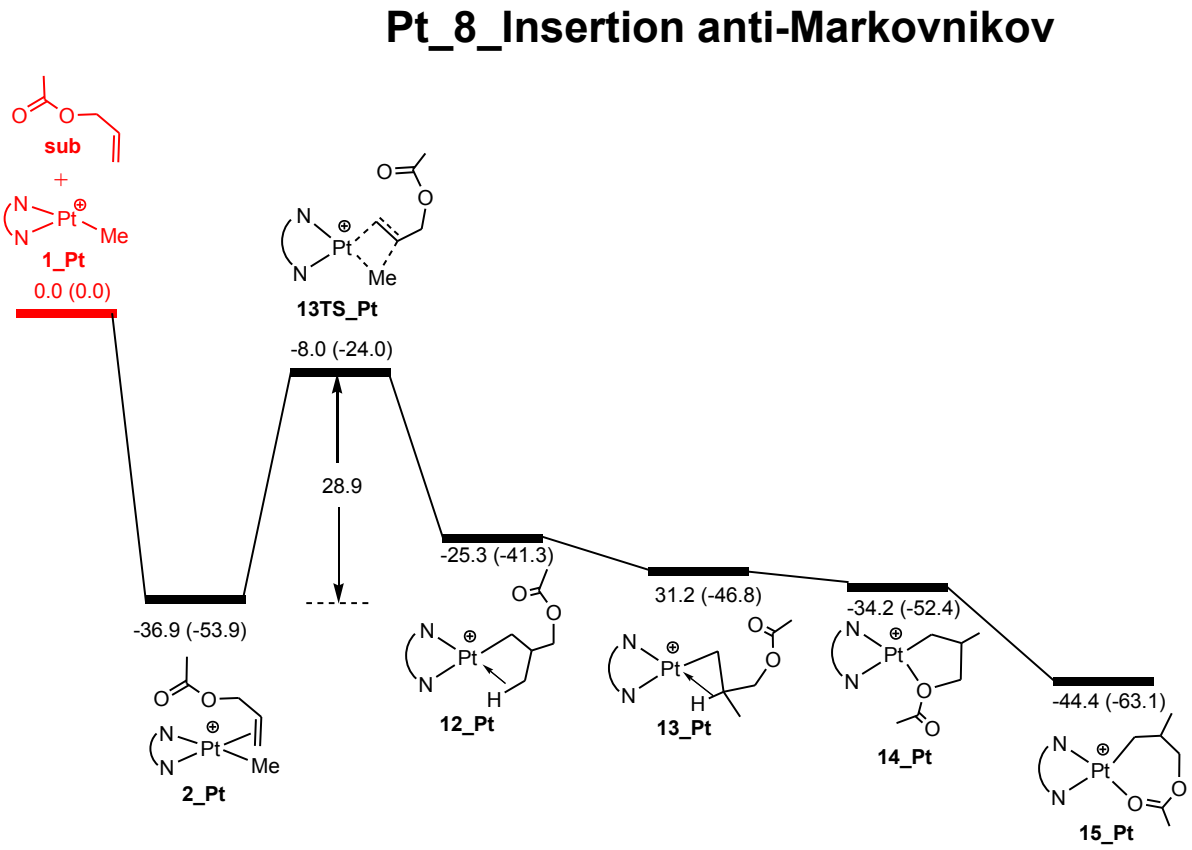


Figure S21: Calculated potential energy diagram for the reaction of $[(phen)Pt(CH_3)]^+$ and allyl acetate proceeding *via* the anti-Markovinikov insertion pathway. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

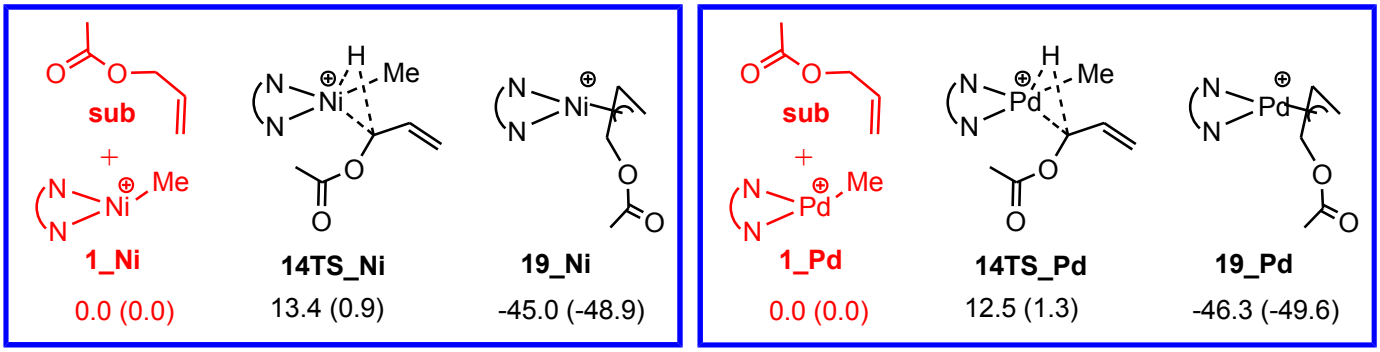


Figure S22: Calculated relative energies for **14_M** (key transition structure for formation of the allyl complex) and **19_M** for (a) M = Ni and (b) M = Pd. The relative Gibbs and electronic energies (in parentheses) obtained from the M06 calculations are given in kcal mol^{-1}.

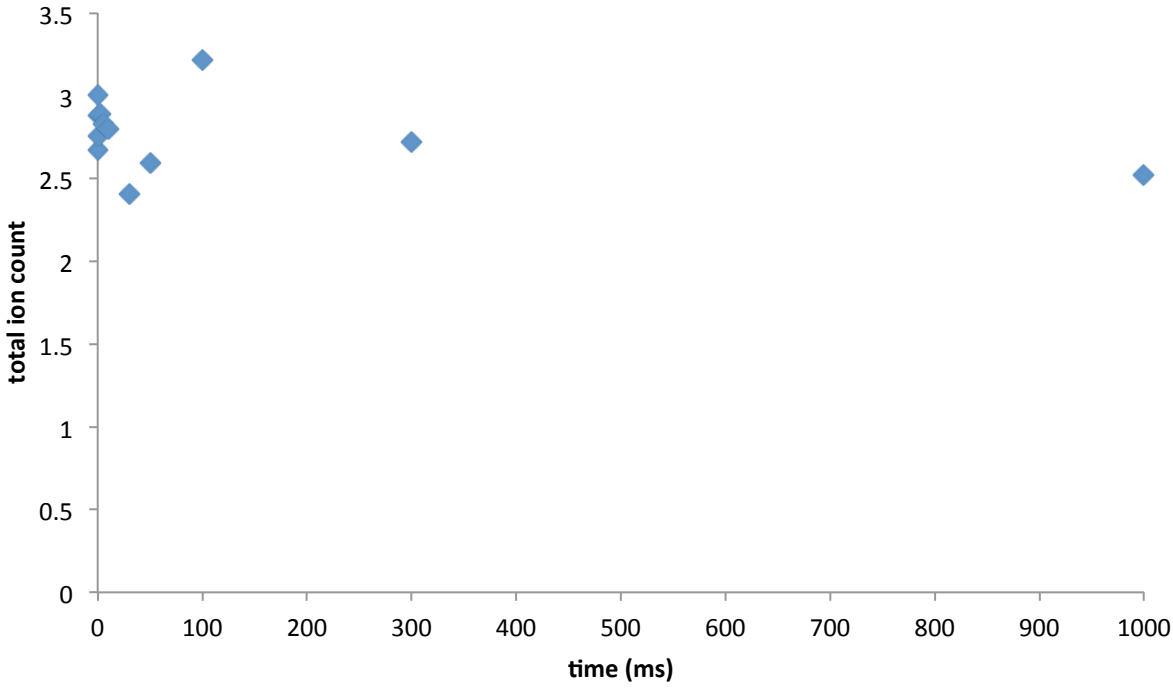


Figure S23: Plot of total ion count (x 10^6 ions) vs. time (ms) for the reaction of $[(phen)Ni(CH_3)]^+$ with allyl acetate. Note that at 1,000 ms < 5% of the reactant remains.

Table S2: DFT calculation of the energetics associated with the reactions of $[(phen)M(CH_3)]^+$, **1,** with allyl acetate.

Reaction	Species	M = Ni	M = Pd	M = Pt
[a]Oxidative addition path 1,2	**1_M + $C_3H_5CO_2CH_3$**	0	0	0
	2_M	-21.2	-25.4	-36.9
	2TS_M	12.6	15.2	3.8
	1TS_M	28.2	27.2	19.1
	3_M	7.4	4.0	-14.8
	3TS_M	10.8	27.8	23.9
	4_M	-41.4	-34.3	-44.2
[a]Oxidative addition path 3,4	**1_M + $C_3H_5CO_2CH_3$**	0	0	0
	5_M	-19.9	-17.8	-23.8
	5TS_M	15.4	10.0	-1.0
	4TS_M	b	17.1	17.1
	6_M	8.4	7.6	-10.6
	6TS_M	9.3	19.0	12.7
	4_M	-41.4	-8.8	-44.2
[a]Oxidative addition path 5,6	**1_M + $C_3H_5CO_2CH_3$**	0	0	0
	7_M	-10.8	-10.6	-14.8
	8TS_M	10.7	10.8	1.7
	7TS_M	24.6	26.6	17.2
	8_M	0.2	2.3	2.3
	9TS_M	9.1	19.5	13.8
	4_M	41.4	-34.3	44.2
[a]Insertion path 7	**1_M + $C_3H_5CO_2CH_3$**	0	0	0
	2_M	-21.2	-25.4	-36.9
	10TS_M	-8.0	-8.2	-9.4
	9_M	-20.6	-24.8	-26.3
	11TS_M	b	-23.7	-21.9
	10_M	-42.0	-39.5	-44.9
	12TS_M	-21.8	-17.2	-24.0
	4_M	-41.4	-34.2	-44.1
	11_M	-52.1	-33.9	-41.1
[a]Insertion path 8	**1_M + $C_3H_5CO_2CH_3$**	0	0	0
	2_M	-21.2	-25.4	-36.9
	13TS_M	-5.2	-6.3	-8.0
	12_M	-35.3	-23.6	-25.3
	13_M	-43.6	-29.5	-31.2
	14_M	-44.1	-30.1	-34.2
	15_M	-52.3	-38.6	-44.4

(a) In the case of the DFT calculations of the reaction of $[(phen)M(CH_3)]^+$ with allyl acetate, all energies are relative to separated reactants. (b) barrierless pathway

Table S3. Cartesian coordinates and total energies for all of the calculated structures

sub

E = -345.565469 au

H = -345.433293 au

G = -345.474920 au

C	-0.87484700	-0.81217900	-0.65108800
C	-1.83850400	-0.40098600	0.41115100
H	-1.96050400	-1.09536700	1.24577300
H	-1.09607800	-1.81538000	-1.03326400
H	-0.87391100	-0.09874100	-1.48395300
C	-2.52275100	0.74093700	0.37475800
H	-3.22903200	1.01212200	1.15755700
H	-2.39056700	1.45384100	-0.43999000
O	0.81549700	1.26185400	-0.54476200
C	1.19156500	0.20655900	-0.09140000
C	2.51760100	-0.03841700	0.56191000
O	0.45691300	-0.92496500	-0.11393700
H	3.12038100	0.87204000	0.52587000
H	3.04450000	-0.85831900	0.06037400
H	2.36755400	-0.34079000	1.60523700

1_Pd

E = -738.767411 au

H = -738.544297 au

G = -738.598586 au

N	-0.37567700	-1.47611500	-0.00167100
C	-1.18610700	-0.38621200	-0.00034900
C	-2.59237300	-0.49305800	0.00093900
C	-3.14425700	-1.79162500	0.00130300
C	-2.31119300	-2.88716700	0.00020900
C	-0.92243500	-2.68210400	-0.00144600
Pd	1.72299800	-0.83797300	-0.00085900
H	-4.22694000	-1.91314900	0.00239900
H	-2.70518500	-3.90005100	0.00046500
H	-0.23730700	-3.52939600	-0.00265300
N	0.78731200	1.00643000	-0.00097900
C	1.36475400	2.20258100	-0.00156100
C	0.62355000	3.39066100	-0.00139300
C	-0.75087200	3.32287200	-0.00044300
C	-1.38889700	2.06618300	0.00010500
C	-0.57525200	0.91316400	-0.00040400
H	2.45148600	2.22654300	-0.00207800
H	1.14708100	4.34300700	-0.00189900
H	-1.35516600	4.22943300	-0.00011500
C	-2.81314800	1.92263700	0.00122900
C	-3.39199100	0.69304100	0.00175100
H	-3.42368200	2.82443300	0.00166500
H	-4.47610100	0.58959800	0.00269300
C	3.58228700	-0.10095800	0.00598100
H	3.76381900	0.48456500	0.91540400
H	4.18645800	-1.02436300	0.00896600
H	3.77179600	0.48382300	-0.90231100

2_Pd

E = -1084.399667 au

H = -1084.041322 au

G = -1084.113975 au

N	-0.35411400	1.20480600	-0.82574400
C	-1.56584200	0.84554500	-0.33195200
C	-2.57557900	1.79277000	-0.05469500
C	-2.29061400	3.14766700	-0.31450700
C	-1.06280800	3.49733300	-0.82656300
C	-0.12281400	2.48433200	-1.06654900
Pd	1.00513000	-0.56534000	-0.94738000
H	-3.04909100	3.90335300	-0.11239800
H	-0.81126500	4.53150900	-1.04740300
H	0.85669000	2.73920000	-1.47296500
N	-0.84609700	-1.45565600	-0.36632800
C	-1.08339300	-2.74345300	-0.15409600
C	-2.30324200	-3.22082000	0.34143600
C	-3.30110400	-2.31790600	0.62774200
C	-3.08008300	-0.94319000	0.41577300
C	-1.82348800	-0.54729300	-0.09053200
H	-0.27463900	-3.43538500	-0.38271000
H	-2.44042300	-4.28850300	0.49110000
H	-4.26301500	-2.65163500	1.01602500
C	-4.07887900	0.04379300	0.69212400
C	-3.83596300	1.36069500	0.46606700
C	1.91948300	-2.36790600	-1.14464800
H	1.26241100	-2.95071900	-1.80333600
H	-5.03933700	-0.28746000	1.08466700
H	-4.59745300	2.11160100	0.67257700
H	1.99333900	-2.82054300	-0.14643000
H	2.91479700	-2.30083600	-1.59813800
C	3.03114800	1.24829100	0.54555800
C	3.04952900	0.21100700	-0.53433900
H	3.64441000	-0.67127900	-0.28702600
H	3.97691800	1.80612900	0.50638300
H	2.20130300	1.95783800	0.43868800
C	2.70123100	0.44504700	-1.85056300
H	3.05515100	-0.21107200	-2.64521900
H	2.34818800	1.42577800	-2.17563100
O	0.75930600	0.66916500	1.85740200
C	1.80787200	0.42539700	2.41156100
C	1.97089000	-0.15872800	3.77581800
O	3.01270500	0.65733100	1.84154300
H	2.48645300	-1.12446100	3.71049000
H	0.99198500	-0.29320900	4.24106300
H	2.59491000	0.49383100	4.39688500

1TS_Pd

E = -1084.311500 au

H = -1083.956644 au

G = -1084.029945 au

N	0.24227300	1.10921700	0.56905100
C	1.54582200	0.89093100	0.25219400
C	2.50397000	1.92801900	0.25570100
C	2.06287300	3.22506900	0.58617600
C	0.73762700	3.43544200	0.88412400
C	-0.14277100	2.34302700	0.86232400
Pd	-0.97795900	-0.77550000	0.38867400
H	2.77741600	4.04756100	0.59457300
H	0.35693500	4.42367700	1.12760100
H	-1.20023000	2.49750200	1.06455100
N	1.01207800	-1.42536700	-0.13727800
C	1.38784200	-2.65955300	-0.44780700
C	2.71015500	-2.99777000	-0.76184000
C	3.66828300	-2.01072600	-0.75407500
C	3.30535700	-0.69183300	-0.42037200
C	1.95132000	-0.43831600	-0.10510400
H	0.61426100	-3.42518700	-0.45480800
H	2.95390300	-4.02762200	-1.00939100
H	4.70569600	-2.23477300	-1.00055800
C	4.25305700	0.37941300	-0.39485200
C	3.86594000	1.64106800	-0.07322700
C	-1.75466900	-2.59718600	-0.09963100
H	-1.44605800	-3.33487200	0.65021400
H	5.29049300	0.15934700	-0.64275100
H	4.58605000	2.45807600	-0.05947900
H	-1.31259000	-2.76979200	-1.08752200
H	-2.84144200	-2.52708700	-0.19207700
C	-3.19588100	0.21507200	0.85023100
C	-2.70510200	-0.73364600	1.78914800
H	-3.22493200	-1.68868700	1.86208000
H	-4.13652700	0.00783400	0.35005700
H	-2.87767800	1.25644000	0.83794700
C	-1.55582000	-0.55983700	2.56213400
H	-1.24779500	-1.34553300	3.24955600
H	-1.11222100	0.42219200	2.72471400
O	-2.29640400	2.19767800	-1.04838700
C	-2.46515600	1.18479700	-1.72530800
C	-2.62720600	1.24823100	-3.22615600
O	-2.56498300	-0.02604300	-1.24248800
H	-2.08676900	0.43333400	-3.71883000
H	-2.28612200	2.21816000	-3.59883500
H	-3.68948500	1.12918800	-3.47341800

2TS_Pd

E = -1084.332714 au

H = -1083.977355 au

G = -1084.049137 au

N	-0.26244100	1.17752100	-0.60774600
C	-1.54905500	0.88780700	-0.27951600
C	-2.54804200	1.88540200	-0.20818000
C	-2.16990800	3.21469100	-0.47990500
C	-0.86251300	3.49565000	-0.80129600
C	0.05795100	2.43913400	-0.85046500
Pd	1.07498400	-0.65204900	-0.37992100
H	-2.91846200	4.00479600	-0.42909400

H	-0.53187700	4.50915500	-1.01291000
H	1.09945300	2.64688700	-1.08956900
N	-0.93987800	-1.43301800	-0.05850300
C	-1.26751300	-2.69861100	0.15521100
C	-2.57318100	-3.10597400	0.45973400
C	-3.55993100	-2.15144100	0.54758700
C	-3.24449000	-0.79935000	0.31082100
C	-1.90422000	-0.47843200	-0.00325300
H	-0.46722100	-3.43388700	0.08480100
H	-2.78181300	-4.15954900	0.62651000
H	-4.58546100	-2.42595600	0.79273100
C	-4.22766800	0.23748300	0.37724600
C	-3.89156800	1.52971200	0.13058000
C	1.94928400	-2.41247100	0.15802900
H	1.92308800	-3.10371400	-0.69249100
H	-5.25169700	-0.03386100	0.63037200
H	-4.63956800	2.31959700	0.18392700
H	1.33520000	-2.73714600	1.00308100
H	2.96994400	-2.20664200	0.49379100
C	3.24292500	0.76685200	-1.01103400
C	2.85850000	-0.45372400	-1.61477800
H	3.53705100	-1.29760900	-1.49070900
H	4.24588100	0.87809000	-0.61271400
H	2.74853200	1.69313000	-1.28892300
C	1.70062900	-0.63860900	-2.41421900
H	1.59884200	-1.56933500	-2.97177000
H	1.17945600	0.21967100	-2.84382000
O	1.28954300	-0.12858600	1.73270700
C	2.16088300	0.77258600	1.89734300
C	2.33540000	1.31204900	3.29558600
O	2.88402000	1.29027500	0.99468000
H	2.17280600	0.51888600	4.03148200
H	1.57690900	2.08634300	3.46652500
H	3.32248500	1.76384200	3.42282900

3_Pd

E = -1084.350053 au

H = -1083.993640 au

G = -1084.067000 au

N	-0.25729200	1.17595500	-0.62222900
C	-1.52205100	0.77612900	-0.33380700
C	-2.60892700	1.67819100	-0.33670000
C	-2.33623400	3.02843100	-0.63397700
C	-1.04459000	3.42110100	-0.89784400
C	-0.02719900	2.45463500	-0.87663800
Pd	1.23175500	-0.50186200	-0.33649100
H	-3.15343600	3.74907100	-0.64292500
H	-0.79723600	4.45693100	-1.11483900
H	1.00775900	2.74292900	-1.05444000
N	-0.70045300	-1.46001400	0.03615300
C	-0.90648900	-2.73335500	0.33637100
C	-2.17800600	-3.24936400	0.62075300
C	-3.25797100	-2.39674700	0.59781500
C	-3.06858400	-1.03673800	0.28405800

C	-1.75465200	-0.60325300	-0.00231100
H	-0.03168000	-3.38191800	0.35851300
H	-2.28921600	-4.30381800	0.85938100
H	-4.26092000	-2.75897900	0.82141800
C	-4.14893900	-0.09941800	0.25549500
C	-3.92678300	1.20813800	-0.03847000
C	2.29923200	-2.13257200	0.33270300
H	2.15357800	-2.94440900	-0.38923300
H	-5.15219000	-0.45762800	0.48204600
H	-4.74840700	1.92298500	-0.05138100
H	1.84111900	-2.31612700	1.30762300
H	3.35260900	-1.85923700	0.44185600
C	2.98514900	0.45310400	-1.17749500
C	2.65195700	-0.64351000	-2.00946700
H	3.27471800	-1.53839600	-1.98619200
H	3.88685300	0.43075700	-0.56831500
H	2.60195500	1.45114900	-1.38187600
C	1.36816300	-0.72513100	-2.55982100
H	1.02520400	-1.65726900	-3.00705200
H	0.81817200	0.17436400	-2.83726000
O	2.30826000	1.90127200	1.16843800
C	1.80240700	1.13275100	1.98208000
C	1.77909300	1.43253200	3.46133800
O	1.25486000	-0.01589100	1.68455200
H	0.85618900	1.07503700	3.92853300
H	1.90456900	2.50643200	3.62478100
H	2.61543800	0.90961800	3.94204600

3TS_Pd

E = -1084.31072 au

H = -1083.955183 au

G = -1084.029067 au

N	-0.23800400	1.05058100	-0.46954100
C	-1.55698900	0.84429700	-0.21124300
C	-2.47751400	1.91622600	-0.31717600
C	-1.98803600	3.18499700	-0.68015600
C	-0.64356400	3.36395800	-0.91358400
C	0.20891200	2.26122700	-0.79677900
Pd	1.20730700	-0.48762400	-0.25938900
H	-2.68588200	4.01753200	-0.76529700
H	-0.23188000	4.33268300	-1.18392400
H	1.28459900	2.35315700	-0.95297300
N	-1.15702100	-1.47408600	0.31207900
C	-1.59422800	-2.65737900	0.69923600
C	-2.94289200	-2.92837100	0.98736100
C	-3.85383500	-1.90529100	0.85944100
C	-3.41895300	-0.62719300	0.45369800
C	-2.03829200	-0.46019800	0.18853000
H	-0.84168600	-3.44375300	0.79684300
H	-3.24684400	-3.92272800	1.30528600
H	-4.91042700	-2.06563100	1.07307900
C	-4.32079300	0.47415100	0.31978700
C	-3.86636100	1.69836700	-0.04998300
C	2.48302100	-2.05372900	0.71383500

H	2.34247900	-3.10183200	0.44685800
H	-5.37760500	0.31118000	0.52818200
H	-4.54820700	2.54233700	-0.14513200
H	1.83757600	-1.78172000	1.55617300
H	3.51957700	-1.79818700	0.94180300
C	2.83595000	-1.63942100	-1.33984800
C	1.55250500	-1.80717100	-1.96872300
H	1.05617800	-2.77743300	-1.89708300
H	3.47616500	-2.50854900	-1.22320100
H	3.39273600	-0.71548400	-1.52294400
C	0.85973100	-0.71019800	-2.45250400
H	-0.17496400	-0.81465200	-2.77678000
H	1.38259200	0.19768300	-2.75861700
O	3.18198100	1.44090100	0.25305700
C	2.64028100	1.26527400	1.34519000
C	3.08434100	1.96678600	2.59958100
O	1.63757400	0.44333800	1.52652900
H	2.22960200	2.24057500	3.22627700
H	3.67395200	2.85106000	2.34227900
H	3.71492300	1.28709100	3.18664900

4_Pd

E = -1084.413824 au

H = -1084.054707 au

G = -1084.128020 au

N	-0.98484400	-1.39219700	0.12924800
C	-2.09232100	-0.59879500	0.03683400
C	-3.39914500	-1.10670800	0.17109900
C	-3.53574900	-2.48866200	0.41188500
C	-2.41069800	-3.27806200	0.50341300
C	-1.14715900	-2.68928800	0.35630200
Pd	0.78041200	-0.27420300	-0.02453500
H	-4.52962800	-2.92052800	0.52476600
H	-2.48160100	-4.34659500	0.68832800
H	-0.24586500	-3.29771400	0.42524400
N	-0.62048500	1.24017100	-0.32060300
C	-0.38583900	2.52217200	-0.55272000
C	-1.43160400	3.45023400	-0.68123700
C	-2.73433900	3.01962400	-0.55954700
C	-3.00326600	1.65670600	-0.31393700
C	-1.89787900	0.79443500	-0.20382000
H	0.66049500	2.81065200	-0.64315500
H	-1.19722900	4.49397200	-0.87286700
H	-3.56229900	3.72174600	-0.65144500
C	-4.32158400	1.11667200	-0.17279000
C	-4.51087700	-0.21033100	0.06160500
H	-5.17224500	1.79165800	-0.25436000
H	-5.51527000	-0.61670600	0.17133400
C	2.17177900	-1.77306900	0.78801600
C	2.13988300	-2.03629700	-0.56565300
H	1.37099800	-2.71838600	-0.94339200
H	1.52460500	-2.29489900	1.49379200
H	3.00606200	-1.23327800	1.23528200
C	3.20186300	-1.68705000	-1.56431000
O	2.31043800	1.01354700	-0.20796000

C	2.56461200	1.58584700	0.95283100
C	3.73919800	2.52527100	0.91239300
O	1.92007700	1.35476800	1.96727500
H	3.88392000	2.96147500	-0.08108500
H	4.64766600	1.96267200	1.16674000
H	3.61290000	3.30767800	1.66658600
H	2.78658400	-0.97198100	-2.29330000
H	3.37871400	-2.60600500	-2.14671200
C	4.51265100	-1.16955400	-0.99779400
H	4.38500900	-0.19261900	-0.51761700
H	4.93793100	-1.87109600	-0.26760800
H	5.24634100	-1.04790000	-1.80238900

5_Pd

E = -1084.383772 au

H = -1084.025820 au

G = -1084.101870 au

N	0.46454200	1.27881600	-0.21920000
C	1.78082900	1.03132400	-0.00193500
C	2.71255900	2.06560500	0.22816100
C	2.22894700	3.38967000	0.21853600
C	0.89267600	3.62650600	-0.01259500
C	0.04029800	2.53237300	-0.22832900
Pd	-0.61173200	-0.61813100	-0.57006100
H	2.92194300	4.21261700	0.39083300
H	0.49111900	4.63640800	-0.03224600
H	-1.02228900	2.68604400	-0.41875400
N	1.31069500	-1.32198500	-0.26148800
C	1.72215400	-2.58433900	-0.29066300
C	3.05786600	-2.95114200	-0.07896900
C	3.99110400	-1.97068900	0.16641700
C	3.58837300	-0.62114100	0.19874600
C	2.22419000	-0.33433700	-0.02045000
H	0.96683800	-3.34135500	-0.49052700
H	3.33225200	-4.00216500	-0.11370200
H	5.03777000	-2.22196700	0.33474000
C	4.50747500	0.44994400	0.43878900
C	4.08800800	1.74240600	0.45183600
C	-1.37073900	-2.45982700	-0.91862700
H	-2.45215700	-2.36959000	-1.06616300
H	5.55478000	0.20344300	0.60813300
H	4.79272400	2.55352800	0.62985500
H	-1.15884900	-3.10479200	-0.05586200
H	-0.89022500	-2.83714100	-1.83143400
C	-2.83470400	0.55683400	1.75189900
C	-3.27120900	-0.76522800	2.27992200
H	-4.31731100	-0.83598400	2.58431100
C	-2.44308500	-1.79693000	2.42913800
H	-2.77341500	-2.73916200	2.86156200
H	-1.39499900	-1.73063900	2.12811300
O	-2.52652500	0.17750500	-1.02925000
C	-3.52696700	0.72074300	-0.56514400
C	-4.66422800	1.14077900	-1.43322200
O	-3.73739900	1.00122600	0.70672900

H	-5.06126600	2.10943300	-1.11406600
H	-5.47421600	0.40724700	-1.32966500
H	-4.35031200	1.17194900	-2.47890900
H	-2.91700500	1.34762700	2.50621000
H	-1.80228600	0.52554600	1.37430100

5TS_Pd

E = -1084.339908 au

H = -1083.984883 au

G = -1084.057358 au

N	0.21923800	1.22704100	-0.17752500
C	1.56707200	1.08012600	-0.09739500
C	2.44593000	2.18220900	-0.03934900
C	1.87332600	3.47051600	-0.09113200
C	0.50732100	3.60402900	-0.18580800
C	-0.29275200	2.44883400	-0.22021700
Pd	-0.76340600	-0.77325400	-0.37256200
H	2.52066200	4.34644800	-0.05801300
H	0.03582200	4.58248700	-0.23134600
H	-1.37963200	2.51020600	-0.26471800
N	1.24474500	-1.30916400	-0.17029300
C	1.73443100	-2.54426500	-0.15575200
C	3.10429600	-2.81401100	-0.04546100
C	3.98641000	-1.76134900	0.04570800
C	3.49908000	-0.44002300	0.02770100
C	2.10350700	-0.25147100	-0.07656400
H	1.01553900	-3.35662300	-0.24348400
H	3.44572200	-3.84571600	-0.03998800
H	5.05895700	-1.93466800	0.12724700
C	4.36145400	0.69966900	0.10091000
C	3.85553600	1.96060400	0.06266300
C	-1.40610400	-2.67429900	-0.71220600
H	-2.48656600	-2.62520800	-0.87369800
H	5.43479700	0.53278900	0.17912300
H	4.51558300	2.82593300	0.10747400
H	-1.16264600	-3.31975700	0.14220600
H	-0.89223700	-3.00838700	-1.62294700
C	-2.69439100	0.48332400	2.34248100
C	-2.25326600	-0.81542900	2.15821900
H	-2.97278000	-1.63036400	2.07333900
H	-3.72360100	0.70847200	2.60447300
H	-1.97513500	1.28815700	2.47978300
C	-0.90275500	-1.07322500	1.97367600
H	-0.52329400	-2.09372700	2.00005400
H	-0.17283400	-0.28904000	2.18536500
O	-2.64722800	-0.24939200	-1.02788600
C	-3.42448900	0.64291200	-0.54499900
C	-4.74668800	0.80252500	-1.24096400
O	-3.16634700	1.36647900	0.45093500
H	-5.04303700	1.85643300	-1.24886100
H	-5.51273400	0.25254500	-0.67824300
H	-4.71269700	0.40380400	-2.25864100

4TS_Pd

E = -1084.323873 au

H = -1083.969774 au

G = -1084.046012 au

N	0.45312900	1.26974600	-0.16840300
C	1.76271900	0.98128600	0.03969200
C	2.73058300	1.98290300	0.26293900
C	2.28913600	3.32219300	0.26178500
C	0.95758000	3.59944400	0.05369400
C	0.06476800	2.53528900	-0.15712600
Pd	-0.69500600	-0.57763900	-0.61800700
H	3.01024200	4.12253200	0.42583800
H	0.58607700	4.62093600	0.04914600
H	-0.99875800	2.71535700	-0.30591600
N	1.21016600	-1.35385400	-0.19574000
C	1.57590000	-2.63059300	-0.21707200
C	2.89803100	-3.04553100	-0.01124000
C	3.86836500	-2.09631000	0.21644200
C	3.51638100	-0.73250600	0.23913000
C	2.16080700	-0.39891300	0.02787000
H	0.79247600	-3.36102000	-0.41027000
H	3.13499500	-4.10586400	-0.03909500
H	4.90680500	-2.38423400	0.37729200
C	4.47398200	0.30762200	0.46184200
C	4.09667300	1.61331800	0.47308800
C	-1.50379900	-2.38346600	-1.05667300
H	-2.56977200	-2.25337800	-1.26866500
H	5.51448100	0.02767500	0.62063400
H	4.83019800	2.40123700	0.63947800
H	-1.35042800	-3.07612900	-0.21608100
H	-0.97933100	-2.74312900	-1.95240300
C	-4.20265100	-0.89817600	2.32257700
C	-2.99737400	-1.33978800	1.88143400
H	-2.88581100	-2.34809400	1.48393800
H	-5.07970000	-1.54258200	2.33670500
H	-4.32535400	0.12569900	2.67601700
C	-1.86253000	-0.50838600	1.97746500
H	-0.86551800	-0.91939700	1.82298400
H	-1.92831000	0.45769200	2.46738400
O	-2.46529800	0.22252600	-1.28209900
C	-3.09264700	1.02859200	-0.51865600
C	-4.34270200	1.64095700	-1.09691300
O	-2.76194300	1.30621900	0.65512400
H	-4.50800200	2.64020800	-0.68334400
H	-5.19523700	1.01288000	-0.80310700
H	-4.30326100	1.67216700	-2.18906000

6_Pd

E = au

H = au

G = au

N	0.41008100	1.30342400	-0.09236100
C	1.72984400	1.00395400	0.01913900

C	2.71921500	1.99506500	0.18576900
C	2.29073100	3.33835500	0.23051300
C	0.95116700	3.62693400	0.12006200
C	0.03378200	2.57330600	-0.03730700
Pd	-0.79378200	-0.56543300	-0.47758800
H	3.02826800	4.13056500	0.35658700
H	0.58656000	4.65017600	0.15717200
H	-1.03758600	2.75541400	-0.09217800
N	1.15276400	-1.32806200	-0.20009500
C	1.50582400	-2.60888800	-0.24221300
C	2.83449700	-3.03239700	-0.12355900
C	3.82265300	-2.08802800	0.04065600
C	3.48291100	-0.72225700	0.09022600
C	2.11800100	-0.37679500	-0.03145900
H	0.70857600	-3.33582800	-0.38323300
H	3.06224200	-4.09411900	-0.16643700
H	4.86750400	-2.38303200	0.13184000
C	4.46112200	0.30812000	0.25607800
C	4.09339900	1.61568200	0.30133000
C	-1.59345300	-2.36179800	-1.00221800
H	-2.67219500	-2.22397700	-1.10452900
H	5.50749200	0.01961400	0.34376400
H	4.84066000	2.39816000	0.42713000
H	-1.35135800	-3.12474500	-0.25299300
H	-1.12127800	-2.58325000	-1.96907800
C	-3.68825300	-0.84836100	2.21151600
C	-2.59839100	-1.54170300	1.82251600
H	-2.64919600	-2.62750500	1.73317300
H	-4.61731700	-1.35543900	2.46536100
H	-3.66258600	0.23821400	2.29666700
C	-1.33023600	-0.89430100	1.61978100
H	-0.43990700	-1.47473200	1.87581300
H	-1.29247400	0.16961300	1.86921100
O	-2.57490700	0.16040100	-1.08054500
C	-3.17606900	1.12427200	-0.43870500
C	-4.49476100	1.51116100	-1.05385400
O	-2.75542000	1.65264300	0.59005900
H	-4.70846000	2.56416500	-0.84781500
H	-5.28314700	0.90897900	-0.58102600
H	-4.52104000	1.31182600	-2.12893800

6TS_Pd

E = -1084.325379 au

H = -1083.969717 au

G = -1084.042982 au

N	0.63551900	1.29025400	-0.25463900
C	1.89241200	0.84484200	0.00710500
C	2.97151100	1.72252700	0.21638200
C	2.69954300	3.10497900	0.14671100
C	1.42088400	3.53729100	-0.12629300
C	0.40240600	2.59118800	-0.32485100
Pd	-0.74111100	-0.28651800	-0.44093200
H	3.50600800	3.82009000	0.30538600
H	1.18366800	4.59589700	-0.18936300

H	-0.61940800	2.88730000	-0.55264300
N	1.02337900	-1.37733700	-0.16797700
C	1.20037700	-2.69221300	-0.17670600
C	2.45099200	-3.28463600	0.04561500
C	3.54328300	-2.47956700	0.28374300
C	3.39058800	-1.07858400	0.28544800
C	2.09987300	-0.56701900	0.04690700
H	0.32254500	-3.30533300	-0.37524200
H	2.53866700	-4.36761700	0.02637500
H	4.52632400	-2.91398500	0.46249200
C	4.47219700	-0.16628600	0.50634300
C	4.27052200	1.17899500	0.47515900
C	-1.91088400	-1.82620200	-1.39645100
H	-2.89078900	-1.40997700	-1.63237600
H	5.46381700	-0.57496200	0.69500300
H	5.09789400	1.86750500	0.64075500
H	-1.94645600	-2.90391100	-1.22620500
H	-1.20054600	-1.63429300	-2.22075600
C	-4.35466600	-1.18973000	1.41007100
C	-3.50700600	-1.96882600	0.72525600
H	-3.88313600	-2.84491900	0.19284700
H	-5.41590200	-1.42547600	1.46044600
H	-4.00909300	-0.30612400	1.94939700
C	-2.06102000	-1.73663300	0.72586300
H	-1.45060200	-2.62972900	0.87547100
H	-1.79148400	-0.93957400	1.43658900
O	-2.28058200	0.94125700	-0.83468400
C	-2.79595600	1.53265400	0.21893100
C	-3.98961500	2.38785500	-0.11126700
O	-2.37115400	1.39190700	1.36093800
H	-4.12289400	3.15411700	0.65795100
H	-4.88345400	1.74908800	-0.11924000
H	-3.90506500	2.84216700	-1.10353100

7_Pd

E = -1084.370699 au

H = -1084.013086 au

G = -1084.090444 au

N	0.40404800	1.19364700	-0.10881900
C	1.74358400	0.98518100	-0.07910900
C	2.67128500	2.04565400	-0.12594300
C	2.15318200	3.35413400	-0.21418000
C	0.79064200	3.54898400	-0.25259600
C	-0.05593600	2.42984400	-0.19592200
Pd	-0.66183000	-0.70432500	-0.06365900
H	2.83922100	4.19963500	-0.25526800
H	0.36374900	4.54580100	-0.32843400
H	-1.14046900	2.53815200	-0.22460800
N	1.29311600	-1.38004200	0.02499700
C	1.71877600	-2.63580100	0.08405100
C	3.07930400	-2.97074600	0.11738600
C	4.01843000	-1.96549800	0.08629600
C	3.59810500	-0.62250000	0.02260800
C	2.21130400	-0.36881400	-0.00614300

H	0.95555900	-3.41106600	0.10504800
H	3.36824000	-4.01738200	0.16383400
H	5.08350600	-2.19387400	0.10801100
C	4.51669100	0.47529600	-0.01866200
C	4.07260800	1.75814300	-0.09049900
C	-1.45144600	-2.56506000	-0.05704300
H	-2.54628500	-2.49827600	-0.11939100
H	5.58343300	0.25682900	0.00521800
H	4.77642700	2.58863900	-0.12566500
H	-1.16251700	-3.07852200	0.87062100
H	-1.07100700	-3.09463400	-0.94040500
C	-3.56160200	0.09262900	1.07277000
C	-2.68191900	0.10251700	2.27124800
H	-2.08694500	-0.79700800	2.44866700
H	-4.18549400	-0.81141100	1.02774400
H	-4.20436400	0.98147600	1.04885600
C	-2.62817700	1.13390300	3.11319900
H	-1.99931200	1.11653300	4.00064500
H	-3.22857500	2.03140400	2.95819600
O	-2.43611200	0.11740400	-2.29934800
C	-3.22466700	0.19327300	-1.39955800
C	-4.69946000	0.38435300	-1.52893400
O	-2.71127900	0.10685200	-0.11549300
H	-5.02389700	1.32436900	-1.06552200
H	-5.25265700	-0.43081400	-1.04594300
H	-4.94967700	0.40685800	-2.59162000

8TS_Pd

E = -1084.336966 au

H = -1083.982312 au

G = -1084.056194 au

N	0.32473000	1.24543600	0.06593000
C	1.65932500	1.00918800	0.04398100
C	2.60643600	2.04998700	0.13522700
C	2.11203100	3.36652800	0.24011700
C	0.75305400	3.59041600	0.24604700
C	-0.11413200	2.48941100	0.15577200
Pd	-0.80337300	-0.62781700	-0.16430400
H	2.81449900	4.19646800	0.31087500
H	0.34563100	4.59561800	0.31770600
H	-1.19788900	2.61756700	0.15079300
N	1.16702700	-1.33927300	-0.20268000
C	1.57144400	-2.59623400	-0.33785100
C	2.92586600	-2.95649100	-0.36102000
C	3.88200200	-1.97316000	-0.24488800
C	3.48526700	-0.62797800	-0.10738800
C	2.10232200	-0.35060400	-0.08820700
H	0.79313900	-3.35118400	-0.43911800
H	3.19745500	-4.00262300	-0.47512500
H	4.94300300	-2.22022500	-0.26287100
C	4.42322100	0.44870300	0.00147400
C	4.00243800	1.73646200	0.11464800
C	-1.64138500	-2.43666400	-0.51432400
H	-2.73057600	-2.32110300	-0.52410900

H	5.48599500	0.21102700	-0.01544300
H	4.72193400	2.55069500	0.18987000
H	-1.33617700	-3.14732100	0.26592300
H	-1.27774100	-2.74351400	-1.50400900
C	-3.36655400	0.17622100	1.94152500
C	-2.60428900	-0.93946900	2.28786200
H	-3.07351800	-1.92279400	2.29454800
H	-4.44230700	0.10490600	1.79562400
H	-2.96127000	1.17828300	2.07184200
C	-1.23361100	-0.83232400	2.33816900
H	-0.60141600	-1.69602000	2.53970600
H	-0.75798400	0.14609100	2.42312400
O	-2.38387600	0.55386500	-2.16711800
C	-3.11724800	0.67510700	-1.20065600
C	-4.48020700	1.29614100	-1.22666300
O	-2.70541400	0.22842400	-0.01780600
H	-4.58959200	2.04124000	-0.42841200
H	-5.24274500	0.52378100	-1.06212300
H	-4.65916700	1.76579200	-2.19711400

7TS_Pd

E = -1084.309267 au

H = -1083.954997 au

G = -1084.030944 au

N	0.40096000	1.18412000	-0.27958600
C	1.73053800	0.93179300	-0.21123400
C	2.69656800	1.94962700	-0.34965400
C	2.22587600	3.26161700	-0.56502400
C	0.87113300	3.49936600	-0.63978900
C	-0.01683700	2.42077800	-0.49327600
Pd	-0.76172400	-0.66180400	-0.09068600
H	2.94331900	4.07383000	-0.67936500
H	0.48176900	4.49894900	-0.81618000
H	-1.09739000	2.55448200	-0.55401500
N	1.18863600	-1.39527500	0.10965300
C	1.56904300	-2.65742000	0.26251800
C	2.91618400	-3.04178600	0.31769900
C	3.89295400	-2.07869200	0.20722400
C	3.52306300	-0.72946700	0.03637500
C	2.14612800	-0.42826300	-0.01094000
H	0.77714500	-3.40007300	0.34184900
H	3.16514800	-4.09229100	0.44296100
H	4.94871600	-2.34539200	0.24370500
C	4.48133700	0.32643300	-0.09829500
C	4.08608100	1.61426500	-0.28158500
C	-1.62232000	-2.49822800	0.04976000
H	-2.71487100	-2.44210900	0.02956700
H	5.53942100	0.07132400	-0.05671400
H	4.82192100	2.41003500	-0.38993300
H	-1.27948100	-2.98154400	0.97697700
H	-1.28440100	-3.04537100	-0.83961000
C	-1.75643700	1.76421800	2.96834900
C	-2.72653500	1.17517400	2.23395400
H	-3.61366400	1.72301900	1.91869800

H	-1.83456100	2.79424600	3.31057600
H	-0.85555500	1.21547800	3.24750200
C	-2.61940600	-0.19756400	1.90352100
H	-3.48236200	-0.77009100	1.57540500
H	-1.77497800	-0.77144800	2.28605900
O	-3.09410100	-0.90600000	-2.11748600
C	-3.39302000	-0.09400900	-1.26888100
C	-4.72819800	0.60264300	-1.20317700
O	-2.56715300	0.30263800	-0.29513900
H	-4.59608700	1.69048900	-1.16472100
H	-5.25996200	0.30722200	-0.28707500
H	-5.33887100	0.33427800	-2.06889900

8_Pd

E = -1084.353170 au

H = -1083.997887 au

G = -1084.069735 au

N	0.20414400	1.24928700	0.04813400
C	1.52510900	0.97104300	-0.04976600
C	2.50469700	1.98373100	-0.08747800
C	2.05142900	3.31832200	-0.02561000
C	0.70236700	3.58245800	0.06650600
C	-0.20032200	2.50621300	0.10145500
Pd	-0.98997500	-0.60931800	-0.01939200
H	2.77704700	4.13064400	-0.05483700
H	0.32878300	4.60218600	0.11199200
H	-1.27772100	2.66010500	0.17923200
N	0.95287200	-1.37258300	-0.10037000
C	1.30253000	-2.65018200	-0.17935600
C	2.63943500	-3.05603000	-0.28183200
C	3.62975700	-2.09941100	-0.30257100
C	3.28707200	-0.73460900	-0.22513400
C	1.91837500	-0.40776000	-0.12383100
H	0.49650400	-3.38162600	-0.16585200
H	2.87106000	-4.11590000	-0.34471700
H	4.67827700	-2.38469100	-0.38101200
C	4.26013600	0.31602400	-0.25227500
C	3.88569400	1.62187500	-0.18870900
C	-1.97159400	-2.38810800	-0.20186100
H	-3.02821000	-2.19650100	0.00744500
H	5.31166900	0.04363500	-0.33028600
H	4.63235500	2.41427900	-0.21690500
H	-1.55906500	-3.12801800	0.49292400
H	-1.81453600	-2.66982000	-1.24964000
C	-2.10435400	0.97053500	3.13860100
C	-2.08953100	-0.26062300	2.60121000
H	-3.01375400	-0.83824700	2.54140900
H	-3.01206000	1.40775700	3.54842500
H	-1.19363500	1.56873700	3.20324500
C	-0.88058900	-0.86266800	2.07445700
H	-0.78262500	-1.94472900	2.20119700
H	0.04465500	-0.33156500	2.32715200
O	-1.83735000	0.02305200	-2.12406800
C	-2.81046500	0.46033900	-1.47556500
C	-3.97428300	1.13133200	-2.12523600

O	-2.82164900	0.32533100	-0.18461700
H	-4.61732100	1.62256400	-1.38975300
H	-4.56331900	0.37777800	-2.66247200
H	-3.61918300	1.85316400	-2.86840400

9TS_Pd

E = -1084.323279 au

H = -1083.967433 au

G = -1084.042253 au

N	-0.61335700	1.25546300	-0.28581700
C	-1.89233200	0.80609900	-0.20055000
C	-2.99862800	1.66606200	-0.32212100
C	-2.72982100	3.03364800	-0.53981200
C	-1.42614200	3.46970000	-0.62584000
C	-0.38052500	2.54204500	-0.49226400
Pd	0.78940500	-0.27571900	0.00254100
H	-3.55799500	3.73467500	-0.63785500
H	-1.19093400	4.51735500	-0.79350800
H	0.66484700	2.83808700	-0.55819900
N	-0.98365000	-1.38105400	0.13582300
C	-1.14204300	-2.67986900	0.35264200
C	-2.40635400	-3.27499000	0.46443000
C	-3.53221100	-2.48912700	0.34977700
C	-3.39711700	-1.10453500	0.12293500
C	-2.08978800	-0.59007400	0.02217800
H	-0.23552300	-3.27577500	0.44661900
H	-2.47820400	-4.34474400	0.64179800
H	-4.52660500	-2.92594000	0.43606800
C	-4.50899600	-0.21053900	-0.00302200
C	-4.31795900	1.11968200	-0.21734700
C	2.02893200	-1.65702700	1.10946400
H	3.02687200	-1.23775300	1.23768100
H	-5.51457900	-0.62042300	0.07941400
H	-5.16861800	1.79335800	-0.30955300
H	2.04236900	-2.74882700	1.10007300
H	1.37020900	-1.31632500	1.92838400
C	4.35715800	-1.14947400	-1.67534600
C	3.55522800	-1.99901500	-1.02162800
H	3.98114400	-2.85728700	-0.49781600
H	5.43305200	-1.30531800	-1.71877900
H	3.96083300	-0.27227800	-2.18631900
C	2.09915600	-1.84186200	-0.99298600
H	1.52780200	-2.77257500	-1.01978400
H	1.76517900	-1.16541700	-1.79564600
O	2.36417500	0.95505200	-0.20354800
C	2.64255600	1.59418500	0.91760300
C	3.88957300	2.43055400	0.81743800
O	1.96431200	1.50188400	1.93060800
H	3.96259500	3.09352000	1.68353100
H	3.90653900	3.01097800	-0.11174400
H	4.76541700	1.76863300	0.79892000

10TS_Pd

E = -1084.372668 au

H = -1084.014575 au

G = -1084.086514 au

N	0.53754100	1.25041900	-0.57757300
C	1.75088800	0.81289400	-0.14806300
C	2.80139600	1.70220300	0.16352000
C	2.56152700	3.08084300	0.00535800
C	1.33338400	3.50807600	-0.44463900
C	0.34541300	2.55368900	-0.72260000
Pd	-0.89068600	-0.31837600	-0.84608800
H	3.35262000	3.79354800	0.23607500
H	1.11511300	4.56338600	-0.58634500
H	-0.63425900	2.87080600	-1.07681300
N	0.94524700	-1.43501000	-0.35417100
C	1.12831700	-2.74053700	-0.25056400
C	2.33474800	-3.31070700	0.18261100
C	3.37793800	-2.47765600	0.51777800
C	3.21467200	-1.08138500	0.41897800
C	1.96410600	-0.60125100	-0.02453600
H	0.28313900	-3.37563300	-0.52277500
H	2.42852500	-4.39171200	0.24597800
H	4.33017500	-2.88260100	0.85930900
C	4.25540600	-0.15358200	0.74171200
C	4.05658100	1.18473800	0.61669000
C	-2.04025100	-2.15813700	-1.14198200
H	-1.87831000	-2.50125900	-0.11122500
H	5.21192000	-0.54403500	1.08672700
H	4.85086400	1.89013100	0.85713300
H	-1.26011800	-2.49462600	-1.83839500
C	-2.99519900	1.53213400	0.17946500
C	-2.57784700	0.82539900	-1.08855800
H	-2.37523000	1.50432400	-1.92527300
H	-2.20803500	2.20345200	0.54700300
H	-3.89483500	2.13195000	-0.01587000
C	-3.12547700	-0.44961300	-1.41662100
O	-1.25682200	0.56436800	1.99173600
C	-2.41340100	0.22024300	2.07896300
C	-2.98672900	-0.69758100	3.10848800
O	-3.37382800	0.62849200	1.21432000
H	-2.20376300	-1.01556800	3.80021000
H	-3.43590100	-1.57386000	2.62436400
H	-3.78904500	-0.19386700	3.65988600
H	-2.97441200	-2.59395100	-1.49335800
H	-3.30743200	-0.65802900	-2.46982600
H	-3.88663700	-0.83652800	-0.73902300

9_Pd

E = -1084.400213 au

H = -1084.040551 au

G = -1084.112971 au

N	0.59763100	1.26710500	-0.47426400
C	1.81835500	0.78939800	-0.10505300
C	2.87778500	1.65508000	0.24196000

C	2.63878700	3.04197000	0.18711700
C	1.40173900	3.50523300	-0.19954300
C	0.40296200	2.57666100	-0.52130600
Pd	-0.82620200	-0.25646100	-0.80373000
H	3.43876500	3.73371900	0.44886300
H	1.18466900	4.56853900	-0.25843000
H	-0.58566000	2.91501500	-0.82933100
N	1.00237800	-1.44077100	-0.43898600
C	1.18171300	-2.75178500	-0.42195500
C	2.39630500	-3.34986600	-0.05171100
C	3.44936200	-2.54080600	0.31038400
C	3.28916200	-1.14024400	0.30330900
C	2.03009800	-0.63153300	-0.08068600
H	0.32730300	-3.36312700	-0.71439800
H	2.48892000	-4.43278500	-0.05721100
H	4.40774900	-2.96828000	0.60375800
C	4.33955900	-0.23714700	0.66204500
C	4.14172200	1.10672100	0.63032800
C	-2.91136500	-1.53231700	-1.26166700
H	-3.02585400	-1.79993000	-0.20467700
H	5.30249200	-0.65037300	0.95931800
H	4.94290500	1.79350300	0.89983700
H	-1.85443300	-1.74333500	-1.60395600
C	-2.89002400	1.49977800	0.33389900
C	-2.47041400	0.90954400	-0.99069900
H	-2.20972000	1.71802600	-1.69060600
H	-2.08839700	2.09109000	0.79710200
H	-3.75863500	2.15729900	0.17759500
C	-3.41768000	-0.11514100	-1.58803500
O	-1.25121600	0.05406800	1.90534100
C	-2.44782500	-0.09671700	2.04343500
C	-3.10627900	-0.98612500	3.04671700
O	-3.36140700	0.52926100	1.27580400
H	-2.34962300	-1.53768900	3.60868300
H	-3.79064900	-1.68365400	2.54844300
H	-3.71325000	-0.38612100	3.73503100
H	-3.45245100	-2.28426100	-1.84956400
H	-3.45685600	0.00402700	-2.67765200
H	-4.44484100	-0.00166900	-1.20888400

11TS_Pd

E = -1084.399745 au

H = -1084.040946 au

G = -1084.111190 au

N	0.74078400	1.31960900	-0.28962600
C	1.94404100	0.75221400	0.00320300
C	3.06423200	1.53257400	0.36336700
C	2.90491300	2.93151900	0.40565800
C	1.68362300	3.48718800	0.09977000
C	0.62266800	2.63883600	-0.24349400
Pd	-0.77483900	-0.11168500	-0.71881000
H	3.75299300	3.55857700	0.67895300
H	1.52646500	4.56247100	0.11772700
H	-0.35335000	3.05395600	-0.49205400

N	0.98608600	-1.40470700	-0.42404800
C	1.08303400	-2.72311100	-0.47701200
C	2.26947700	-3.41197900	-0.18038700
C	3.38265400	-2.68741600	0.18124400
C	3.30876800	-1.28131600	0.25127500
C	2.07199900	-0.67847600	-0.06066500
H	0.18245800	-3.26554500	-0.76672900
H	2.29417800	-4.49683800	-0.24141300
H	4.32269600	-3.18630900	0.41538000
C	4.42340900	-0.46291500	0.61877700
C	4.30598600	0.88981900	0.67027200
C	-2.91383100	-1.19430400	-1.59082100
H	-3.19201900	-1.60460200	-0.61402100
H	5.36983600	-0.94811500	0.85408300
H	5.15626400	1.51150600	0.94747500
H	-1.83752500	-1.44545600	-1.80701900
C	-2.87150100	1.55641100	0.46067400
C	-2.34228800	1.14860600	-0.89333700
H	-1.97495500	2.04246800	-1.42021400
H	-2.07867900	1.95526900	1.10952600
H	-3.63476600	2.33832400	0.33017300
C	-3.26297700	0.29737400	-1.74904300
O	-1.64247400	-0.47118800	1.74950800
C	-2.85402200	-0.39844800	1.82239100
C	-3.73095400	-1.30235400	2.62430800
O	-3.57471100	0.52308800	1.16102600
H	-3.13521500	-2.10216200	3.06929700
H	-4.52291400	-1.72400100	1.99364100
H	-4.22839800	-0.73099900	3.41714400
H	-3.42570000	-1.79090000	-2.35610100
H	-3.14200000	0.57464800	-2.80341400
H	-4.32279800	0.45036300	-1.49279900

10_Pd

E = -1084.425211 au

H = -1084.064338 au

G = -1084.136385 au

N	0.82973700	-1.22836100	-0.36555400
C	2.02250600	-0.57571300	-0.23523800
C	3.25691600	-1.23164000	-0.42676400
C	3.22792400	-2.58796900	-0.80514200
C	2.01677500	-3.21595700	-0.98789700
C	0.83667200	-2.49769300	-0.75415400
Pd	-0.82704800	-0.00569100	0.00300400
H	4.16526000	-3.12052000	-0.96293200
H	1.95637100	-4.25459700	-1.30206900
H	-0.13368200	-2.97214200	-0.88862800
N	0.80816400	1.43913300	0.18232400
C	0.76273600	2.73046500	0.46555000
C	1.92207400	3.49946000	0.66199400
C	3.15258300	2.89189100	0.54797900
C	3.22824600	1.51706400	0.24260400
C	2.01153900	0.82463100	0.07759000
H	-0.23074200	3.17237700	0.54179800

H	1.83379700	4.55731000	0.89601600
H	4.07180400	3.45986600	0.68834800
C	4.46468400	0.81447500	0.08422500
C	4.47712000	-0.50441800	-0.24528800
H	5.39695100	1.36098600	0.22077900
H	5.41948600	-1.03321400	-0.38192000
C	-3.60577600	-0.87355000	0.18259800
C	-2.23678800	-1.48737500	0.01511900
H	-2.16688400	-1.97876900	-0.97107400
H	-4.39032300	-1.62702600	0.03335500
H	-3.73210500	-0.43694300	1.18212000
C	-1.98806200	-2.47851000	1.15041100
O	-2.32789400	1.48025000	0.00429900
C	-3.34370400	1.30583700	-0.68246200
C	-4.00278500	2.40392700	-1.43784200
O	-3.95804400	0.14955700	-0.77925700
H	-3.30553700	3.22810800	-1.60239600
H	-4.85774200	2.77170300	-0.85574800
H	-4.39560800	2.03041700	-2.38879500
H	-1.10968700	-3.09668000	0.91948000
H	-2.83336000	-3.19081400	1.17925000
C	-1.80012800	-1.86624800	2.53479500
H	-0.91191100	-1.21943200	2.56613700
H	-2.66015600	-1.26302800	2.85392200
H	-1.66471500	-2.65173000	3.28797700

12TS_Pd

E = -1084.386941 au

H = -1084.028764 au

G = -1084.100848 au

N	0.99888600	-1.34160600	-0.16649300
C	2.10908200	-0.54496300	-0.11275600
C	3.41832700	-1.05874600	-0.21063800
C	3.56285000	-2.45245400	-0.35704700
C	2.44061900	-3.24799700	-0.38107400
C	1.17553500	-2.65228900	-0.28130900
Pd	-0.77577300	-0.19832100	-0.04260500
H	4.55880500	-2.88608100	-0.44061400
H	2.51194400	-4.32816400	-0.47704500
H	0.28427700	-3.27561800	-0.29221800
N	0.64907200	1.31404900	0.18743400
C	0.42353900	2.60237900	0.39447300
C	1.47375900	3.52958800	0.49013900
C	2.77307300	3.09059700	0.36657400
C	3.03245300	1.72053500	0.15543700
C	1.92241400	0.85866200	0.07378400
H	-0.62274700	2.89060000	0.48953800
H	1.24545400	4.57829900	0.66151900
H	3.60631300	3.78915800	0.43518500
C	4.34888400	1.17420900	0.03069500
C	4.53263300	-0.16176000	-0.14592400
H	5.20152500	1.84950000	0.08481400
H	5.53527600	-0.57753400	-0.23521200
C	-3.11738100	-1.48181800	-1.00479100

C	-2.07813400	-1.94878300	-0.20220700
H	-1.36906900	-2.54594800	-0.78584300
H	-3.05418300	-1.53818800	-2.08737400
H	-4.10879400	-1.28288800	-0.60326300
C	-2.32600600	-2.42941100	1.22029100
O	-2.18275000	1.22945300	0.25046800
C	-3.12087800	1.43380800	-0.61096600
C	-3.83416400	2.75261200	-0.44689600
O	-3.44000700	0.64779400	-1.51079900
H	-3.12412300	3.57460300	-0.60077500
H	-4.22385200	2.84337900	0.57313600
H	-4.64903900	2.83797300	-1.16912800
H	-1.35550200	-2.62937500	1.70041200
H	-2.82960400	-3.40901500	1.16244900
C	-3.13865700	-1.49131300	2.10033900
H	-2.62190900	-0.53718500	2.26264900
H	-4.12281400	-1.26364600	1.66908000
H	-3.31772700	-1.94931200	3.07984500

11_Pd

E = -157.0801748 au

H = -156.965795 au

G = -156.998936 au

N	0.32464100	1.32271200	0.00044100
C	1.53890000	0.70968200	0.00023300
C	2.74833800	1.42164800	-0.00012500
C	2.65748900	2.82988700	-0.00013300
C	1.41858400	3.43636400	0.00013900
C	0.25702000	2.64649900	0.00037100
Pd	-1.23550100	0.00046000	0.00032100
H	3.56721100	3.42933600	-0.00035700
H	1.32177100	4.51871700	0.00015300
H	-0.74094500	3.08377300	0.00050800
N	0.32392400	-1.32295200	0.00071100
C	0.25570500	-2.64671700	0.00055800
C	1.41692200	-3.43710200	-0.00003900
C	2.65611900	-2.83120400	-0.00043100
C	2.74766100	-1.42301900	-0.00025000
C	1.53852300	-0.71051800	0.00027100
H	-0.74248800	-3.08345900	0.00101000
H	1.31971400	-4.51942000	-0.00019700
H	3.56555700	-3.43108900	-0.00088200
C	3.97491600	-0.68243800	-0.00063200
C	3.97524000	0.68050700	-0.00053300
H	4.91396100	-1.23390000	-0.00101100
H	4.91453600	1.23154400	-0.00080700
O	-2.98014100	-1.08288000	-0.00015200
C	-3.65731000	0.00432200	-0.00089200
C	-5.13563600	0.00075900	-0.00076400
H	-5.50148000	-0.51909500	0.89263500
H	-5.52202300	1.02330000	-0.01929600
H	-5.50217600	-0.55349800	-0.87275400
O	-2.97678300	1.08816900	-0.00091000

1_Pt

E = -730.223461 au

H = -729.999851 au

G = -730.054377 au

N	0.49123900	-1.41771100	-0.00004500
C	1.45869900	-0.46641100	-0.00001300
C	2.83259300	-0.77297900	0.00000800
C	3.18485700	-2.13899100	0.00003900
C	2.19534400	-3.09676300	0.00003500
C	0.85025800	-2.69300400	-0.00002400
H	4.23650900	-2.42327100	0.00006600
H	2.43559300	-4.15670400	0.00007400
H	0.04646600	-3.42817700	-0.00005800
N	-0.30549200	1.16661800	-0.00001000
C	-0.72999400	2.43059500	-0.00000200
C	0.16633500	3.50481800	0.00001100
C	1.52205900	3.26035900	0.00000600
C	1.99164500	1.93269300	-0.00001200
C	1.03605000	0.89802800	-0.00001000
H	-1.80391100	2.58971300	-0.00000700
H	-0.22857900	4.51714900	0.00002700
H	2.23650700	4.08254000	-0.00000300
C	3.38270300	1.59217300	-0.00000600
C	3.78729000	0.29341900	0.00001000
H	4.11193500	2.40077800	-0.00002900
H	4.84723900	0.04351700	0.00000400
C	-3.28358100	0.48627400	0.00006700
H	-3.45519300	1.09037700	-0.90066500
H	-4.00758100	-0.35210600	0.00022400
H	-3.45508100	1.09059600	0.90067000
Pt	-1.49525200	-0.44971800	-0.00000700

2_Pt

E = -1075.874861 au

H = -1075.515800 au

G = -1075.588164 au

N	-0.40824200	0.97394500	-1.02581700
C	-1.65188200	0.72442500	-0.54205400
C	-2.68207100	1.68574200	-0.57550300
C	-2.38369000	2.94094000	-1.14169700
C	-1.12717900	3.17272600	-1.65177200
C	-0.16759800	2.15377700	-1.57328700
H	-3.15431000	3.71003400	-1.17915900
H	-0.86579900	4.12360900	-2.10856500
H	0.83415400	2.31686800	-1.97107700
N	-0.90567200	-1.48731800	0.04315900
C	-1.14166000	-2.69850100	0.53784400
C	-2.39421600	-3.07911000	1.03275500
C	-3.42352100	-2.16458900	1.01815300
C	-3.20387300	-0.87231500	0.50231000
C	-1.91589100	-0.57090900	0.01306600
H	-0.30532600	-3.39371100	0.54698300
H	-2.53110600	-4.08411400	1.42287000
H	-4.40941100	-2.42713800	1.40059000

C	-4.22687700	0.12719400	0.45990500
C	-3.97425400	1.35883300	-0.05540500
C	1.96971000	-2.46787300	-0.17963200
H	1.46421800	-3.27652500	-0.72732800
H	-5.21307200	-0.12321800	0.84802400
H	-4.75413500	2.11830400	-0.08868400
H	1.93757500	-2.67116500	0.90096100
H	3.02004800	-2.45637000	-0.49795100
C	2.74136300	1.57575800	0.49895800
C	2.88394400	0.25470700	-0.19320600
H	3.48414600	-0.46773000	0.36538700
H	3.70491000	2.10165000	0.44170600
H	1.96790200	2.20681200	0.04782100
C	2.70813800	0.07159900	-1.56770100
H	3.21523100	-0.74284900	-2.08557100
H	2.41250800	0.90772300	-2.20574100
O	0.30737900	1.93608800	1.62618400
C	1.22804200	1.61554500	2.34319100
C	1.16468200	1.42593000	3.82308000
O	2.48384800	1.39599100	1.88784600
H	1.63795500	0.48214000	4.11483900
H	0.12473000	1.45164100	4.15592900
H	1.72123300	2.23067600	4.31902000
Pt	0.97637300	-0.72555000	-0.58240700

2TS_Pt

E = -1075.808411 au

H = -1075.453241 au

G = -1075.523296 au

N	-0.46889300	1.24121300	-0.62363500
C	-1.73267600	0.87196600	-0.28408500
C	-2.79951800	1.79643500	-0.22877500
C	-2.51733800	3.14172100	-0.53442200
C	-1.23663500	3.50239900	-0.88259400
C	-0.24290300	2.51416900	-0.91324500
Pt	0.98389100	-0.51368300	-0.35865500
H	-3.31765700	3.87994300	-0.49610200
H	-0.98071000	4.52913800	-1.13076800
H	0.77376100	2.78656500	-1.18751500
N	-0.95698800	-1.39287300	-0.05785200
C	-1.19372600	-2.68480500	0.13367800
C	-2.46949100	-3.18229500	0.42571800
C	-3.52227700	-2.30203500	0.52532200
C	-3.30324900	-0.92882600	0.30524600
C	-1.99012200	-0.50978600	0.00090700
H	-0.34373700	-3.35839400	0.05328800
H	-2.60405400	-4.25051200	0.57344000
H	-4.52590600	-2.65292100	0.76280200
C	-4.35667500	0.03681700	0.37062300
C	-4.11326800	1.34888100	0.11782200
C	1.99598600	-2.22747200	0.14310700
H	2.14603900	-2.87510200	-0.73000500
H	-5.35899100	-0.30564600	0.62374600
H	-4.91561600	2.08378000	0.16536300
H	1.39170100	-2.72351400	0.91078000

H	2.95916400	-1.96250600	0.59325400
C	3.06616800	1.22796300	-0.64525700
C	2.85260800	-0.01039400	-1.29342100
H	3.61437200	-0.77204200	-1.12330100
H	4.01483600	1.42248900	-0.15484800
H	2.51161100	2.11407500	-0.93714800
C	1.81854700	-0.31624200	-2.26151300
H	1.96893800	-1.21145100	-2.86572800
H	1.31422800	0.49592600	-2.79227400
O	0.93767000	-0.04406000	1.81764300
C	1.69870200	0.92633300	2.10472400
C	1.74648200	1.35943500	3.54780000
O	2.44298400	1.56626800	1.30304100
H	0.84278000	1.04552100	4.07719200
H	1.88765500	2.44132500	3.62394100
H	2.61037200	0.87894500	4.02410400

1TS_Pt

E = -1075.781182 au

H = -1075.425500 au

G = -1075.498905 au

N	-0.40577500	1.03329400	-0.86897300
C	-1.65973600	0.68233900	-0.48448300
C	-2.74435800	1.58228200	-0.52832000
C	-2.48404400	2.89428400	-0.97255300
C	-1.21050200	3.23798900	-1.35822300
C	-0.19823700	2.27104700	-1.28823700
H	-3.29596300	3.61960900	-1.00967700
H	-0.97012200	4.23978400	-1.70311700
H	0.81609500	2.53626000	-1.58281200
N	-0.80921200	-1.50839500	0.01883600
C	-1.01043200	-2.78418500	0.33984300
C	-2.27686400	-3.28866900	0.65308300
C	-3.35987000	-2.43781000	0.64387900
C	-3.18200500	-1.08786400	0.28530600
C	-1.87865900	-0.66181100	-0.04554100
H	-0.13698300	-3.43151400	0.35238100
H	-2.38121000	-4.34001300	0.90734100
H	-4.35544100	-2.79724500	0.90163700
C	-4.26123900	-0.15002800	0.23803600
C	-4.04805800	1.13688000	-0.14371800
C	2.11819500	-2.20365100	0.38774800
H	2.24951300	-2.97031300	-0.38664200
H	-5.25747500	-0.49226400	0.51401900
H	-4.87073500	1.84967800	-0.17753100
H	1.52932000	-2.59060200	1.22862000
H	3.08958800	-1.89098700	0.78486400
C	2.90811300	1.09987100	-0.06669100
C	3.02184700	0.05633900	-1.02021700
H	3.80320200	-0.68384300	-0.84830000
H	3.65324100	1.15955800	0.72034500
H	2.29368700	1.99015500	-0.19624300
C	2.15777600	-0.16596400	-2.13109400
H	2.38404700	-1.00570700	-2.78677900

H	1.60470200	0.64618200	-2.60449500
O	0.82329300	2.61559700	1.32287700
C	1.10835500	1.70676400	2.10680200
C	0.75768600	1.79728200	3.57585500
O	1.74976600	0.61969400	1.78763500
H	0.39687900	0.83633700	3.95758800
H	0.01234700	2.58151600	3.73700100
H	1.66243400	2.05097300	4.14224400
Pt	1.06596800	-0.58942000	-0.33374900

3_Pt

E = -1075.837178 au

H = -1075.479828 au

G = -1075.552976 au

N	-0.48188200	1.23635900	-0.54209900
C	-1.72822600	0.74769600	-0.31446400
C	-2.87282200	1.57189500	-0.35459600
C	-2.67959900	2.94204700	-0.62318400
C	-1.40646700	3.42498900	-0.82082200
C	-0.32586600	2.53191300	-0.76728300
H	-3.54226200	3.60659600	-0.65938100
H	-1.22072900	4.47880900	-1.01062300
H	0.69308000	2.89258700	-0.89213200
N	-0.75935600	-1.42214200	0.06589800
C	-0.87436900	-2.70761800	0.36680100
C	-2.11307000	-3.31424200	0.61228600
C	-3.25481100	-2.54838600	0.54489300
C	-3.15981200	-1.17738400	0.23366500
C	-1.87382900	-0.64650300	-0.00425300
H	0.04752100	-3.28407700	0.41763400
H	-2.15127500	-4.37276600	0.85522600
H	-4.23396800	-2.98820300	0.73191100
C	-4.30276200	-0.31925900	0.16223100
C	-4.16411700	1.00345400	-0.11701200
C	2.29010200	-1.94596900	0.28692100
H	2.20780700	-2.76131500	-0.44341500
H	-5.28631500	-0.75005900	0.34447500
H	-5.03499600	1.65604700	-0.15988200
H	1.89672700	-2.23038800	1.26823100
H	3.33441400	-1.63379100	0.39599900
C	2.78447700	0.77958200	-1.01406100
C	2.55709500	-0.28871300	-1.92917000
H	3.24174400	-1.13750200	-1.93829600
H	3.68218300	0.77380300	-0.39781200
H	2.38636800	1.77405700	-1.21020500
C	1.27833700	-0.44403200	-2.50085100
H	1.03628900	-1.37545400	-3.01119700
H	0.69793000	0.42772100	-2.80645300
O	1.87940000	2.06124600	1.41910900
C	1.43474600	1.19134700	2.15879200
C	1.35197800	1.35955400	3.65380100
O	0.99841500	0.01927700	1.75503300
H	0.42630900	0.93244100	4.05293200
H	1.42997500	2.41844600	3.91434100

H	2.18697800	0.82302900	4.12150500
Pt	1.10541600	-0.35328100	-0.29583000

3TS_Pt

E = -1075.772342 au

H = -1075.416379 au

G = -1075.491305 au

N	-0.41400100	1.04906900	-0.46231700
C	-1.74076900	0.85034600	-0.21154600
C	-2.65142300	1.92463600	-0.38321100
C	-2.15740600	3.17314000	-0.80252200
C	-0.81109800	3.34068500	-1.02977200
C	0.03640800	2.24708400	-0.84606800
H	-2.85555500	3.99886700	-0.93635600
H	-0.39382800	4.29297600	-1.34549400
H	1.11324200	2.33366900	-0.99425400
N	-1.39412800	-1.45677500	0.41618700
C	-1.85974900	-2.61455500	0.84266700
C	-3.21731000	-2.85003200	1.12101300
C	-4.10434000	-1.81544400	0.93733900
C	-3.63827900	-0.56344400	0.48701700
C	-2.24896700	-0.43062600	0.23804000
H	-1.12465900	-3.41126300	0.98038600
H	-3.54611700	-3.82478500	1.47325400
H	-5.16755900	-1.94510100	1.13841400
C	-4.52404300	0.54007700	0.29118400
C	-4.04672000	1.73834200	-0.12779600
C	2.61118100	-1.77385400	0.81917000
H	2.35859100	-2.83307500	0.88584700
H	-5.58596600	0.39964800	0.48958600
H	-4.71339100	2.58679000	-0.27507000
H	2.22680100	-1.25122800	1.70234600
H	3.68688300	-1.59499200	0.75812100
C	2.60733900	-1.83879900	-1.24463600
C	1.25119300	-1.94327100	-1.72682500
H	0.67135600	-2.84109900	-1.50665000
H	3.15113000	-2.76210900	-1.06785200
H	3.23729200	-1.04004700	-1.64340700
C	0.64863400	-0.82929900	-2.31280600
H	-0.41094300	-0.87017000	-2.56355700
H	1.24128400	-0.07163100	-2.82943800
O	3.07576000	1.66288500	0.28924500
C	2.47151700	1.51640600	1.34659000
C	2.83007100	2.24905800	2.60829400
O	1.45429800	0.68909700	1.49197000
H	1.93829300	2.51249700	3.18579300
H	3.41370100	3.14185200	2.36795200
H	3.44563100	1.59438600	3.23882300
Pt	1.08965200	-0.40897200	-0.21823100

4_Pt

E = -1075.886065 au

H = -1075.526501 au

G = -1075.599746 au

N	-1.08509300	-1.34772500	0.16082100
C	-2.20180600	-0.56753500	0.04423900
C	-3.50444400	-1.08655800	0.16193900
C	-3.63137300	-2.46749900	0.41409500
C	-2.49882200	-3.24238600	0.53443200
C	-1.23826600	-2.64539500	0.40218000
H	-4.62215200	-2.90908700	0.51481000
H	-2.56129100	-4.30923600	0.73149000
H	-0.33266100	-3.24246200	0.49494200
N	-0.73523100	1.27496600	-0.29916100
C	-0.50428600	2.55923600	-0.53472300
C	-1.55359700	3.47848200	-0.68355300
C	-2.85635500	3.04147300	-0.58167500
C	-3.12188800	1.67813800	-0.33469300
C	-2.01402400	0.82416500	-0.20166900
H	0.54016300	2.85436600	-0.61227000
H	-1.32211100	4.52269100	-0.87560400
H	-3.68597200	3.73908600	-0.69061500
C	-4.43801000	1.12794100	-0.21346100
C	-4.62073800	-0.19934600	0.02627400
H	-5.29257000	1.79527400	-0.31399300
H	-5.62374000	-0.61260600	0.12154400
C	2.05681300	-1.71007100	0.80923200
C	1.97366100	-1.98038600	-0.55474900
H	1.22525400	-2.70645100	-0.88819900
H	1.47768600	-2.27474800	1.54128300
H	2.92081800	-1.18315200	1.21554500
C	3.01768700	-1.66489800	-1.59036400
O	2.24857600	1.02920600	-0.18991300
C	2.49533900	1.69434900	0.92653500
C	3.71896200	2.56290200	0.84098700
O	1.80369200	1.59517500	1.92984800
H	3.86370400	2.96623300	-0.16654200
H	4.60192600	1.95594900	1.08331200
H	3.65465100	3.36926500	1.57689000
H	2.61331700	-0.92261300	-2.29704500
H	3.13585800	-2.58457900	-2.18519500
C	4.37037600	-1.21643400	-1.06419200
H	4.30942800	-0.23830200	-0.57551900
H	4.78322200	-1.94264300	-0.35111100
H	5.08252500	-1.12692300	-1.89219300
Pt	0.67770100	-0.24042100	0.00272300

5_Pt

E = -1075.849583 au

H = -1075.491098 au

G = -1075.567297 au

N	0.60114200	1.35482300	-0.15543100
C	1.91248200	1.07774700	0.05767400
C	2.87533700	2.08480400	0.26904300
C	2.42767400	3.42134600	0.24732900
C	1.09491800	3.68956800	0.02493100
C	0.20878600	2.61966500	-0.17346100

H	3.14268600	4.22839200	0.40360700
H	0.72079500	4.70975300	-0.00211000
H	-0.85045800	2.79966800	-0.35755500
N	1.34625200	-1.24939800	-0.16651800
C	1.70345600	-2.53231600	-0.17672700
C	3.02409800	-2.94513200	0.03607300
C	4.00230100	-2.00275300	0.25971800
C	3.65696600	-0.63727200	0.27172000
C	2.30675000	-0.29852600	0.05565000
H	0.91450000	-3.25660200	-0.36119600
H	3.25323600	-4.00732100	0.01822200
H	5.03761100	-2.29751300	0.42646700
C	4.61341400	0.40636300	0.48916300
C	4.24012400	1.71385700	0.48684700
C	-1.37281400	-2.34887000	-0.80557200
H	-2.45323900	-2.24286700	-0.96459200
H	5.65282000	0.12680200	0.65520300
H	4.97566200	2.50066100	0.64858700
H	-1.21440300	-3.01738700	0.05330300
H	-0.93137900	-2.79541900	-1.70893100
C	-2.78226300	0.68868200	1.85134200
C	-3.33346200	-0.59465800	2.36507400
H	-4.38873400	-0.58624900	2.64487700
C	-2.58822400	-1.68626600	2.52540000
H	-2.99707800	-2.60325400	2.94467500
H	-1.53328800	-1.69572600	2.24438100
O	-2.39047400	0.32867000	-0.96084400
C	-3.38294800	0.89859400	-0.50034700
C	-4.48329700	1.35147100	-1.39802800
O	-3.61208400	1.18078900	0.76192300
H	-4.87368700	2.32186000	-1.07641100
H	-5.30789000	0.62994500	-1.33094700
H	-4.13636900	1.39137000	-2.43289400
H	-2.84569200	1.49357900	2.59210100
H	-1.74012400	0.58113700	1.51767500
Pt	-0.52277000	-0.51964500	-0.47928700

5TS_Pt

E = -1075.813268 au

H = -1075.457627 au

G = -1075.530932 au

N	0.34940500	1.30990200	-0.20667100
C	1.69400900	1.14783300	-0.09772100
C	2.58793500	2.23716300	-0.05787500
C	2.03522200	3.53077000	-0.15507700
C	0.67178800	3.68039600	-0.27307400
C	-0.14512500	2.53776800	-0.28909600
H	2.69355800	4.39876200	-0.13677600
H	0.21561200	4.66398700	-0.35174300
H	-1.22999300	2.61684900	-0.35091300
N	1.31709600	-1.22901000	-0.09679800
C	1.77777200	-2.47676400	-0.02702900
C	3.13985000	-2.76700400	0.11438100
C	4.04721100	-1.73357900	0.17984300

C	3.59032900	-0.40331400	0.10868800
C	2.20330400	-0.18881600	-0.02419400
H	1.03931900	-3.27199100	-0.09694700
H	3.45694900	-3.80532700	0.16225500
H	5.11382400	-1.92983600	0.28255200
C	4.47228000	0.72324300	0.15730800
C	3.99150800	1.99224500	0.07233100
C	-1.34728300	-2.59390800	-0.58272900
H	-2.42073200	-2.55408600	-0.80074600
H	5.54098900	0.53930500	0.25734000
H	4.66761800	2.84564100	0.10139200
H	-1.18797800	-3.19856600	0.32342600
H	-0.83171500	-3.06519300	-1.43173200
C	-2.60478000	0.83963600	2.31358800
C	-2.20864900	-0.50637700	2.27582800
H	-2.96526600	-1.29073400	2.24366400
H	-3.60027900	1.11127400	2.65252100
H	-1.84265100	1.60375800	2.45829600
C	-0.87964300	-0.83186500	2.13242200
H	-0.54556800	-1.86554000	2.21115300
H	-0.11437100	-0.06951700	2.29164100
O	-2.55540800	-0.11630200	-0.91613800
C	-3.30990000	0.78232100	-0.43320200
C	-4.62509500	0.98953500	-1.12144300
O	-3.04027600	1.51368900	0.56946500
H	-4.87357700	2.05547100	-1.14713400
H	-5.41087400	0.48858300	-0.54018600
H	-4.61561400	0.56979700	-2.13061600
Pt	-0.64786800	-0.68389300	-0.34432700

4TS_Pt

E = -1075.795971 au

H = -1075.441141 au

G = -1075.516548 au

N	0.56004300	1.33606500	-0.20385600
C	1.86024800	1.03922500	0.05271700
C	2.83564600	2.03239700	0.27335400
C	2.41353500	3.37684600	0.21490600
C	1.09393600	3.66343700	-0.05181800
C	0.19121500	2.60713800	-0.25610200
H	3.13894700	4.17357600	0.37695600
H	0.73788900	4.68889200	-0.10732600
H	-0.86048500	2.79754900	-0.45679000
N	1.26561800	-1.28332300	-0.14468800
C	1.60656900	-2.57004400	-0.14446900
C	2.91653400	-3.00201000	0.09576400
C	3.90099100	-2.07024600	0.33793300
C	3.57530000	-0.69973800	0.33403900
C	2.23403700	-0.34394100	0.08484400
H	0.81101000	-3.28363100	-0.34544100
H	3.13384700	-4.06678200	0.08378600
H	4.92888400	-2.37717800	0.52779900
C	4.54250200	0.33076800	0.56235700
C	4.18778900	1.64319400	0.53339600

C	-1.49757700	-2.32801400	-0.88830200
H	-2.57686000	-2.19646200	-1.03126600
H	5.57363400	0.03862600	0.75608600
H	4.93065200	2.42184100	0.70183100
H	-1.32556900	-3.03321900	-0.06000100
H	-1.07318100	-2.75218200	-1.81097000
C	-3.91981500	-0.78178600	2.61673500
C	-2.67753600	-1.10953100	2.18163500
H	-2.44846400	-2.12477700	1.85997400
H	-4.71054900	-1.52422300	2.70629200
H	-4.16318700	0.24614500	2.88715200
C	-1.65060800	-0.14256500	2.18704600
H	-0.61465100	-0.43691100	2.03280800
H	-1.82479600	0.83861400	2.61672600
O	-2.40285800	0.30136800	-1.13194600
C	-3.01834600	1.14064100	-0.38507900
C	-4.29981900	1.68530800	-0.95621400
O	-2.64627900	1.49448900	0.75235400
H	-4.49672600	2.68904500	-0.56886500
H	-5.12278600	1.03290500	-0.63329800
H	-4.27967800	1.68544900	-2.04952000
Pt	-0.61425700	-0.51769000	-0.54828000

6_Pt

E = -1075.827622 au

H = -1075.471655 au

G = -1075.546283 au

N	0.53102000	1.37511200	-0.09582600
C	1.84741300	1.05895600	0.02364600
C	2.85197900	2.03693000	0.16749700
C	2.44369300	3.38736700	0.17839900
C	1.10840500	3.69264000	0.05918800
C	0.17249700	2.65209900	-0.07205900
H	3.19198000	4.17201300	0.28665300
H	0.75978100	4.72198800	0.07063700
H	-0.89614600	2.84904900	-0.12843400
N	1.22640800	-1.26183700	-0.14171000
C	1.54983900	-2.55356800	-0.14719700
C	2.86911100	-2.99788200	-0.01193800
C	3.87773600	-2.07103200	0.12982100
C	3.56726400	-0.69739500	0.14216000
C	2.21170800	-0.32656700	0.00785700
H	0.73505600	-3.26282700	-0.27072500
H	3.07416200	-4.06493200	-0.02456500
H	4.91535600	-2.38655800	0.23286100
C	4.56309600	0.31954600	0.28459900
C	4.21868600	1.63468700	0.29548300
C	-1.55069800	-2.31302200	-0.85312200
H	-2.63035100	-2.17738000	-0.96720900
H	5.60386900	0.01514800	0.38344100
H	4.97967800	2.40631300	0.40434500
H	-1.34586000	-3.05806800	-0.07307200
H	-1.11124000	-2.64069300	-1.80713100
C	-3.40726100	-0.53494100	2.46981800

C	-2.40506800	-1.28590500	1.98279700
H	-2.54118500	-2.36186100	1.86547200
H	-4.35126400	-0.98327700	2.77409700
H	-3.30212800	0.54358400	2.58506100
C	-1.09433400	-0.72785900	1.68973100
H	-0.25412000	-1.36820200	1.98109800
H	-0.97203100	0.31743800	1.99343800
O	-2.50209900	0.22651700	-0.97605700
C	-3.07660300	1.22966800	-0.35620000
C	-4.42721200	1.56622200	-0.92162000
O	-2.59649200	1.81392500	0.61010300
H	-4.67395300	2.60989400	-0.70730400
H	-5.17491700	0.93068500	-0.42744200
H	-4.48107600	1.36600300	-1.99581700
Pt	-0.70462000	-0.50210800	-0.41023300

6TS_Pt

E = -1075.792891 au

H = -1075.436520 au

G = -1075.509132 au

N	0.77229000	1.30580900	-0.20367100
C	2.02917700	0.84892000	0.04861100
C	3.11957600	1.71325100	0.24121700
C	2.86317600	3.09808500	0.16318800
C	1.58555300	3.54199600	-0.10042600
C	0.55118500	2.61144400	-0.28147000
H	3.67817300	3.80607700	0.30860000
H	1.36035400	4.60282800	-0.16903500
H	-0.47010700	2.91528900	-0.49939600
N	1.11139500	-1.34542600	-0.10446600
C	1.25613200	-2.66618200	-0.10303700
C	2.49530800	-3.28215700	0.11720700
C	3.61036500	-2.50315600	0.34044000
C	3.49132200	-1.09873300	0.33054900
C	2.21198000	-0.56258500	0.09748600
H	0.36097700	-3.25653400	-0.29053000
H	2.55706100	-4.36701200	0.10807700
H	4.58315000	-2.96090900	0.51638900
C	4.58938200	-0.20164700	0.53500900
C	4.41069500	1.14741200	0.49385600
C	-1.91426900	-1.77077000	-1.28131000
H	-2.86247100	-1.30172500	-1.54838400
H	5.57570900	-0.62443100	0.72011600
H	5.25177500	1.82170600	0.64785900
H	-2.01654000	-2.85226400	-1.16779600
H	-1.18622100	-1.62195700	-2.10316300
C	-4.31516600	-1.13077500	1.48332800
C	-3.50727400	-1.91101700	0.75840400
H	-3.91885700	-2.75897100	0.20641100
H	-5.38212900	-1.33557300	1.54638500
H	-3.93556800	-0.27442800	2.04302200
C	-2.04449000	-1.71613800	0.72336600
H	-1.46626600	-2.62341900	0.91674500
H	-1.77358800	-0.93695800	1.45596200

O	-2.15740500	1.04393300	-0.73735100
C	-2.70064600	1.62413400	0.31489300
C	-3.89125200	2.47282800	-0.03493900
O	-2.29872100	1.47437100	1.46194300
H	-4.04257300	3.23817100	0.73165600
H	-4.78207600	1.83022100	-0.05682100
H	-3.79245600	2.92759000	-1.02564000
Pt	-0.61948300	-0.22290100	-0.37254400

7_Pt

E = -1075.83474 au

H = -1075.476646 au

G = -1075.552836 au

N	0.52189400	1.27899100	-0.09665800
C	1.85857200	1.04896300	-0.07700500
C	2.80714300	2.08769000	-0.13386500
C	2.31337600	3.40554700	-0.22113500
C	0.95347600	3.62409900	-0.24849300
C	0.08305100	2.52422800	-0.18319500
H	3.01382800	4.23855400	-0.27025300
H	0.54504200	4.62867800	-0.32266400
H	-0.99889600	2.65284100	-0.20455600
N	1.33603500	-1.29272700	0.04039500
C	1.72148900	-2.56432400	0.11804000
C	3.07142200	-2.93477500	0.15155400
C	4.04465500	-1.96217300	0.10153400
C	3.66711500	-0.60723600	0.02460300
C	2.29060500	-0.31201700	-0.00086500
H	0.93320000	-3.31160000	0.15365900
H	3.32666100	-3.98935100	0.21251400
H	5.10123000	-2.22661900	0.12077400
C	4.61194000	0.46816400	-0.03046300
C	4.20069700	1.76243700	-0.10722600
C	-1.44318400	-2.45562700	-0.05729700
H	-2.52675300	-2.37638600	-0.23555900
H	5.67298000	0.22334100	-0.01191900
H	4.92688800	2.57285400	-0.15257200
H	-1.29185500	-2.96903000	0.90493500
H	-1.02696700	-3.07081600	-0.86792600
C	-3.42286300	0.19301500	1.08698100
C	-2.55629900	0.30173000	2.28955300
H	-1.94190900	-0.56703400	2.53474500
H	-3.97718100	-0.75504900	1.06133900
H	-4.12482500	1.03300500	1.03225700
C	-2.54566000	1.38746700	3.06299000
H	-1.93137500	1.44398700	3.95902200
H	-3.16623200	2.25687100	2.84069000
O	-2.35682200	0.38956200	-2.31200800
C	-3.12566000	0.37187000	-1.39671800
C	-4.61090400	0.48893600	-1.48140800
O	-2.57967300	0.24138800	-0.11633600
H	-4.96549300	1.42167400	-1.02509700
H	-5.11233200	-0.34328400	-0.97259100
H	-4.88903400	0.48836400	-2.53748800

Pt	-0.57172200	-0.60603100	-0.04851600

8TS_Pt

E = -1075.807050 au

H = -1075.451960 au

G = -1075.526629 au

N	0.46884200	1.31390100	0.10301900
C	1.80183500	1.06425600	0.06873200
C	2.76297500	2.09109200	0.14949200
C	2.28611000	3.41364900	0.25848100
C	0.92928900	3.65230900	0.27838500
C	0.04580600	2.56437100	0.19727800
H	2.99820400	4.23579800	0.32193000
H	0.53458300	4.66223300	0.35393400
H	-1.03557500	2.70800500	0.20341600
N	1.25932100	-1.26867500	-0.16623300
C	1.63515700	-2.53808700	-0.29728500
C	2.98186400	-2.92134500	-0.33062200
C	3.96179200	-1.95926100	-0.23014800
C	3.59504500	-0.60533700	-0.09584100
C	2.22021600	-0.29959400	-0.06503600
H	0.83946000	-3.27469900	-0.38385900
H	3.22953900	-3.97381900	-0.44035100
H	5.01654700	-2.23045600	-0.25681000
C	4.55092300	0.45706900	0.00138500
C	4.15310900	1.75249800	0.11576000
C	-1.55778900	-2.36322000	-0.45946600
H	-2.64654700	-2.23879500	-0.52620200
H	5.60947000	0.20223500	-0.02412600
H	4.88757600	2.55385400	0.18333100
H	-1.33329100	-3.07521300	0.34971600
H	-1.19289000	-2.76457000	-1.41616500
C	-3.35277700	0.34726900	1.77140800
C	-2.65885300	-0.76675600	2.26470400
H	-3.14336100	-1.74222800	2.25223500
H	-4.41198200	0.28453800	1.53095000
H	-2.96425100	1.34886500	1.95323500
C	-1.30242500	-0.67318300	2.44127400
H	-0.70227700	-1.53658500	2.72259800
H	-0.82066700	0.30134300	2.53297800
O	-2.25590700	0.79481100	-2.17398000
C	-2.98616900	0.85803700	-1.20723000
C	-4.34881900	1.47962800	-1.19024200
O	-2.57409600	0.34311400	-0.03898000
H	-4.44471300	2.20562800	-0.37272700
H	-5.11339800	0.70680500	-1.03861600
H	-4.53744400	1.97708500	-2.14459700
Pt	-0.67345900	-0.55244100	-0.12411400

7TS_Pt

E = -1075.781182 au

H = -1075.426560 au

G = -1075.501937 au

N	0.54542100	1.26297500	-0.27986600
C	1.87159800	0.98851600	-0.20376900
C	2.85808800	1.98349700	-0.34876500
C	2.41330100	3.30189900	-0.57989000
C	1.06260300	3.56332000	-0.66036300
C	0.15118500	2.50633200	-0.50648400
H	3.14517400	4.10001400	-0.70104800
H	0.69339900	4.56840900	-0.84816000
H	-0.92597000	2.66101600	-0.57152500
N	1.26446900	-1.31277900	0.13822600
C	1.60647600	-2.58606300	0.31393100
C	2.94206700	-3.00215700	0.38723800
C	3.94891500	-2.07016400	0.27138200
C	3.61915500	-0.71376900	0.07765600
C	2.25337200	-0.37511200	0.01452800
H	0.79140800	-3.30130800	0.39541800
H	3.15973800	-4.05719600	0.53112900
H	4.99574400	-2.36752100	0.32105700
C	4.60197800	0.31867900	-0.06583400
C	4.23861000	1.61353200	-0.26888400
C	-1.57757700	-2.38349300	0.07332000
H	-2.67029100	-2.29240900	0.03490000
H	5.65370600	0.04037500	-0.01471000
H	4.99443000	2.38943300	-0.38351100
H	-1.29938000	-2.89768300	1.00756400
H	-1.27635800	-2.99275000	-0.79081900
C	-1.74930500	1.97292700	2.95787200
C	-2.71069400	1.38097200	2.21487200
H	-3.58107300	1.93588000	1.86673500
H	-1.81921700	3.01259500	3.27156100
H	-0.86510300	1.41751900	3.27435500
C	-2.61980300	-0.00166200	1.92231700
H	-3.48209000	-0.56830600	1.58240600
H	-1.79194800	-0.58119600	2.32990400
O	-2.93179200	-0.67201500	-2.20920900
C	-3.27200600	0.04155300	-1.29380000
C	-4.63611600	0.66484300	-1.16383200
O	-2.45570600	0.39200200	-0.28607800
H	-4.55499800	1.75383200	-1.06094500
H	-5.14159600	0.28758600	-0.26340100
H	-5.24572100	0.42261700	-2.03781000
Pt	-0.64564300	-0.56620600	-0.07485000

8_Pt

E = -1075.841385 au

H = -1075.484377 au

G = -1075.558501 au

N	0.40052900	1.32233900	-0.02030300
C	1.70819900	0.98001500	-0.10885100
C	2.73551700	1.94146800	-0.16628300
C	2.34588200	3.29746100	-0.13204200
C	1.01046600	3.62633900	-0.04325000
C	0.05475000	2.59819700	0.01366500

H	3.10802900	4.07464500	-0.17908600
H	0.68644800	4.66344700	-0.01591700
H	-1.01278900	2.80532200	0.09865200
N	1.01145500	-1.32641000	-0.09838600
C	1.28994400	-2.62537000	-0.14700700
C	2.60285800	-3.10114300	-0.24685300
C	3.64450800	-2.20104600	-0.29349000
C	3.37652800	-0.81840800	-0.24574600
C	2.02991500	-0.41552300	-0.14906900
H	0.44427700	-3.30811900	-0.11082300
H	2.77629000	-4.17309100	-0.28630300
H	4.67526200	-2.54529500	-0.36949600
C	4.40193200	0.18043700	-0.29689800
C	4.09553100	1.50553200	-0.25979700
C	-1.96346700	-2.22616000	-0.06930700
H	-3.01012800	-1.99231100	0.15793100
H	5.43796900	-0.14675400	-0.37015900
H	4.88217500	2.25737100	-0.30482300
H	-1.59491200	-2.96480800	0.65360000
H	-1.88467200	-2.61622900	-1.09277300
C	-1.67991600	1.26444500	3.26226600
C	-1.82319800	0.07240900	2.66905700
H	-2.81285600	-0.38405700	2.59711700
H	-2.52150400	1.79010500	3.70812300
H	-0.70048300	1.73927200	3.34917500
C	-0.70183200	-0.66168600	2.07521800
H	-0.70521200	-1.73838900	2.28252800
H	0.27510100	-0.22885400	2.33193700
O	-1.77328800	0.09980800	-2.11595700
C	-2.72179200	0.59052800	-1.46557900
C	-3.90565900	1.22659600	-2.10585400
O	-2.67868700	0.52789900	-0.16807700
H	-4.43084700	1.88330900	-1.40660400
H	-4.59971700	0.43849900	-2.42448800
H	-3.59978200	1.77653900	-3.00112900
Pt	-0.88053500	-0.48369600	-0.00327500

9TS_Pt

E = -1075.790449 au

H = -1075.434131 au

G = -1075.507406 au

N	-0.76105900	1.27917600	-0.25500900
C	-2.03950600	0.81842000	-0.18487700
C	-3.15245000	1.66698600	-0.30246300
C	-2.89530600	3.03979400	-0.50016400
C	-1.59388800	3.48777900	-0.56979200
C	-0.53733100	2.57341900	-0.44207700
H	-3.72825400	3.73532400	-0.59529800
H	-1.36745600	4.53982300	-0.72080700
H	0.50497700	2.87935900	-0.49577600
N	-1.09162500	-1.34400700	0.13242400
C	-1.22163600	-2.64929300	0.34141500
C	-2.47482300	-3.26801700	0.44405900
C	-3.61893800	-2.50752400	0.32947900

C	-3.51310500	-1.11853200	0.11327900
C	-2.21738000	-0.57923100	0.02174600
H	-0.30102300	-3.22239000	0.43618400
H	-2.52457700	-4.34000600	0.61515000
H	-4.60317500	-2.96762600	0.40931000
C	-4.63646300	-0.23799200	-0.01062000
C	-4.46364600	1.09769400	-0.21101900
C	1.98883000	-1.60637500	1.08962900
H	2.96329500	-1.14368000	1.24891500
H	-5.63698200	-0.66162700	0.06275500
H	-5.32444800	1.75863500	-0.30035200
H	2.05121600	-2.69540800	1.15297200
H	1.30726900	-1.28134300	1.90088000
C	4.32219600	-1.10613400	-1.60156900
C	3.54282300	-1.96541900	-0.93912800
H	3.98533500	-2.81384800	-0.41223200
H	5.40056400	-1.24176400	-1.65052900
H	3.90616900	-0.23511000	-2.10832100
C	2.07277000	-1.83291100	-0.88913600
H	1.53103000	-2.78030000	-0.95032500
H	1.74768100	-1.18462300	-1.72106400
O	2.22925500	1.03326400	-0.23672200
C	2.59087500	1.68050800	0.86041900
C	3.87485700	2.44256200	0.68225700
O	1.96182200	1.64204400	1.90616600
H	3.98124500	3.19063200	1.47236500
H	3.93306700	2.91247300	-0.30529000
H	4.71417100	1.73746800	0.75539700
Pt	0.65042100	-0.21473100	-0.00871800

10TS_Pt

E = -1075.831618 au

H = -1075.472883 au

G = -1075.544403 au

N	0.52079600	1.12046600	-0.61311800
C	1.80735400	0.87884000	-0.23587300
C	2.78045100	1.89524600	-0.18682300
C	2.38244000	3.19758200	-0.54688800
C	1.07927400	3.42650100	-0.92555600
C	0.17330200	2.35875400	-0.94344000
Pt	-0.74526500	-0.53996300	-0.56798100
H	3.10841800	4.00922200	-0.51850900
H	0.73544000	4.41838000	-1.20596500
H	-0.86443700	2.51861500	-1.22395000
N	1.18579600	-1.40286900	0.06076000
C	1.48357600	-2.64974900	0.39217600
C	2.76702600	-3.03906300	0.80274200
C	3.76442500	-2.09126400	0.86837500
C	3.47815200	-0.75500500	0.52398000
C	2.15984800	-0.45979300	0.12245800
H	0.67522000	-3.37940800	0.33117000
H	2.95563600	-4.07782300	1.06127400
H	4.77200400	-2.36113600	1.18303200
C	4.44931700	0.29565900	0.56499100

C	4.11281500	1.56824000	0.22329300
C	-1.76567800	-2.53064600	-0.41256500
H	-1.51575200	-2.60651200	0.65517400
H	5.46465200	0.05428500	0.87632800
H	4.85368000	2.36575800	0.25767600
H	-1.01208800	-2.98461800	-1.07024100
C	-3.20206700	1.25327500	-0.17725800
C	-2.54744500	0.27544000	-1.12890700
H	-2.44827000	0.69029100	-2.14085300
H	-2.69254800	2.22484000	-0.17324400
H	-4.24844800	1.41859600	-0.46852400
C	-2.96643100	-1.10881200	-1.07397000
O	-1.46699600	1.99461700	1.73638900
C	-2.30862900	1.17498100	2.02263700
C	-2.45342500	0.48818600	3.34113500
O	-3.25421700	0.74324100	1.15413900
H	-1.74602200	0.90785900	4.05968600
H	-2.25722900	-0.58495700	3.21550000
H	-3.47738400	0.58609600	3.71841900
H	-2.66546500	-3.13017400	-0.54869400
H	-3.13113200	-1.60768600	-2.02888600
H	-3.71784800	-1.34076000	-0.31763200

9_Pt

E = -1075.859553 au

H = -1075.499247 au

G = -1075.571329 au

N	0.49406900	1.05401500	-0.73157500
C	1.76655200	0.79698100	-0.31060900
C	2.73297200	1.81436300	-0.20567500
C	2.35046400	3.12082400	-0.56671300
C	1.07226400	3.35309500	-1.02222200
C	0.16556100	2.28979400	-1.08989100
H	3.07316000	3.93220500	-0.48971800
H	0.74810700	4.34536600	-1.32370100
H	-0.85332700	2.44422800	-1.43551600
N	1.15100400	-1.49756100	-0.12810900
C	1.44789000	-2.75902200	0.14716000
C	2.72237000	-3.15798400	0.57861400
C	3.70768400	-2.20637600	0.72605700
C	3.42194100	-0.85608300	0.43844500
C	2.11426900	-0.55237100	0.01085900
H	0.64789500	-3.48834700	0.02033800
H	2.91416200	-4.20714100	0.78844100
H	4.70681100	-2.48484200	1.05965100
C	4.38224800	0.19850300	0.55654900
C	4.05014800	1.48042700	0.24660100
C	-2.74954600	-1.92731000	-0.28617800
H	-2.66453800	-1.82747000	0.80145700
H	5.38762100	-0.04776100	0.89516100
H	4.78487700	2.27953700	0.33368400
H	-1.72593500	-2.16142000	-0.76983400
C	-2.92558300	1.43262600	0.20601300
C	-2.57850900	0.44896600	-0.89332000

H	-2.55912800	0.99065000	-1.85273800
H	-2.28390700	2.32194200	0.20084000
H	-3.96955900	1.76083400	0.09666100
C	-3.50053800	-0.76694000	-0.94799100
O	-0.80904300	1.70338500	1.85232900
C	-1.74697000	1.03921000	2.23678700
C	-1.81746400	0.30770100	3.53852200
O	-2.86520800	0.83463100	1.50901500
H	-1.05529600	0.68922200	4.22212600
H	-1.62689200	-0.75965200	3.35916500
H	-2.81248400	0.39134600	3.98717300
H	-3.19975200	-2.90627900	-0.50007900
H	-3.72613400	-1.02932600	-1.98921100
H	-4.46198000	-0.60712100	-0.43680900
Pt	-0.78384300	-0.52786800	-0.61561700

11TS_Pt

E = -1075.851787 au

H = -1075.492906 au

G = -1075.564262 au

N	-0.97801200	-1.30556300	-0.05888400
C	-2.17772100	-0.67957000	0.13327600
C	-3.34795000	-1.39429600	0.45874500
C	-3.24887700	-2.79351900	0.58286700
C	-2.03071500	-3.40644900	0.39043300
C	-0.91253000	-2.62746800	0.07028000
H	-4.13487200	-3.37601000	0.83271800
H	-1.91713600	-4.48362300	0.47938100
H	0.05994800	-3.08756300	-0.08916900
N	-1.07482600	1.38650100	-0.29922300
C	-1.07822400	2.70768200	-0.38848800
C	-2.23935000	3.47257900	-0.19403100
C	-3.42139300	2.83110800	0.10379100
C	-3.44271000	1.42614400	0.21846300
C	-2.22827300	0.74435000	0.00852900
H	-0.12352800	3.18050100	-0.61874900
H	-2.18968600	4.55487300	-0.28002600
H	-4.34017900	3.39573400	0.25885600
C	-4.61893100	0.67691800	0.54000800
C	-4.57241100	-0.67736900	0.65435000
C	2.85839700	0.79418100	-1.66850700
H	3.43835600	1.28258200	-0.87978500
H	-5.55351100	1.21407200	0.69591800
H	-5.46825700	-1.24466300	0.90292200
H	1.79163000	1.16908900	-1.56104400
C	2.82201200	-1.55544600	0.74552800
C	2.14467400	-1.36521600	-0.60148300
H	1.78828200	-2.35676700	-0.92237900
H	2.08858300	-1.73382500	1.54627300
H	3.50226900	-2.41731700	0.70325800
C	3.01617000	-0.73538800	-1.68399700
O	2.00861100	0.96035100	1.51139000
C	3.18994800	0.66935400	1.58341000
C	4.25576400	1.56039900	2.13302500

O	3.69879100	-0.48983800	1.15396700
H	3.82527500	2.51719200	2.43597300
H	5.03786700	1.72052800	1.38039100
H	4.73872200	1.08106300	2.99258100
H	3.14036700	1.23829800	-2.63100500
H	2.69141900	-1.11139500	-2.66230500
H	4.08161200	-0.99512300	-1.58077700
Pt	0.59546400	-0.03546500	-0.49149200

10_Pt

E = -1075.890158 au

H = -1075.530134 au

G = -1075.600964 au

N	0.93330900	-1.20598000	-0.35186100
C	2.13958900	-0.57299900	-0.21071100
C	3.36418100	-1.24755800	-0.38229100
C	3.31880600	-2.60501200	-0.75464000
C	2.09847000	-3.21056600	-0.95511300
C	0.92416300	-2.47810700	-0.74387600
H	4.24817100	-3.15522400	-0.89672600
H	2.02487800	-4.24833600	-1.26909500
H	-0.05134700	-2.93229300	-0.89599900
N	0.93470300	1.44482900	0.16249900
C	0.88981200	2.74043800	0.43188600
C	2.05152000	3.50266300	0.63715600
C	3.28231800	2.88991800	0.54921500
C	3.35618200	1.51150100	0.26080500
C	2.13891600	0.82599900	0.08571700
H	-0.10194400	3.18761200	0.48947400
H	1.96451100	4.56336400	0.85818300
H	4.20081400	3.45673800	0.69778300
C	4.58646800	0.79286200	0.12712900
C	4.58881100	-0.52993700	-0.18954400
H	5.52321800	1.32957500	0.27109400
H	5.52748000	-1.06937000	-0.30815000
C	-3.51337300	-0.86902000	0.16757100
C	-2.14186600	-1.47641600	-0.03950200
H	-2.12671500	-1.96548500	-1.03051000
H	-4.30936100	-1.59940800	-0.02126600
H	-3.63173300	-0.48327800	1.18874000
C	-1.94902800	-2.53977100	1.05372700
O	-2.16936000	1.48434700	0.03176500
C	-3.23605400	1.35550100	-0.59806000
C	-3.91437300	2.51428200	-1.23413000
O	-3.86862800	0.22201400	-0.72719500
H	-3.21065800	3.33414100	-1.39244400
H	-4.72262800	2.85972500	-0.57639200
H	-4.37492300	2.20931000	-2.17913400
H	-1.09281600	-3.18093500	0.80147000
H	-2.81979100	-3.22023100	1.03745700
C	-1.74908200	-2.01432100	2.47088900
H	-0.83192600	-1.41346200	2.54598500
H	-2.58204100	-1.38600700	2.81360600
H	-1.66453300	-2.84493200	3.18236500

Pt	-0.69427700	-0.00386000	-0.03185700

12TS_Pt

E = -1075.853989 au

H = -1075.495575 au

G = -1075.567572 au

N	1.08981500	-1.31103300	-0.15953700
C	2.21859500	-0.53673500	-0.10559300
C	3.51767500	-1.07340600	-0.19326100
C	3.63781000	-2.47040900	-0.32878600
C	2.49955400	-3.24340000	-0.34945700
C	1.24398600	-2.62815100	-0.25981500
H	4.62537800	-2.92371200	-0.40536300
H	2.55078600	-4.32554700	-0.43484800
H	0.34369400	-3.23606400	-0.26553000
N	0.78121200	1.33486200	0.17812400
C	0.56742700	2.62866700	0.38027000
C	1.62879200	3.54131400	0.47746100
C	2.92519200	3.08972400	0.36196400
C	3.17094000	1.71632900	0.15725500
C	2.05259900	0.86794200	0.07296000
H	-0.47561400	2.92860400	0.46779900
H	1.41068500	4.59299000	0.64361000
H	3.76454800	3.78059100	0.43200900
C	4.47935800	1.14890500	0.04096500
C	4.64391500	-0.19100100	-0.12805100
H	5.34220000	1.81099400	0.09534400
H	5.64102900	-0.62112600	-0.21051600
C	-2.99781600	-1.44239800	-1.02021100
C	-1.98286400	-1.90561800	-0.17713800
H	-1.30448200	-2.55523700	-0.74281500
H	-2.88628700	-1.48272600	-2.10024000
H	-4.00788800	-1.25341200	-0.66219600
C	-2.31314800	-2.39206500	1.22989800
O	-2.05766000	1.28961000	0.23707600
C	-3.03749600	1.48244300	-0.58753700
C	-3.76182900	2.78595200	-0.38731900
O	-3.37013500	0.69389000	-1.47796800
H	-3.11801300	3.61172700	-0.71655700
H	-3.98172300	2.94291700	0.67409500
H	-4.68338400	2.80347500	-0.97372100
H	-1.37252800	-2.64584100	1.74237600
H	-2.86994900	-3.33986700	1.14524900
C	-3.10063800	-1.41248600	2.08725800
H	-2.53133900	-0.49370100	2.27747100
H	-4.05108800	-1.12051700	1.61949800
H	-3.34760400	-1.86445800	3.05474900
Pt	-0.65481500	-0.15945600	-0.04446900

11_Pt

E = -157.0801748 au

H = -156.965795 au

G = -156.998936 au

N	0.52645800	1.30928600	0.00032600
C	1.74770700	0.70786900	0.00026400
C	2.95315000	1.42348300	0.00021400
C	2.85528400	2.83087300	0.00034500
C	1.61108000	3.42812400	0.00048100
C	0.45273700	2.63558500	0.00043400
H	3.76062700	3.43667400	0.00034200
H	1.50780700	4.50984900	0.00060200
H	-0.54761100	3.06644300	0.00048600
N	0.52581500	-1.30967700	0.00032200
C	0.45163300	-2.63595000	0.00020900
C	1.60968700	-3.42893300	-0.00000800
C	2.85412700	-2.83217200	-0.00011900
C	2.95254800	-1.42482300	0.00000100
C	1.74736500	-0.70876600	0.00021100
H	-0.54887700	-3.06642900	0.00028200
H	1.50604000	-4.51062200	-0.00010500
H	3.75924500	-3.43831200	-0.00030100
C	4.17931300	-0.68266900	-0.00010200
C	4.17960500	0.68084300	0.00002000
H	5.11885800	-1.23317700	-0.00028400
H	5.11937400	1.23096900	-0.00005300
O	-2.81012900	-1.07987700	-0.00075100
C	-3.49355500	0.00421800	-0.00131600
C	-4.97085100	0.00055400	-0.00006300
H	-5.33547000	-0.51769700	0.89471100
H	-5.35760400	1.02243800	-0.02067000
H	-5.33754300	-0.55646300	-0.87012700
O	-2.80688600	1.08496200	-0.00115000
Pt	-1.03658500	0.00037100	0.00003000

15_Pt

E = -1035.384682 au

H = -1035.076891 au

G = -1035.144468 au

N	-1.06667900	-1.29405000	-0.08552400
C	-2.19176700	-0.51840800	-0.00272200
C	-3.48412300	-1.07622900	0.03448100
C	-3.59138200	-2.48059500	-0.00516600
C	-2.44857800	-3.24607800	-0.07039300
C	-1.19759500	-2.61833100	-0.10894400
H	-4.57577300	-2.94624200	0.02246800
H	-2.49445400	-4.33148500	-0.09403600
H	-0.27906100	-3.19788700	-0.15548700
N	-0.76029200	1.38403700	0.03949800
C	-0.56657500	2.69281100	0.09575900
C	-1.63170000	3.60383200	0.17754900
C	-2.92405300	3.12735900	0.19982800
C	-3.15724400	1.73766400	0.14026000
C	-2.02845800	0.90079500	0.05780100
H	0.46891600	3.02902900	0.07323400
H	-1.42308900	4.66959800	0.22181900
H	-3.76990000	3.81110000	0.26314100

C	-4.46131400	1.14789900	0.16348500
C	-4.61655000	-0.20267600	0.11490200
H	-5.32917600	1.80308800	0.22385100
H	-5.61035000	-0.64748200	0.13860900
C	3.51600700	-1.01900800	1.25492700
C	3.02821300	-2.00087900	0.24272600
H	3.67820000	-2.84819800	0.01260000
H	2.70104600	-0.60039400	1.85802200
H	4.27900400	-1.42853600	1.92035900
C	1.86368600	-1.82844200	-0.39368700
H	1.57422600	-2.56037100	-1.15846800
O	2.32768300	1.04271800	-0.24116400
C	3.55669400	1.00321700	-0.05938200
C	4.43564800	2.05626500	-0.63956600
O	4.21134700	0.10246500	0.61931500
H	5.25563800	2.29945100	0.04220500
H	3.85323200	2.94726000	-0.88527100
H	4.87898800	1.66642000	-1.56535100
Pt	0.67517500	-0.24528100	-0.13887000

1_Ni

E = -781.836664 au

H = -781.613408 au

G = -781.666151 au

N	0.60082400	-1.43412900	0.00006900
C	1.02353500	-0.14401800	-0.00002500
C	2.37874500	0.22749300	-0.00005700
C	3.32526000	-0.81889400	0.00000100
C	2.89213600	-2.12715700	0.00009100
C	1.51391500	-2.39650600	0.00012500
H	4.38911800	-0.58400700	-0.00002200
H	3.59705100	-2.95428400	0.00014800
H	1.14920800	-3.42289900	0.00020800
N	-1.28778500	0.42328100	0.00002000
C	-2.26575500	1.32462700	0.00015300
C	-2.00589200	2.70236500	0.00016000
C	-0.70323900	3.15127500	0.00003700
C	0.35317900	2.21768000	-0.00005000
C	0.00618100	0.85573300	-0.00003700
H	-3.28427000	0.94650600	0.00025500
H	-2.84280500	3.39553200	0.00024200
H	-0.48078700	4.21772400	0.00000800
C	1.74118000	2.57398900	-0.00011000
C	2.71295500	1.62036700	-0.00011600
H	2.00457400	3.63067100	-0.00014800
H	3.76440200	1.90402900	-0.00016000
C	-3.24069400	-1.61112200	-0.00022800
H	-3.73228900	-1.23390100	-0.90527100
H	-3.26379800	-2.72245600	-0.00082900
H	-3.73188000	-1.23474000	0.90539500
Ni	-1.39817300	-1.44004400	-0.00000400

2_Ni

E = -1127.460713 au

H = -1127.102041 au

G = -1127.174917 au

N	-0.31009100	1.30838600	-0.58596300
C	-1.49756800	0.85371300	-0.11051200
C	-2.51213500	1.70520000	0.37529700
C	-2.26844000	3.09114200	0.34093500
C	-1.07085400	3.55039500	-0.15834900
C	-0.12220200	2.62092400	-0.60739000
H	-3.02744300	3.78254900	0.70562700
H	-0.84534000	4.61249200	-0.20823700
H	0.82994400	2.98298700	-0.99405700
N	-0.71245100	-1.33460600	-0.63639400
C	-0.89365200	-2.64888100	-0.64552900
C	-2.05757300	-3.26802500	-0.16862800
C	-3.07232800	-2.48993400	0.33734400
C	-2.91483600	-1.09107100	0.36845300
C	-1.70641000	-0.55989400	-0.12482700
H	-0.08757200	-3.25480500	-1.05099900
H	-2.13817600	-4.35100000	-0.21019600
H	-3.99246500	-2.93735700	0.71197900
C	-3.92097600	-0.20555600	0.87096200
C	-3.72940800	1.13976600	0.87111600
C	1.74709000	-1.87342900	-1.79035900
H	1.03280600	-2.30472800	-2.50410700
H	-4.84776500	-0.63478800	1.24939800
H	-4.49883800	1.81215500	1.24803200
H	1.90428000	-2.53810800	-0.92861500
H	2.70164200	-1.71757500	-2.30510900
C	2.93831400	1.26013000	0.42297100
C	2.83460100	0.45514600	-0.83657900
H	3.49201300	-0.41733400	-0.83754700
H	3.76880000	1.97192100	0.32879100
H	2.02377000	1.82010800	0.65057200
C	2.29281400	0.88261100	-2.02943900
H	2.54721500	0.37931900	-2.96121600
H	1.86536600	1.87734900	-2.14815700
O	1.25890900	-0.48919400	1.51260500
C	2.35610000	-0.38131200	2.02132500
C	2.84340200	-1.12118800	3.22150300
O	3.29902600	0.45340200	1.54300800
H	3.74398000	-1.69417400	2.97119300
H	2.06422600	-1.79337700	3.58681500
H	3.12545300	-0.41358000	4.00974800
Ni	0.91274200	-0.29395000	-1.11971800

1TS_Ni

E = -1127.382895 au

H = -1127.027064 au

G = -1127.096167 au

N	0.16551700	0.93158000	-0.87504500
C	-1.12654500	0.72256300	-0.51684900
C	-2.08990200	1.74938200	-0.47235000

C	-1.67158500	3.04535200	-0.83343000
C	-0.37211000	3.24491000	-1.23594400
C	0.51276000	2.15708300	-1.23686100
H	-2.38326100	3.86960700	-0.80540100
H	-0.01405500	4.22489400	-1.53915500
H	1.54514900	2.31465400	-1.55002800
N	-0.53803600	-1.57278200	-0.28555100
C	-0.89815800	-2.84303000	-0.14471900
C	-2.21880200	-3.23848900	0.10772400
C	-3.19511200	-2.27630800	0.24111300
C	-2.85578900	-0.92086500	0.06543300
C	-1.50903200	-0.62243500	-0.22621900
H	-0.11306700	-3.59209900	-0.22351100
H	-2.44639900	-4.29641500	0.20887600
H	-4.22570500	-2.54986300	0.46505400
C	-3.80614200	0.14677100	0.14778700
C	-3.43611800	1.43106400	-0.10416200
C	2.03232100	-2.41469300	0.32670300
H	2.09621300	-3.13978900	-0.49421400
H	-4.83715200	-0.09483900	0.40257300
H	-4.16526800	2.23836200	-0.05133700
H	1.31195400	-2.69589700	1.09936500
H	3.00503600	-2.24609800	0.79434900
C	3.11182500	0.57803900	0.05412500
C	3.20443400	-0.41760800	-0.96235800
H	3.92025300	-1.21870100	-0.78553200
H	3.82494700	0.52845100	0.87171800
H	2.65209500	1.55372000	-0.07995600
C	2.37935100	-0.55594100	-2.08747200
H	2.54267000	-1.41749100	-2.73371200
H	1.83585400	0.26971600	-2.54104800
O	1.31738600	2.26503300	1.52079900
C	1.16720400	1.15339200	2.00937700
C	0.30342900	0.92046200	3.22451700
O	1.71177200	0.04916500	1.53754600
H	-0.57419600	0.32178400	2.94372300
H	-0.02621400	1.87789100	3.63682100
H	0.84771500	0.34991600	3.98523700
Ni	1.29948700	-0.76717400	-0.36017500

2TS_Ni

E = -1127.408373 au

H = -1127.052245 au

G = -1127.121008 au

N	0.03533400	1.09413900	-0.34725400
C	-1.29882700	0.97856900	-0.13232200
C	-2.17232500	2.08598200	-0.10501500
C	-1.60315700	3.36209400	-0.28117600
C	-0.24125000	3.47541400	-0.44685000
C	0.54554900	2.31339500	-0.47084500
H	-2.24226300	4.24446700	-0.26917400
H	0.23664400	4.44523400	-0.56028800
H	1.62855200	2.38058100	-0.56581300
N	-0.92801700	-1.36481400	0.14437300

C	-1.38992300	-2.58875100	0.36691700
C	-2.74827100	-2.86291000	0.57718400
C	-3.65285600	-1.82568800	0.55942400
C	-3.19623500	-0.51494400	0.32476100
C	-1.81414100	-0.33368900	0.10846800
H	-0.66200200	-3.39686000	0.38993500
H	-3.06212600	-3.88759200	0.75816000
H	-4.71425700	-2.00441100	0.72848400
C	-4.06421500	0.62325200	0.31031600
C	-3.57109600	1.87442900	0.11106400
C	1.64547200	-2.52397900	0.24130800
H	1.33057700	-3.27377000	-0.49540000
H	-5.12897600	0.46497000	0.47599200
H	-4.23222900	2.73995000	0.11716400
H	1.21540200	-2.68034200	1.23483800
H	2.73415600	-2.44844200	0.30933300
C	2.84798900	0.16819700	-1.76047800
C	2.15933400	-1.03458400	-1.95361300
H	2.73816800	-1.95586000	-1.91325900
H	3.93115800	0.18283200	-1.71201900
H	2.36767300	1.11679000	-1.98301100
C	0.77105800	-1.11409000	-2.20597700
H	0.33867300	-2.08100700	-2.46572500
H	0.22680100	-0.24311500	-2.57589500
O	1.80646200	-0.23440000	1.41573400
C	2.81213500	0.54149000	1.31587800
C	3.48019200	0.94481400	2.60315000
O	3.28999200	0.97498800	0.23689300
H	3.93190700	1.93656800	2.51151000
H	4.28542800	0.22932600	2.81366000
H	2.77208100	0.91302600	3.43610900
Ni	0.95447100	-0.79022600	-0.25030800

3_Ni

E = -1127.416686 au

H = -1127.059285 au

G = -1127.129283 au

N	0.04440100	1.08582700	-0.60720700
C	-1.25676300	0.86470900	-0.29398600
C	-2.22197500	1.89219100	-0.27166100
C	-1.78373900	3.19793000	-0.56957600
C	-0.45478700	3.41737000	-0.84982900
C	0.43247700	2.32900300	-0.85400300
H	-2.49842900	4.02024500	-0.56226900
H	-0.07560800	4.41372600	-1.06119400
H	1.49394700	2.49111900	-1.03113700
N	-0.66967600	-1.42543700	0.05514800
C	-1.00749300	-2.67040000	0.36148900
C	-2.31878500	-3.04564900	0.68385300
C	-3.30610500	-2.08655000	0.69319000
C	-2.98182400	-0.75523000	0.36962500
C	-1.63782900	-0.47194900	0.04475000
H	-0.21364600	-3.41460100	0.36341700
H	-2.53226200	-4.08326700	0.92694500

H	-4.33378400	-2.34338600	0.94821700
C	-3.94448300	0.30398300	0.36432600
C	-3.57816200	1.57729400	0.05935100
C	2.04516900	-2.29735000	0.29097000
H	1.80743100	-3.12208600	-0.39046800
H	-4.97709100	0.06748500	0.61728500
H	-4.31155400	2.38246500	0.06596800
H	1.60249200	-2.40261300	1.28294300
H	3.11929100	-2.10596100	0.35685400
C	2.81683100	-0.00682300	-1.40860100
C	2.26220400	-1.11757200	-2.07269100
H	2.79802400	-2.06555000	-2.05555000
H	3.78966400	-0.07787800	-0.92785900
H	2.50254300	1.00260700	-1.65482800
C	0.90973700	-1.11051100	-2.41067300
H	0.41320400	-2.04274400	-2.67982600
H	0.40061100	-0.19211600	-2.69881800
O	2.83666000	1.58406400	0.83995100
C	2.23359400	0.92367200	1.68008200
C	2.32830900	1.22514900	3.15633300
O	1.46666400	-0.10311800	1.42412700
H	1.36242900	1.09217500	3.65412300
H	2.70263400	2.24150200	3.30545200
H	3.03392700	0.52278100	3.61759100
Ni	1.16600900	-0.67392100	-0.36295600

3TS_Ni

E = -1127.409232 au

H = -1127.052799 au

G = -1127.123990 au

N	-0.05597100	1.15506100	-0.23541700
C	1.29409300	1.08261900	-0.11844800
C	2.11977700	2.20765900	0.04535200
C	1.48077100	3.46420500	0.09153900
C	0.11056800	3.52952700	-0.03195000
C	-0.63127300	2.34859800	-0.19795500
H	2.07369700	4.36913600	0.21947100
H	-0.41294700	4.48150300	-0.00379700
H	-1.71153100	2.37884000	-0.30426200
N	0.98670500	-1.25142100	-0.35205300
C	1.48462200	-2.48061000	-0.42402100
C	2.85741500	-2.75075500	-0.34093000
C	3.74416500	-1.70900000	-0.17192300
C	3.25230500	-0.39210200	-0.08899500
C	1.85908400	-0.22008200	-0.18711400
H	0.77444400	-3.29545900	-0.54260900
H	3.20009700	-3.77985800	-0.40907000
H	4.81576800	-1.89249600	-0.10232100
C	4.07851500	0.76537900	0.08487500
C	3.53515000	2.01217600	0.15013400
C	-1.57102500	-2.25538200	-1.31512800
H	-1.02736900	-3.19977400	-1.28530700
H	5.15595900	0.62712000	0.16181200
H	4.17229400	2.88570900	0.28034800

H	-1.26330500	-1.66818300	-2.19871500
H	-2.65031900	-2.40139800	-1.35045300
C	-1.75351100	-2.08917500	0.81477700
C	-0.79730400	-1.73672900	1.87589200
H	0.06178700	-2.39815000	2.00590200
H	-1.83606200	-3.16533400	0.66878400
H	-2.73071000	-1.61509600	0.91118000
C	-0.98716700	-0.71897400	2.73332600
H	-0.30896600	-0.56827400	3.57167800
H	-1.83147600	-0.03899900	2.61843000
O	-3.26342900	0.66306600	1.14154900
C	-3.38779100	0.62279300	-0.07687900
C	-4.59928400	1.16005600	-0.79370300
O	-2.49319600	0.13304600	-0.90211500
H	-4.30269900	1.89926500	-1.54800400
H	-5.28646100	1.61316300	-0.07465800
H	-5.10933800	0.35090900	-1.32979800
Ni	-0.88498800	-0.61850800	-0.40660300

4_Ni

E = -1127.494496 au

H = -1127.134848 au

G = -1127.207055 au

N	-0.77270200	-1.37255500	0.15444100
C	-1.89492000	-0.60857200	0.04181400
C	-3.19997800	-1.11455400	0.17443500
C	-3.32725800	-2.49085900	0.44530600
C	-2.19133400	-3.26341300	0.55798600
C	-0.93172800	-2.66809200	0.40511000
H	-4.31634300	-2.93260300	0.56208800
H	-2.25074800	-4.32865200	0.76468800
H	-0.03363000	-3.27740800	0.48903600
N	-0.40360700	1.17060700	-0.33847500
C	-0.14735000	2.44096000	-0.61478200
C	-1.17561300	3.38132200	-0.79205100
C	-2.49063300	2.98570500	-0.67258600
C	-2.78641000	1.63761100	-0.38387700
C	-1.69309300	0.77046100	-0.23203100
H	0.90403500	2.71063700	-0.70068100
H	-0.91780100	4.41239700	-1.01939300
H	-3.30104100	3.70245300	-0.80080800
C	-4.10875700	1.10527100	-0.24082000
C	-4.30623600	-0.21492500	0.02935700
H	-4.95668800	1.77949200	-0.35168500
H	-5.31409400	-0.61273400	0.13869900
C	2.20378300	-1.77572300	0.59167100
C	2.08306000	-1.90115900	-0.76884900
H	1.27357400	-2.51996000	-1.16847900
H	1.58924200	-2.33831300	1.29340500
H	3.07086200	-1.28776300	1.03311400
C	3.06556000	-1.42795500	-1.79678100
O	2.24526900	0.90821000	-0.04260100
C	2.37202200	1.34385900	1.19085500
C	3.46471600	2.35152700	1.39029300

O	1.64364900	0.93093100	2.09179200
H	3.41542000	3.13819400	0.62791300
H	4.44226200	1.86334500	1.28019300
H	3.39595600	2.78780200	2.39010000
H	2.60902900	-0.60489400	-2.37130400
H	3.16223300	-2.24990700	-2.52438400
C	4.43672000	-1.02168600	-1.28557300
H	4.38403500	-0.12708700	-0.65563100
H	4.90524600	-1.83151200	-0.71051100
H	5.09733100	-0.79262400	-2.12920400
Ni	0.84745100	-0.28460800	0.01823900

5_Ni

E = -1127.456586 au

H = -1127.098342 au

G = -1127.172803 au

N	0.45201800	1.29405500	-0.19545400
C	1.73299500	0.91675800	0.02745800
C	2.75220300	1.81151100	0.39862300
C	2.38806000	3.16675400	0.53685400
C	1.08345300	3.54634200	0.30347200
C	0.13845000	2.57428500	-0.06502400
H	3.14004200	3.90134800	0.82321300
H	0.77508000	4.58458600	0.39565400
H	-0.89817100	2.84018400	-0.26800800
N	0.96967800	-1.27023000	-0.50663100
C	1.21291300	-2.56588600	-0.67853500
C	2.48372300	-3.13013600	-0.49509000
C	3.53934600	-2.32750600	-0.12335600
C	3.32032500	-0.94856100	0.06459200
C	2.01361400	-0.47071100	-0.14111000
H	0.37141900	-3.18630100	-0.97628800
H	2.61409200	-4.19761900	-0.65275600
H	4.53543600	-2.74392900	0.02314800
C	4.34519300	-0.02183800	0.44643500
C	4.07433200	1.30265300	0.60722700
C	-1.66039800	-1.84093200	-1.20439500
H	-2.72229900	-1.61209600	-1.36198600
H	5.35316100	-0.40339400	0.60370200
H	4.86202200	1.99736400	0.89558300
H	-1.58526700	-2.60817300	-0.42101700
H	-1.23852700	-2.21055500	-2.15027700
C	-2.78214200	0.03519100	1.69005400
C	-3.16779600	-1.30469400	2.20647200
H	-4.20541300	-1.42168100	2.52358800
C	-2.29494400	-2.30250100	2.32878000
H	-2.57703200	-3.26174100	2.75722000
H	-1.25505800	-2.18989800	2.01378400
O	-2.20690700	0.80206000	-0.97993100
C	-3.35941400	0.83162600	-0.53546200
C	-4.49672400	1.30824800	-1.36869100
O	-3.72581900	0.44865900	0.66482000
H	-5.26808200	1.78927500	-0.76136600
H	-4.94924000	0.43398400	-1.85722400

H	-4.13298500	1.97896500	-2.15118700
H	-2.86381100	0.81344200	2.46008700
H	-1.75855000	0.03190600	1.28815800
Ni	-0.66521500	-0.29256500	-0.70494200

4TS_Ni

E = -1127.396903 au

H = -1127.042437 au

G = -1127.116628 au

N	0.31176200	1.24443700	-0.26237400
C	1.59415400	0.93601300	0.04185800
C	2.54489500	1.88767100	0.45167200
C	2.10279800	3.22387900	0.54905700
C	0.79657000	3.53163600	0.23426200
C	-0.07484100	2.50717400	-0.17494300
H	2.79864500	4.00074900	0.86458200
H	0.43040400	4.55353300	0.29066500
H	-1.10839100	2.71436300	-0.44851200
N	0.97934300	-1.29492700	-0.50569200
C	1.31435300	-2.56442400	-0.71409600
C	2.61495800	-3.04934100	-0.51100200
C	3.60026900	-2.19126200	-0.07409500
C	3.28786600	-0.83375100	0.13851900
C	1.96050800	-0.43509100	-0.10404500
H	0.52384400	-3.22774900	-1.05819300
H	2.82427900	-4.09873300	-0.70192300
H	4.61582800	-2.54677700	0.09730000
C	4.23883300	0.14860600	0.56843500
C	3.88262700	1.45373300	0.72345900
C	-1.67916000	-1.99982000	-1.20116700
H	-2.75962000	-1.82470700	-1.16000800
H	5.26128000	-0.17166400	0.76418800
H	4.61548300	2.19160500	1.04732600
H	-1.41012800	-2.83000000	-0.53199300
H	-1.38491200	-2.23532000	-2.23518900
C	-3.68652000	-1.51566600	2.61666900
C	-2.51304100	-1.81727100	2.00243700
H	-2.30426300	-2.83683100	1.68028800
H	-4.42555400	-2.28153500	2.84454700
H	-3.92582100	-0.48727200	2.88549700
C	-1.53163600	-0.82671800	1.81611900
H	-0.53388800	-1.11287600	1.48899500
H	-1.65214200	0.16496700	2.23975400
O	-2.18905800	0.59376500	-1.33256700
C	-3.12591500	0.92367600	-0.52476000
C	-4.30354500	1.62250400	-1.15396600
O	-3.11583900	0.69664100	0.70008900
H	-4.82966400	2.23460600	-0.41655900
H	-5.00023100	0.86184600	-1.52937600
H	-3.98863200	2.22783300	-2.00971400
Ni	-0.73157500	-0.40268400	-0.77792400

6_Ni

E = -1127.411039 au

H = -1127.054450 au

G = -1127.127737 au

N	0.23698300	1.19708000	-0.08701500
C	1.56640000	0.95803900	0.03190700
C	2.52026900	1.97127800	0.23941200
C	2.03950400	3.29411200	0.32675500
C	0.68892900	3.53025900	0.21089000
C	-0.18741000	2.45044600	0.00433100
H	2.74126500	4.11208600	0.48673200
H	0.28275000	4.53598900	0.28060300
H	-1.26084300	2.60677700	-0.05939600
N	1.01264000	-1.33978900	-0.28414500
C	1.38723300	-2.61166700	-0.39284000
C	2.72205900	-3.02382600	-0.29453400
C	3.70542300	-2.08409000	-0.07901800
C	3.34992700	-0.72669600	0.03692200
C	1.98220000	-0.40252300	-0.07147400
H	0.60539700	-3.34463800	-0.57227200
H	2.95826800	-4.07995400	-0.39369600
H	4.75196600	-2.37682200	-0.00133000
C	4.30142900	0.32137200	0.25054000
C	3.90303300	1.61855000	0.34745300
C	-1.55057800	-2.21289000	-1.05876200
H	-2.63003300	-2.07956800	-1.14172400
H	5.35460100	0.05610800	0.33011200
H	4.63302200	2.41108600	0.50649100
H	-1.30161400	-3.05229800	-0.40263700
H	-1.08175800	-2.31388000	-2.04877600
C	-3.76832000	-1.28114600	2.00406400
C	-2.56526400	-1.81014200	1.69288100
H	-2.43854800	-2.89362200	1.68051100
H	-4.61142100	-1.91660000	2.26879200
H	-3.91966400	-0.20127600	2.01711900
C	-1.41428200	-0.97979900	1.47984200
H	-0.44860100	-1.40102400	1.77029800
H	-1.56583000	0.09073700	1.65414100
O	-2.29858600	0.23416000	-1.09519800
C	-3.13375400	1.03399800	-0.48608400
C	-4.30901100	1.41935400	-1.34330500
O	-3.01187600	1.42809700	0.67247800
H	-4.72505500	2.37143000	-1.00167800
H	-5.08506500	0.64958000	-1.23374900
H	-4.04121700	1.46839600	-2.40312200
Ni	-0.78242900	-0.56176300	-0.46965800

6TS_Ni

E = -1127.41017 au

H = -1127.054926 au

G = -1127.126241 au

N	0.36843600	1.23139200	-0.23010500
C	1.65963700	0.89115000	-0.00059700
C	2.68403800	1.82962200	0.21302400

C	2.31649800	3.19092100	0.17771600
C	1.00609000	3.53094000	-0.07360400
C	0.05517400	2.51707000	-0.27623200
H	3.07188200	3.95890900	0.34140400
H	0.69105100	4.57021600	-0.11463300
H	-0.98254000	2.76275200	-0.48331800
N	0.91299700	-1.35319900	-0.23256200
C	1.17050900	-2.65748700	-0.25693700
C	2.45173200	-3.18576100	-0.05661700
C	3.50563300	-2.33029600	0.17993600
C	3.27405600	-0.94195800	0.21054600
C	1.95346000	-0.50212200	-0.00396200
H	0.33250200	-3.32432500	-0.44505000
H	2.59245800	-4.26272900	-0.09173700
H	4.51232700	-2.71495200	0.33988400
C	4.30096500	0.02995100	0.43972300
C	4.01785800	1.36121100	0.44109900
C	-1.57856900	-1.83510100	-1.54095700
H	-2.62725400	-1.59077000	-1.71094200
H	5.31778200	-0.32116900	0.60882000
H	4.80488500	2.09479800	0.61057100
H	-1.44029800	-2.87084000	-1.22169800
H	-0.95361700	-1.59942500	-2.41679900
C	-4.14360900	-1.31117100	1.48470100
C	-3.13940500	-1.98162500	0.89132000
H	-3.34603700	-2.94130700	0.41371500
H	-5.15224400	-1.71941400	1.50800000
H	-3.97530300	-0.35390700	1.97949800
C	-1.76238000	-1.54225700	0.96340500
H	-1.03080400	-2.34211400	1.08904400
H	-1.59085600	-0.65432600	1.59017900
O	-2.27025000	0.57454500	-0.88993000
C	-2.87801600	1.28855800	0.02767300
C	-4.10611800	1.98490800	-0.49362400
O	-2.51640500	1.37215500	1.19715300
H	-4.94854100	1.28048500	-0.44610000
H	-3.99287700	2.28425600	-1.54059300
H	-4.34543800	2.84744900	0.13497400
Ni	-0.79782800	-0.42299500	-0.47585800

7_Ni

E = -1127.442416 au

H = -1127.084346 au

G = -1127.158278 au

N	0.17113100	1.04622300	-0.13674000
C	1.51951500	0.92995700	-0.10954200
C	2.39576900	2.02797600	-0.17583100
C	1.80701800	3.30470100	-0.28121000
C	0.43355200	3.41704300	-0.31474500
C	-0.35377300	2.25677400	-0.23816400
H	2.44086900	4.18916000	-0.33668600
H	-0.04866100	4.38744700	-0.40148800
H	-1.44165700	2.31426500	-0.25798600
N	1.11627500	-1.40834000	0.03397300

C	1.57231900	-2.65392000	0.11413400
C	2.94055300	-2.95990300	0.15151300
C	3.86737900	-1.94299500	0.10266300
C	3.42054500	-0.61011800	0.01663700
C	2.03100100	-0.39687700	-0.01454900
H	0.83150100	-3.44775900	0.14959600
H	3.24617800	-4.00090400	0.21497400
H	4.93557000	-2.15581700	0.12721900
C	4.29722900	0.52194500	-0.04489600
C	3.80712600	1.78849300	-0.13790000
C	-1.43192500	-2.51775500	-0.01231000
H	-2.52904300	-2.48426400	-0.07896100
H	5.37166800	0.34554100	-0.01864000
H	4.48271600	2.64139900	-0.18661400
H	-1.15379900	-3.03026100	0.92038900
H	-1.05423600	-3.07436700	-0.88134800
C	-3.35180700	0.00962900	1.08088500
C	-2.46956400	0.06861800	2.27591300
H	-1.85829300	-0.81431400	2.47713100
H	-3.95797700	-0.90669700	1.06504800
H	-4.01064600	0.88573500	1.03400600
C	-2.44523600	1.11797400	3.09677100
H	-1.82245000	1.13265900	3.98859100
H	-3.06500200	1.99823800	2.91969100
O	-2.26904600	-0.11108000	-2.30402700
C	-3.05015900	-0.01812300	-1.40068000
C	-4.53383300	0.07799700	-1.51153400
O	-2.51180500	0.01030000	-0.11796900
H	-4.91475900	1.00529400	-1.06610600
H	-5.02184100	-0.76048000	-0.99791700
H	-4.80062400	0.05303600	-2.57008600
Ni	-0.68317100	-0.76661900	-0.05672800

8_TS

E = -1127.406906 au

H = -1127.052047 au

G = -1127.124135 au

N	0.09564100	1.12077000	0.08958100
C	1.43995800	0.97079900	0.05631200
C	2.34067700	2.04806000	0.14781700
C	1.78141300	3.33601900	0.27330100
C	0.41082400	3.48249200	0.29869100
C	-0.40269000	2.34159400	0.20246600
H	2.43637200	4.20387000	0.34365200
H	-0.04842000	4.46367200	0.38884300
H	-1.49063600	2.41950000	0.21283000
N	0.99058100	-1.35382600	-0.19812500
C	1.42388800	-2.60160800	-0.34471100
C	2.78592700	-2.93391700	-0.38204400
C	3.73110300	-1.93833800	-0.27383300
C	3.30937600	-0.60246000	-0.12649900
C	1.92313900	-0.36376500	-0.08960100
H	0.66655300	-3.37511800	-0.44647600
H	3.07263900	-3.97521800	-0.50319700

H	4.79525600	-2.16977600	-0.30527800
C	4.20988300	0.50750000	-0.02257300
C	3.74662500	1.78085600	0.10587300
C	-1.58992800	-2.37054800	-0.54249000
H	-2.68104200	-2.27785400	-0.56319000
H	5.28029600	0.30899400	-0.05490400
H	4.44007500	2.61770000	0.17658900
H	-1.29601600	-3.12641400	0.19884300
H	-1.21635300	-2.62891200	-1.54312600
C	-3.31879300	0.03486100	1.87339300
C	-2.58493400	-1.10141900	2.22211100
H	-3.06707300	-2.07770400	2.19033400
H	-4.38677300	-0.01752000	1.67142700
H	-2.90860500	1.02757400	2.05029100
C	-1.21888800	-1.01120600	2.29895600
H	-0.59543200	-1.88952400	2.45938200
H	-0.72945300	-0.04079200	2.39405400
O	-2.14871500	0.34335100	-2.18551500
C	-2.92420800	0.51446600	-1.25870100
C	-4.28531500	1.12600500	-1.37103500
O	-2.54868700	0.13743100	-0.04283800
H	-4.43607900	1.89423500	-0.60134100
H	-5.05096100	0.35392200	-1.21842300
H	-4.42196500	1.56350200	-2.36305700
Ni	-0.82339500	-0.67162000	-0.15375800

7TS_Ni

E = -1127.383637 au

H = -1127.028842 au

G = -1127.101934 au

N	0.15041400	1.02809400	-0.32921400
C	1.49202000	0.87651700	-0.25552400
C	2.40045400	1.94140500	-0.39509300
C	1.84954700	3.21889800	-0.62472500
C	0.48057000	3.36405200	-0.70824900
C	-0.34315200	2.23552900	-0.55593000
H	2.51017400	4.07725200	-0.74321800
H	0.02942300	4.33502900	-0.89735600
H	-1.42909600	2.30073900	-0.62117800
N	1.01624400	-1.43382900	0.05214300
C	1.43875400	-2.68446400	0.20602000
C	2.79750600	-3.02581200	0.28069000
C	3.75318500	-2.03890200	0.18799200
C	3.34479900	-0.70189000	0.01313000
C	1.96152300	-0.45435100	-0.04962500
H	0.67539000	-3.45557100	0.27020600
H	3.07285000	-4.06966200	0.40634600
H	4.81459500	-2.27914600	0.23981500
C	4.25453900	0.39837400	-0.11533000
C	3.80334900	1.66787000	-0.31098600
C	-1.58361000	-2.48235500	-0.00565300
H	-2.67790200	-2.46222700	-0.00225300
H	5.32298500	0.19386400	-0.06136800
H	4.50535000	2.49393500	-0.41618300
H	-1.22301300	-2.99577600	0.89843400

H	-1.25353800	-3.00450400	-0.91440100
C	-1.37109200	1.68358300	2.90849400
C	-2.39344400	1.07444100	2.26986800
H	-3.31572100	1.60883300	2.04327900
H	-1.43714900	2.71400000	3.25203700
H	-0.43953700	1.15332900	3.11412800
C	-2.30151800	-0.29909100	1.92793900
H	-3.18614000	-0.89109600	1.71324000
H	-1.41325500	-0.85787200	2.22554500
O	-3.13399100	-0.89952600	-2.13616100
C	-3.36160800	-0.22092100	-1.16043000
C	-4.70518700	0.37881300	-0.84330300
O	-2.42351900	0.11273700	-0.26207200
H	-4.62032300	1.46415500	-0.70565100
H	-5.09391600	-0.03925200	0.09652200
H	-5.41560800	0.16497200	-1.64544100
Ni	-0.79399700	-0.74666800	-0.13367200

8_Ni

E = -1127.426185 au

H = -1127.070215 au

G = -1127.140853 au

N	-0.06316300	1.12591200	0.08775200
C	1.27213500	0.94832000	-0.00373100
C	2.18649600	2.01587200	-0.06218600
C	1.64490700	3.31738100	-0.01635200
C	0.27969300	3.48617800	0.07800300
C	-0.55196400	2.35360000	0.12425200
H	2.31051100	4.17908200	-0.05602600
H	-0.16267400	4.47844100	0.11554500
H	-1.63731700	2.43667200	0.19438900
N	0.79813200	-1.39185700	0.02132300
C	1.20768800	-2.65420300	-0.01654500
C	2.56169500	-3.00376200	-0.11102700
C	3.51535000	-2.01194000	-0.17273100
C	3.11395700	-0.66250100	-0.13942800
C	1.73396500	-0.40105700	-0.04144500
H	0.44272000	-3.42508700	0.02570900
H	2.83540500	-4.05512200	-0.13668600
H	4.57384500	-2.25886000	-0.24689700
C	4.02814400	0.43930900	-0.20090900
C	3.58474100	1.72574400	-0.16415000
C	-1.88305600	-2.40959800	-0.11935800
H	-2.94814100	-2.24178300	0.05818600
H	5.09263400	0.22294100	-0.27899600
H	4.28875000	2.55525900	-0.21334500
H	-1.47416200	-3.12792700	0.59672600
H	-1.68104300	-2.69486400	-1.15815200
C	-2.46127500	0.97359700	2.96888600
C	-2.36709700	-0.25237700	2.42694300
H	-3.26735700	-0.85356500	2.28996700
H	-3.41090300	1.37875300	3.31177500
H	-1.57691200	1.59553600	3.11941800
C	-1.10334200	-0.82785200	2.01713100

H	-0.97347200	-1.89402800	2.21437200
H	-0.21995800	-0.24607900	2.30488300
O	-1.38610200	-0.30082700	-2.06811200
C	-2.46300600	0.17478200	-1.64260700
C	-3.50671000	0.76639900	-2.52430800
O	-2.67239800	0.13114200	-0.36520800
H	-4.00755500	1.60538800	-2.02993000
H	-4.27015000	0.00550200	-2.73153600
H	-3.06797300	1.08219700	-3.47486100
Ni	-1.00989200	-0.69252500	0.01413800

9TS_Ni

E = -1127.411035 au

H = -1127.054996 au

G = -1127.126631 au

N	0.30371000	1.17475800	0.29840600
C	1.60836100	0.81934200	0.23338700
C	2.66766600	1.72185300	0.42464700
C	2.31781200	3.05887700	0.70480400
C	0.98704800	3.41059400	0.77870800
C	-0.00096600	2.43489000	0.56658900
H	3.09968300	3.80172800	0.85957300
H	0.68745200	4.43264400	0.99530900
H	-1.06203200	2.67532900	0.61752700
N	0.78418000	-1.35848200	-0.20809900
C	0.99753700	-2.64188200	-0.47802300
C	2.28294300	-3.18798900	-0.59384100
C	3.38314800	-2.37506300	-0.42525500
C	3.19532400	-1.00877400	-0.14073700
C	1.86894000	-0.55056200	-0.04541700
H	0.12108600	-3.27077800	-0.61718200
H	2.39106100	-4.24594500	-0.81759300
H	4.39198900	-2.77716900	-0.51216000
C	4.26421400	-0.07373200	0.05120100
C	4.01172200	1.23628400	0.32412100
C	-2.00017700	-1.78681000	-0.91114400
H	-3.04246200	-1.47089100	-0.95512200
H	5.28852500	-0.43520400	-0.02644600
H	4.83094100	1.93919700	0.46856500
H	-1.91211300	-2.86070100	-0.73399700
H	-1.46565000	-1.50717200	-1.83607400
C	-3.99412700	-0.96703000	2.14123700
C	-3.21901500	-1.85947600	1.51131400
H	-3.64314000	-2.80931600	1.17970800
H	-5.04165300	-1.17152300	2.35224800
H	-3.60186000	-0.00432100	2.46810000
C	-1.79783800	-1.63461800	1.27458100
H	-1.16614000	-2.52276600	1.33731000
H	-1.40041600	-0.81728400	1.89881500
O	-2.37294400	0.73844700	-0.03715900
C	-2.45788800	1.30300500	-1.22225000
C	-3.61755200	2.23992300	-1.39060800
O	-1.64511800	1.05954700	-2.11100600
H	-3.83318400	2.78674100	-0.46611200

H	-4.51414800	1.65863300	-1.64167000
H	-3.41896600	2.93332400	-2.21250300
Ni	-0.89866500	-0.36662200	-0.09375100

10TS_Ni

E = -1127.442474 au

H = -1127.083981 au

G = -1127.153818 au

N	0.43300800	1.31084700	-0.57268800
C	1.58891600	0.76945700	-0.10328600
C	2.67179200	1.54151500	0.36564000
C	2.54662500	2.94163300	0.30411500
C	1.39524100	3.48753900	-0.21571500
C	0.36458000	2.63695500	-0.63661600
H	3.36190200	3.57424600	0.65339800
H	1.26455900	4.56312700	-0.30166600
H	-0.54815900	3.07080800	-1.03615100
N	0.65171300	-1.33288800	-0.66851800
C	0.74969400	-2.65199800	-0.73646800
C	1.86709900	-3.36884100	-0.28337100
C	2.92800600	-2.68269200	0.26077900
C	2.86688000	-1.27829800	0.33971800
C	1.69727400	-0.65270400	-0.13511000
H	-0.08973400	-3.18857600	-1.17574600
H	1.87738800	-4.45198300	-0.37248700
H	3.81291900	-3.20670400	0.62042300
C	3.93253700	-0.47409700	0.85590100
C	3.84151400	0.88203500	0.86180200
C	-1.96914100	-1.67566300	-1.65153000
H	-1.90295700	-2.27810800	-0.73657200
H	4.82602700	-0.97237900	1.22957400
H	4.66135100	1.49309100	1.23677200
H	-1.18254200	-1.90751800	-2.38203700
C	-2.63339700	1.63593100	0.58220300
C	-2.36481500	1.24135100	-0.85049400
H	-2.10694000	2.07590100	-1.50718800
H	-1.72404600	1.98687800	1.08780500
H	-3.37460700	2.44516900	0.60679700
C	-3.00357500	0.14950700	-1.45196700
O	-1.21923400	-0.38816700	1.61139900
C	-2.41119900	-0.36281800	1.83926000
C	-3.16960200	-1.36692400	2.64217100
O	-3.22791500	0.59119800	1.35247500
H	-2.47845100	-2.08790100	3.08417600
H	-3.88564300	-1.89175000	1.99627400
H	-3.75234900	-0.87237700	3.42712600
H	-2.91811200	-1.90316300	-2.13655800
H	-3.20725900	0.19624900	-2.51994200
H	-3.74383100	-0.39903800	-0.86977300
Ni	-0.93914100	-0.08383100	-0.99460600

9_Ni

E = -1127.462743 au

H = -1127.101974 au

G = -1127.173903 au

N	-0.71505400	1.12891600	0.11320800
C	-2.05179600	0.87959800	0.00335700
C	-3.02047500	1.89837400	-0.03675900
C	-2.56064700	3.22885400	0.02785000
C	-1.20860400	3.47294700	0.12658100
C	-0.31327500	2.39489900	0.17016500
H	-3.27614200	4.04982700	-0.00180800
H	-0.81881100	4.48618700	0.17682400
H	0.75604200	2.56999800	0.25913600
N	-1.45720700	-1.40978600	-0.04774300
C	-1.78522700	-2.69244000	-0.11684300
C	-3.11691500	-3.12784100	-0.21187700
C	-4.13102600	-2.19498700	-0.23938000
C	-3.81481800	-0.82198200	-0.17204000
C	-2.45215000	-0.48835800	-0.07381200
H	-0.96705800	-3.41233400	-0.09719600
H	-3.32906300	-4.19256600	-0.26364500
H	-5.17262000	-2.50581100	-0.31331700
C	-4.78550100	0.23096300	-0.20000900
C	-4.40319700	1.53600600	-0.13880700
C	1.90742900	-2.16275400	0.32628200
H	2.73866000	-2.39602100	-0.35065700
H	-5.83940600	-0.03331600	-0.27442000
H	-5.14636800	2.33162300	-0.16595500
H	1.08275400	-1.95141300	-0.41825700
C	2.76972900	0.66624200	-0.62750900
C	1.98626900	0.29064200	0.60190600
H	1.88549600	1.12850500	1.30592200
H	2.79917400	-0.14564100	-1.36522400
H	2.34739600	1.55592300	-1.11145100
C	2.33305500	-1.01596800	1.27512900
O	4.80043900	-1.07692600	-0.66643600
C	5.06228800	0.07372400	-0.39383000
C	6.42657300	0.62262000	-0.13076300
O	4.12225000	1.04077000	-0.30389100
H	7.14158000	-0.19643900	-0.02579100
H	6.42812900	1.24954400	0.76737800
H	6.73063800	1.25948600	-0.97061800
H	1.59913500	-3.06526000	0.86417500
H	1.80799800	-1.08602200	2.23835600
H	3.40385900	-1.13597800	1.49969600
Ni	0.30723700	-0.46422100	0.15762000

10_Ni

E = -1127.499284 au

H = -1127.137974 au

G = -1127.208046 au

N	0.65595700	-1.19701400	-0.40697900
C	1.84100400	-0.53823300	-0.25729300
C	3.09530800	-1.15484800	-0.41607000
C	3.10272600	-2.51286300	-0.78919800

C	1.90417300	-3.15979700	-0.99603800
C	0.70140200	-2.46845400	-0.79160800
H	4.05122300	-3.03145800	-0.92517200
H	1.86995700	-4.20064200	-1.30694500
H	-0.25172000	-2.96945900	-0.94426700
N	0.52506700	1.38276800	0.10389400
C	0.39864800	2.67333300	0.37166100
C	1.50924300	3.50664200	0.58927700
C	2.77938400	2.97621100	0.51566600
C	2.94308800	1.60494900	0.22870000
C	1.76925600	0.85391200	0.04257300
H	-0.61873100	3.05934100	0.41185400
H	1.35209500	4.56006200	0.80688800
H	3.65618800	3.60328400	0.67391500
C	4.20918000	0.94661800	0.10629600
C	4.28082800	-0.37574500	-0.20993000
H	5.11737300	1.52812400	0.25897400
H	5.24752600	-0.86577400	-0.31873300
C	-3.52446800	-1.00750700	0.32071800
C	-2.11487000	-1.50849600	0.12503900
H	-2.08050800	-2.11779600	-0.79482300
H	-4.26551000	-1.80861300	0.20816900
H	-3.65759500	-0.55471400	1.31347300
C	-1.74249900	-2.33795500	1.36090500
O	-2.21982300	1.27278300	-0.12506800
C	-3.31804900	1.10663300	-0.68250400
C	-4.01108900	2.20012200	-1.41264400
O	-3.97607400	-0.01895900	-0.64501300
H	-3.29444500	2.94786800	-1.75998200
H	-4.72241200	2.68426300	-0.73056400
H	-4.58725600	1.79496300	-2.24992600
H	-0.92715000	-3.03408500	1.12133300
H	-2.59613300	-2.98691700	1.63069000
C	-1.33950900	-1.51753400	2.58363400
H	-0.38511800	-0.99414500	2.42031900
H	-2.08798900	-0.75665900	2.84491600
H	-1.21318000	-2.15997700	3.46377300
Ni	-0.86461200	-0.06251600	-0.07059800

12TS_Ni

E = -1127.463500 au

H = -1127.104869 au

G = -1127.175833 au

N	0.83607100	-1.34869700	-0.07004300
C	1.96764100	-0.58852100	-0.07832400
C	3.26720800	-1.11680200	-0.18561200
C	3.38555800	-2.51827100	-0.25879700
C	2.24678100	-3.28987200	-0.19455100
C	0.99305200	-2.66899300	-0.10072400
H	4.36969900	-2.97689400	-0.34871000
H	2.29696600	-4.37512000	-0.22096000
H	0.09688700	-3.28299000	-0.04727800
N	0.50778000	1.23217500	0.23640600
C	0.28128500	2.52285200	0.44160100

C	1.32287600	3.46428500	0.47905600
C	2.62462100	3.04815800	0.30378600
C	2.89257800	1.67895400	0.10247600
C	1.78686000	0.81288700	0.07698900
H	-0.75801200	2.80687600	0.59230100
H	1.08516200	4.51083300	0.65098000
H	3.44760700	3.76154300	0.32969500
C	4.20367300	1.12551000	-0.05622800
C	4.38258400	-0.21726200	-0.19212000
H	5.05902100	1.79953900	-0.05257300
H	5.38294200	-0.63482200	-0.29738200
C	-3.00443900	-1.32552000	-1.22963300
C	-2.06302100	-1.78340600	-0.31408200
H	-1.31600200	-2.39778200	-0.82233900
H	-2.81704200	-1.39629400	-2.29725600
H	-4.03593100	-1.11726100	-0.95462400
C	-2.43395200	-2.21531100	1.10306600
O	-2.10918500	1.00988200	0.35598000
C	-2.93052700	1.39901700	-0.55926600
C	-3.68485800	2.66516500	-0.25601500
O	-3.10581200	0.80552300	-1.63398900
H	-4.71056100	2.58790200	-0.62893500
H	-3.20913000	3.49556200	-0.79477400
H	-3.68115100	2.89038300	0.81451400
H	-1.60222000	-1.99681100	1.79357600
H	-2.52282300	-3.31473500	1.10602800
C	-3.71124800	-1.60497500	1.65589800
H	-3.66610500	-0.50809500	1.65349900
H	-4.59623500	-1.91605200	1.08525900
H	-3.86947400	-1.92840100	2.69084700
Ni	-0.77859300	-0.21579700	0.01366200

11_Ni

E = -970.410127 au

H = -970.168182 au

G = -970.225305 au

N	-0.07778600	-1.29062300	0.00038900
C	-1.30386900	-0.70761600	0.00018000
C	-2.50688200	-1.42395000	-0.00000400
C	-2.39576900	-2.83138500	0.00014100
C	-1.14579900	-3.41753500	0.00042400
C	0.00746900	-2.61394300	0.00050900
H	-3.29503300	-3.44649100	0.00003700
H	-1.03529000	-4.49862800	0.00055600
H	1.01044800	-3.03814400	0.00067000
N	-0.07536500	1.28996300	0.00038000
C	0.01228300	2.61311500	0.00028600
C	-1.13955800	3.41877400	-0.00005800
C	-2.39060400	2.83491600	-0.00031400
C	-2.50429600	1.42767800	-0.00021000
C	-1.30256000	0.70920000	0.00012800
H	1.01606200	3.03541200	0.00047000
H	-1.02715400	4.49967300	-0.00014000
H	-3.28876800	3.45162900	-0.00059300

C	-3.73192700	0.68527900	-0.00045600
C	-3.73315800	-0.67937000	-0.00033800
H	-4.67205000	1.23492100	-0.00074000
H	-4.67426200	-1.22733300	-0.00051800
O	2.84834100	1.06937000	-0.00020600
C	3.54363200	-0.00575900	-0.00079600
C	5.02055600	-0.00115200	-0.00060200
H	5.38462000	0.51891800	0.89348800
H	5.40934200	-1.02231400	-0.02129200
H	5.38558000	0.55752000	-0.87045600
O	2.84538600	-1.07739600	-0.00067400
Ni	1.31184400	-0.00163700	0.00024400

15_Pd

E = -1084.395598 au

H = -1084.036245 au

G = -1084.111046 au

N	0.81385700	1.12193900	0.01829800
C	2.17397000	1.02450500	-0.00818100
C	2.99644100	2.17086500	-0.00521100
C	2.36684700	3.43116300	0.03906400
C	0.99343500	3.50605400	0.08269400
C	0.24668800	2.32087300	0.06928800
Pd	-0.16575000	-0.71348700	-0.00960000
H	2.97657100	4.33414500	0.04283400
H	0.47637000	4.46097600	0.12620200
H	-0.84074900	2.35062000	0.10317600
N	1.95879900	-1.36349200	-0.01073900
C	2.49821900	-2.57197000	-0.02233500
C	3.88485800	-2.78813600	-0.05616300
C	4.72503200	-1.69799000	-0.07617800
C	4.18166300	-0.39643100	-0.06121200
C	2.77581700	-0.28028400	-0.02991400
H	1.80665400	-3.41456700	-0.00299000
H	4.27251900	-3.80353900	-0.06456800
H	5.80675200	-1.82616300	-0.10119900
C	4.98930900	0.78445300	-0.07129000
C	4.41935200	2.01783000	-0.04217100
C	-1.95616900	-2.39937000	0.27018600
H	-1.87781800	-2.37503500	1.36510900
H	6.07247600	0.67377900	-0.09831300
H	5.03625300	2.91540000	-0.04455900
H	-0.92063100	-2.49224200	-0.18388800
C	-2.04190100	0.02765300	-0.03933700
H	-2.11351200	0.78120400	-0.83420500
C	-2.81566600	-1.24803900	-0.28565600
H	-2.36336200	-3.37767800	-0.02084400
H	-2.94215600	-1.40206400	-1.36822700
C	-4.19550600	-1.30234300	0.35755200
H	-4.14746900	-1.00211500	1.41407400
H	-4.59440500	-2.32326600	0.29263900
O	-5.14341000	-0.49359600	-0.33431800
C	-5.27131300	0.79659100	0.05123200
O	-4.56801900	1.30663300	0.89334900

C	-6.38607400	1.46589200	-0.68451700
H	-7.34536900	1.08684900	-0.31054200
H	-6.34246200	2.54507700	-0.52172500
H	-6.34414000	1.23598300	-1.75444600
H	-2.21820400	0.47171700	0.95077300

14TS_Pd

E = -1084.368605 au

H = -1084.010424 au

G = -1084.083579 au

N	0.85812700	1.24001800	-0.35336100
C	2.15415300	0.97807900	-0.02890100
C	3.11026600	2.00369600	0.12258300
C	2.68211800	3.33179600	-0.07323200
C	1.36883800	3.58071800	-0.40035600
C	0.48437600	2.50098600	-0.53108400
Pd	-0.35593300	-0.49059100	-0.49135100
H	3.39678300	4.14653900	0.03856500
H	1.00305300	4.59223200	-0.55589700
H	-0.55906100	2.67498800	-0.78578000
N	1.60209500	-1.35306200	0.01628100
C	1.94564200	-2.61756100	0.19417800
C	3.24808000	-3.01402300	0.53388600
C	4.21595800	-2.04738900	0.68958800
C	3.88197600	-0.68988200	0.50612200
C	2.54632100	-0.38914100	0.16575300
H	1.15780000	-3.36184400	0.06286600
H	3.47227700	-4.06906800	0.66850200
H	5.23836600	-2.31693700	0.95284200
C	4.82977300	0.37244500	0.65153900
C	4.45811900	1.66676000	0.46726500
C	-1.33910800	-2.43823600	-0.56732600
H	-1.05786400	-2.69352800	0.46349600
H	5.85656800	0.12110900	0.91404500
H	5.18162600	2.47297300	0.58034600
H	-0.58450300	-2.73436600	-1.31028300
C	-2.11726000	0.43247000	-0.93486400
H	-2.03124000	0.87023900	-1.93376900
C	-2.67112700	-0.87732300	-0.82188200
H	-2.23606800	-3.00439500	-0.81495500
H	-3.02151100	-1.31981000	-1.75661800
C	-3.53195500	-1.17763200	0.38761900
H	-3.04429800	-0.82858500	1.30729900
H	-3.76199500	-2.24411200	0.47657100
O	-4.79335300	-0.53202400	0.23076000
C	-4.96550900	0.66513400	0.85278900
O	-4.07971800	1.22491200	1.45418900
C	-6.36610000	1.15131400	0.68284400
H	-7.06357400	0.45098400	1.15747500
H	-6.47211900	2.13923000	1.13607000
H	-6.62934200	1.19344300	-0.38026500
H	-2.31631100	1.13300300	-0.11749400

13_Pd

E = -1084.404681 au

H = -1084.046152 au

G = -1084.120563 au

N	1.16836500	-1.33977900	-0.06149900
C	2.30097100	-0.62723400	0.18793400
C	3.49567900	-1.24816900	0.60694600
C	3.48367900	-2.64874200	0.76172700
C	2.32890800	-3.35389100	0.50569000
C	1.18404800	-2.65789700	0.09348200
Pd	-0.45636500	-0.15763400	-0.66595200
H	4.39054000	-3.16029000	1.08276800
H	2.28706100	-4.43426900	0.61569600
H	0.25515800	-3.18454200	-0.11644300
N	1.09157600	1.35736500	-0.38707000
C	1.03629200	2.67129300	-0.55037100
C	2.13659200	3.51239800	-0.32164100
C	3.32694500	2.95601900	0.08945200
C	3.41872100	1.56064900	0.27038400
C	2.26104400	0.79687000	0.01652100
H	0.08109800	3.08018700	-0.87724900
H	2.03381900	4.58412800	-0.47068000
H	4.20017500	3.57964100	0.27832600
C	4.61801200	0.90378400	0.69461200
C	4.65476600	-0.44565700	0.85600100
C	-3.08063600	-0.22554300	-2.83991000
H	-3.88435700	-0.94497700	-3.04337700
H	5.50235800	1.50953300	0.88762200
H	5.56907600	-0.94169600	1.17889600
H	-2.22720300	-0.48036900	-3.47877700
C	-1.94872700	-1.49472100	-0.96006900
H	-2.22343400	-1.96302800	-0.00992400
C	-2.70012400	-0.29446700	-1.36655100
H	-3.43928100	0.77135200	-3.12285100
H	-1.95459600	0.65443700	-1.23067600
C	-3.85637600	0.10144700	-0.46183700
H	-4.66341700	-0.63961800	-0.55671400
H	-4.27130400	1.07734700	-0.74987000
O	-3.39044500	0.14874600	0.87912400
C	-4.35108000	0.41303500	1.81009200
O	-5.50518100	0.57638800	1.50805200
C	-3.76970600	0.48901800	3.18422000
H	-3.28516700	1.46438000	3.31898100
H	-4.56881000	0.39374600	3.92318500
H	-3.01005400	-0.28370800	3.34008400
H	-1.68750600	-2.20442100	-1.75273800

14_Pd

E = -1084.409615 au

H = -1084.049396 au

G = -1084.121388 au

N	1.01427100	-1.36701300	0.26574900
C	2.16510600	-0.64841900	0.12264200
C	3.43535000	-1.24758400	0.25853800
C	3.48577300	-2.61456600	0.59470000

C	2.31437500	-3.31318700	0.77694800
C	1.09294200	-2.65157800	0.59540000
Pd	-0.72568200	-0.26279100	0.01079400
H	4.45324700	-3.10177900	0.71206300
H	2.31516600	-4.36538600	1.04889400
H	0.15261200	-3.18410900	0.72066200
N	0.83716700	1.31242300	-0.24062600
C	0.73580400	2.59007900	-0.57382700
C	1.84870700	3.40342400	-0.83751900
C	3.10795700	2.85685500	-0.73622600
C	3.25152000	1.49565800	-0.39835800
C	2.07218400	0.75278500	-0.17695100
H	-0.27381600	2.99608900	-0.63800500
H	1.70279000	4.44597600	-1.10834700
H	3.99628600	3.45995400	-0.92129500
C	4.52526400	0.85541900	-0.27598500
C	4.61323400	-0.46063800	0.05095400
C	-4.08154300	-2.45694300	-1.37217700
H	-4.53591400	-2.83083900	-0.44403500
H	5.42370500	1.44700400	-0.44630400
H	5.58368700	-0.94404600	0.15514700
H	-3.60032800	-3.30226300	-1.87772200
C	-1.97400900	-1.84521600	-0.13844100
H	-2.34735500	-2.08911800	0.87013400
C	-3.06411200	-1.35424800	-1.07272300
H	-4.88681000	-2.09209200	-2.02312200
H	-2.60314400	-1.03865600	-2.02458300
C	-3.75916100	-0.16768500	-0.45295700
H	-4.37977900	-0.46398300	0.40353000
H	-4.38121100	0.40143500	-1.15196400
O	-2.70885600	0.72052400	0.05759700
C	-3.16751400	1.73148700	0.88409000
O	-4.34328900	1.93145400	0.99942700
C	-2.07991900	2.49091200	1.56925800
H	-1.95260800	3.46254000	1.07551100
H	-2.40413300	2.69912800	2.59375300
H	-1.12423800	1.95692900	1.58485300
H	-1.43144400	-2.70144300	-0.56195900

15_Pd

E = -1084.423538 au

H = -1084.062921 au

G = -1084.134946 au

N	1.05514200	-1.35969900	-0.02963800
C	2.23350300	-0.66902800	0.01297300
C	3.48049500	-1.32937200	0.04622900
C	3.48108700	-2.73766900	0.03899800
C	2.28506500	-3.41633700	-0.00121400
C	1.08998100	-2.68632100	-0.03587700
Pd	-0.62161600	-0.13382400	-0.08071900
H	4.42925400	-3.27375700	0.06494500
H	2.24607700	-4.50230700	-0.00810700
H	0.13217000	-3.20191100	-0.07196600
N	0.98430700	1.37073800	-0.00995800

C	0.92199200	2.69141500	-0.01445400
C	2.06843300	3.50256800	0.01515100
C	3.30721200	2.90310400	0.05022800
C	3.40289800	1.49611900	0.05320100
C	2.19734800	0.76560400	0.02009700
H	-0.07755900	3.12487600	-0.04566800
H	1.96397500	4.58452600	0.00965000
H	4.21726100	3.50194500	0.07327900
C	4.65156800	0.79847300	0.08537000
C	4.68723200	-0.56013500	0.08336200
C	-4.16956400	-2.71111700	-0.24055000
H	-4.02064000	-3.25917100	0.70125200
H	5.57265300	1.37935800	0.11061200
H	5.63755600	-1.09163600	0.10831000
H	-3.85393100	-3.36739900	-1.06075600
C	-1.88917700	-1.71327000	-0.17945900
H	-1.66380100	-2.30542800	0.72582100
C	-3.37231600	-1.40370100	-0.23974600
H	-5.24508400	-2.52215300	-0.35575800
H	-3.59668300	-0.86885800	-1.17668800
C	-3.81741500	-0.51470000	0.92493000
H	-3.04402800	-0.42749500	1.70115900
H	-4.73606200	-0.88245300	1.39182200
O	-4.18884200	0.81973800	0.50862900
C	-3.29560200	1.63473100	0.00073300
O	-2.10403800	1.37015700	-0.17279500
C	-3.86928200	2.96252400	-0.36046700
H	-4.33636500	3.42028600	0.51906400
H	-3.09251000	3.61878300	-0.75873800
H	-4.65921200	2.83035800	-1.10927900
H	-1.57259600	-2.27540900	-1.07240000

13TS_Ni

E = -1127.436447 au

H = -1127.077898 au

G = -1127.149482 au

N	0.67808600	1.13913300	-0.43430100
C	1.97205700	0.93537700	-0.06267100
C	2.89800700	1.98008800	0.12521000
C	2.44677900	3.29545600	-0.09370700
C	1.14141100	3.49878400	-0.47689400
C	0.29053400	2.39593100	-0.63370200
H	3.13203100	4.13148400	0.04117100
H	0.75037400	4.49685800	-0.65608400
H	-0.74110700	2.56058200	-0.92963900
N	1.44118800	-1.37412600	-0.07577600
C	1.80451400	-2.63742300	0.09898200
C	3.09398600	-3.02232300	0.49371800
C	4.04766500	-2.05377600	0.70936400
C	3.70372700	-0.70001400	0.52814700
C	2.38021900	-0.41618200	0.13605600
H	1.04695700	-3.39896400	-0.08154000
H	3.31857000	-4.07821500	0.62043800
H	5.05959700	-2.31893600	1.01379500

C	4.62423700	0.37887800	0.71975100
C	4.23663700	1.66731000	0.52435000
C	-1.08892900	-2.39612000	-0.80770700
H	-0.84680100	-2.76296800	0.19762200
H	5.64379200	0.14482700	1.02279100
H	4.94018100	2.48608900	0.66796600
H	-0.30929400	-2.61946800	-1.54976400
C	-1.94879000	0.48154200	-0.94990300
H	-1.84154400	0.96317200	-1.92544800
C	-2.50559500	-0.80425900	-0.89757800
H	-1.98379900	-2.91841500	-1.14389700
H	-2.86007100	-1.22161400	-1.84078000
C	-3.28838900	-1.22265700	0.32621200
H	-2.79678500	-0.86995300	1.24247900
H	-3.42914600	-2.30632000	0.38061800
O	-4.60356700	-0.67779600	0.23772700
C	-4.82385800	0.51569900	0.84961700
O	-3.94844300	1.14184800	1.39887200
C	-6.26054800	0.90635800	0.74568800
H	-6.88261000	0.18023700	1.28240800
H	-6.40453000	1.89998300	1.17549400
H	-6.58580400	0.89592200	-0.30076600
H	-2.08071600	1.13222400	-0.08136200
Ni	-0.35321800	-0.54571400	-0.59526300

12_Ni

E = -1127.463294 au

H = -1127.103494 au

G = -1127.176306 au

N	0.68258300	1.06381200	-0.31912300
C	2.01931000	0.95728400	-0.06902300
C	2.86722900	2.07255700	0.05344000
C	2.28273500	3.34607300	-0.09745800
C	0.93251000	3.44422900	-0.35076500
C	0.16040900	2.27792400	-0.45373400
H	2.90169900	4.23857600	-0.01321300
H	0.44893500	4.41011800	-0.47103200
H	-0.90802600	2.33653100	-0.64693300
N	1.67047100	-1.38362200	-0.05739200
C	2.12237300	-2.62312100	0.07452700
C	3.46985900	-2.91305500	0.34110000
C	4.36761900	-1.87572000	0.47353100
C	3.91819600	-0.54588900	0.34097500
C	2.55008700	-0.35972200	0.07379900
H	1.39261300	-3.42640200	-0.03302300
H	3.78628200	-3.94828500	0.43845200
H	5.41929800	-2.07175200	0.68035600
C	4.76408000	0.60346700	0.46129200
C	4.25859500	1.85968000	0.32222900
C	-1.54441300	-2.32607800	-0.31365600
H	-1.21033800	-2.26622300	0.73874600
H	5.82292600	0.45231900	0.66669000
H	4.90698800	2.72991400	0.41334200
H	-0.67206400	-2.24900500	-1.03023800

C	-1.91587000	0.03124400	-0.69407700
H	-1.96420300	0.54799300	-1.66202000
C	-2.64083800	-1.30210200	-0.64770800
H	-1.84496400	-3.36779600	-0.48461200
H	-3.05994100	-1.55151000	-1.63424600
C	-3.74642500	-1.39247200	0.38848200
H	-3.38179100	-1.07096700	1.37500000
H	-4.12311100	-2.42137300	0.46207800
O	-4.86913500	-0.59863000	0.01256200
C	-5.01475400	0.61375900	0.59815600
O	-4.20340700	1.08471700	1.36168800
C	-6.30015200	1.25161700	0.18181900
H	-7.13545500	0.73790800	0.67388800
H	-6.30536000	2.30280600	0.47859100
H	-6.45358100	1.15531700	-0.89824300
H	-2.17191800	0.70276400	0.13635500
Ni	-0.16579800	-0.62889300	-0.41592600

13_Ni

E = -1127.476596 au

H = -1127.116883 au

G = -1127.189489 au

N	1.04164600	-1.36952800	-0.07710700
C	2.11789100	-0.56703400	0.14938300
C	3.34872900	-1.04535400	0.62999000
C	3.44433800	-2.42974400	0.87937200
C	2.35223800	-3.23698500	0.64594400
C	1.16169900	-2.67025000	0.16551500
H	4.37841500	-2.84792900	1.25325700
H	2.39393100	-4.30777200	0.82720800
H	0.28781700	-3.28844400	-0.02642600
N	0.72661000	1.19979500	-0.58682500
C	0.52495800	2.48532800	-0.84840500
C	1.52177100	3.45787000	-0.66882200
C	2.76190700	3.07753700	-0.20341000
C	3.00777300	1.71961000	0.08660200
C	1.94677200	0.82254600	-0.12523400
H	-0.46280200	2.76201200	-1.21405000
H	1.30109500	4.49667500	-0.90050200
H	3.55166200	3.81374500	-0.05690600
C	4.25499200	1.21236600	0.57649700
C	4.41844900	-0.11415200	0.83658700
C	-2.90095500	-0.57239900	-2.84663900
H	-3.71277200	-1.29809100	-2.98334700
H	5.07344000	1.91259700	0.73759300
H	5.37000800	-0.49126900	1.20896300
H	-2.06402400	-0.88045500	-3.48419300
C	-1.74628800	-1.72681100	-0.90532900
H	-2.03833600	-2.14508200	0.06344000
C	-2.48962200	-0.54699600	-1.37997700
H	-3.25863400	0.40522700	-3.19294200
H	-1.73872000	0.39945000	-1.33815300
C	-3.61477000	-0.06104800	-0.48083400
H	-4.42421000	-0.80479400	-0.46522100

H	-4.04143700	0.88429900	-0.84484800
O	-3.09002200	0.12028300	0.82977400
C	-3.99399200	0.54485500	1.75749100
O	-5.14811500	0.74671800	1.48037600
C	-3.35212600	0.72371700	3.09519700
H	-2.67130800	1.58350000	3.06827300
H	-4.12324600	0.90279900	3.84777500
H	-2.75922600	-0.15696500	3.36532300
H	-1.49578300	-2.48114500	-1.65951200
Ni	-0.45075500	-0.38016300	-0.72224900

14_Ni

E = -1127.479708 au

H = -1127.119253 au

G = -1127.190239 au

N	0.84265700	-1.37481600	0.28206800
C	1.97057600	-0.62937800	0.10330400
C	3.26899500	-1.15471300	0.22549000
C	3.38244200	-2.51047700	0.59334000
C	2.23950300	-3.24651200	0.81686400
C	0.98371400	-2.64634900	0.64467000
H	4.36838300	-2.96079100	0.70418000
H	2.28919900	-4.29060300	1.11444400
H	0.07086900	-3.21556700	0.80245800
N	0.50608600	1.18875300	-0.26704200
C	0.28885800	2.44567300	-0.62928800
C	1.32992100	3.33834100	-0.93027400
C	2.63566800	2.90375800	-0.84558800
C	2.89993200	1.56695700	-0.48489400
C	1.78717900	0.74726400	-0.22343200
H	-0.75181000	2.76405200	-0.68878100
H	1.09341800	4.35933100	-1.21890900
H	3.46326900	3.57879900	-1.06109600
C	4.21367200	1.00699800	-0.37472800
C	4.38946500	-0.29667100	-0.02446000
C	-3.97080100	-2.28658300	-1.61942600
H	-4.52709300	-2.64849800	-0.74320500
H	5.07209300	1.64692600	-0.57401100
H	5.39106900	-0.71454900	0.06752300
H	-3.51478900	-3.15441800	-2.11039600
C	-1.90906000	-1.85424900	-0.19666900
H	-2.39434100	-2.12988600	0.75554300
C	-2.89930800	-1.28105700	-1.20084300
H	-4.69087300	-1.84560100	-2.32204700
H	-2.34861700	-0.96853700	-2.10571900
C	-3.54101600	-0.06421900	-0.57978600
H	-4.29405800	-0.33778100	0.17035400
H	-3.99147600	0.63608500	-1.29089500
O	-2.45680300	0.63400600	0.13255000
C	-2.88358500	1.53038800	1.10483600
O	-4.02971700	1.87433900	1.13865300
C	-1.81032300	1.97552300	2.04417600
H	-1.51141500	3.00219900	1.79807100
H	-2.23805200	2.00409700	3.05142100

H	-0.92538100	1.33236100	2.03269700
H	-1.38871500	-2.72740200	-0.61245800
Ni	-0.74913300	-0.37009700	0.05058100

15_Ni

E = -1127.495515 au

H = -1127.134028 au

G = -1127.203465 au

N	0.88778400	-1.35616400	-0.07154500
C	2.07316500	-0.68451000	0.00888900
C	3.32398900	-1.32726900	0.06865300
C	3.33079800	-2.73493500	0.04053800
C	2.13358300	-3.40877500	-0.04591300
C	0.93480000	-2.68423600	-0.10012500
H	4.27691000	-3.27341300	0.08452100
H	2.09524300	-4.49449100	-0.07385300
H	-0.01485800	-3.20852000	-0.16968600
N	0.77239600	1.27950000	-0.05235600
C	0.66106300	2.59847900	-0.06356100
C	1.77533000	3.45104500	0.00503100
C	3.03878500	2.90642500	0.08445500
C	3.18953300	1.50457100	0.09155000
C	2.01098600	0.73988400	0.02052200
H	-0.35112300	2.99422700	-0.13518000
H	1.62752200	4.52792800	-0.00744800
H	3.92046400	3.54451400	0.13587900
C	4.45017900	0.82874900	0.15885900
C	4.51239200	-0.53066700	0.14810600
C	-4.12393900	-2.69515000	-0.15001700
H	-3.92121300	-3.22007000	0.79551500
H	5.36018400	1.42466400	0.21451800
H	5.47361900	-1.04052600	0.19719800
H	-3.82302600	-3.36138900	-0.96786600
C	-1.86241700	-1.63645400	-0.22414200
H	-1.61297600	-2.25406800	0.65790000
C	-3.35849300	-1.37138200	-0.21341600
H	-5.20872400	-2.53989700	-0.22441000
H	-3.65681500	-0.85437300	-1.14013300
C	-3.76834000	-0.48894700	0.96312500
H	-3.00981300	-0.48470500	1.75916800
H	-4.72645000	-0.79145000	1.39607500
O	-4.01896400	0.88596300	0.57751300
C	-3.09537000	1.58444100	-0.02562000
O	-1.95056200	1.19652200	-0.27886000
C	-3.53895400	2.96451700	-0.37537900
H	-3.50149600	3.59195600	0.52496100
H	-2.88267200	3.39320700	-1.13702200
H	-4.57633000	2.96138700	-0.72344300
H	-1.58528800	-2.19357500	-1.13428600
Ni	-0.63824200	-0.17640600	-0.14013100

14TS_Pd

E = au

H = au
G = au

N	0.93068600	1.27917900	-0.29601200
C	2.23154000	1.02474100	0.02045900
C	3.18668600	2.05080700	0.15260000
C	2.75371800	3.37552900	-0.05404500
C	1.43560100	3.61662600	-0.37183200
C	0.54798200	2.53882200	-0.48447700
H	3.46567800	4.19439800	0.04230700
H	1.06665100	4.62583200	-0.53431800
H	-0.49854100	2.70254200	-0.73027700
N	1.65508900	-1.28838300	0.09324800
C	1.98297700	-2.55696700	0.28267800
C	3.28426800	-2.96143200	0.61687500
C	4.26746500	-2.00670700	0.75572000
C	3.94910800	-0.64723500	0.56019700
C	2.61579900	-0.33831800	0.22639900
H	1.18654900	-3.29317700	0.16624100
H	3.49646400	-4.01759500	0.76171700
H	5.28755000	-2.28816500	1.01500100
C	4.90215700	0.41359000	0.68629900
C	4.53546500	1.70856400	0.49075200
C	-1.36570200	-2.35672400	-0.45222500
H	-1.09364700	-2.61605600	0.58065400
H	5.92984800	0.16145900	0.94429900
H	5.26443600	2.51148300	0.59077100
H	-0.62832300	-2.69796200	-1.19490600
C	-2.08121400	0.47342000	-0.85580600
H	-2.06680300	0.90851500	-1.86066800
C	-2.64527500	-0.85276000	-0.74040300
H	-2.25702700	-2.93991900	-0.68642000
H	-3.00348400	-1.28054800	-1.67990900
C	-3.54466000	-1.12019800	0.44984500
H	-3.06659600	-0.78543100	1.37988700
H	-3.81562200	-2.17801300	0.53444100
O	-4.77231500	-0.42541500	0.25390100
C	-4.94901600	0.74542700	0.92527000
O	-4.08732400	1.24905600	1.60481100
C	-6.32488500	1.27767100	0.69855600
H	-7.06439700	0.58194500	1.11271500
H	-6.42839700	2.25220300	1.18042800
H	-6.53066100	1.36249000	-0.37453700
H	-2.34902800	1.17907200	-0.06137000
Pt	-0.29243700	-0.40021700	-0.41125100

13TS_Pt

E = -1075.827268 au

H = -1075.469096 au

G = -1075.542186 au

N	0.93068600	1.27917900	-0.29601200
C	2.23154000	1.02474100	0.02045900
C	3.18668600	2.05080700	0.15260000
C	2.75371800	3.37552900	-0.05404500
C	1.43560100	3.61662600	-0.37183200

C	0.54798200	2.53882200	-0.48447700
H	3.46567800	4.19439800	0.04230700
H	1.06665100	4.62583200	-0.53431800
H	-0.49854100	2.70254200	-0.73027700
N	1.65508900	-1.28838300	0.09324800
C	1.98297700	-2.55696700	0.28267800
C	3.28426800	-2.96143200	0.61687500
C	4.26746500	-2.00670700	0.75572000
C	3.94910800	-0.64723500	0.56019700
C	2.61579900	-0.33831800	0.22639900
H	1.18654900	-3.29317700	0.16624100
H	3.49646400	-4.01759500	0.76171700
H	5.28755000	-2.28816500	1.01500100
C	4.90215700	0.41359000	0.68629900
C	4.53546500	1.70856400	0.49075200
C	-1.36570200	-2.35672400	-0.45222500
H	-1.09364700	-2.61605600	0.58065400
H	5.92984800	0.16145900	0.94429900
H	5.26443600	2.51148300	0.59077100
H	-0.62832300	-2.69796200	-1.19490600
C	-2.08121400	0.47342000	-0.85580600
H	-2.06680300	0.90851500	-1.86066800
C	-2.64527500	-0.85276000	-0.74040300
H	-2.25702700	-2.93991900	-0.68642000
H	-3.00348400	-1.28054800	-1.67990900
C	-3.54466000	-1.12019800	0.44984500
H	-3.06659600	-0.78543100	1.37988700
H	-3.81562200	-2.17801300	0.53444100
O	-4.77231500	-0.42541500	0.25390100
C	-4.94901600	0.74542700	0.92527000
O	-4.08732400	1.24905600	1.60481100
C	-6.32488500	1.27767100	0.69855600
H	-7.06439700	0.58194500	1.11271500
H	-6.42839700	2.25220300	1.18042800
H	-6.53066100	1.36249000	-0.37453700
H	-2.34902800	1.17907200	-0.06137000
Pt	-0.29243700	-0.40021700	-0.41125100

12_Pd

E = -1075.855201 au

H = -1075.495506 au

G = -1075.569802 au

N	0.86644500	1.19613200	-0.04291300
C	2.22914800	1.10103400	-0.01226600
C	3.05174400	2.24387000	0.00409500
C	2.42152900	3.50450800	-0.00403800
C	1.04646100	3.57788100	-0.02143800
C	0.29424200	2.39780600	-0.04079000
H	3.02901600	4.40874300	0.00747900
H	0.52871200	4.53330300	-0.02053900
H	-0.79257200	2.42258800	-0.05216200
N	1.97836600	-1.26961100	0.00955500
C	2.49526100	-2.48845200	0.04086500
C	3.87893700	-2.72318400	0.07480700

C	4.74009300	-1.64833600	0.07735300
C	4.21906100	-0.33801000	0.04732300
C	2.81731000	-0.20348000	0.01240300
H	1.78883500	-3.31812200	0.04063700
H	4.24941800	-3.74469100	0.09911900
H	5.81906400	-1.79678900	0.10392700
C	5.03477600	0.83798200	0.05392000
C	4.47389400	2.07679300	0.03375000
C	-1.89434400	-2.25265400	0.17494200
H	-1.79032100	-2.24958600	1.26755000
H	6.11722700	0.72058400	0.07826700
H	5.09869600	2.96872700	0.04193600
H	-0.85946600	-2.29996900	-0.33849600
C	-2.04238000	0.15116300	-0.14227500
H	-2.17021900	0.87453400	-0.95979400
C	-2.81817200	-1.14255400	-0.34946600
H	-2.21873900	-3.25780200	-0.13194800
H	-2.97759400	-1.30846300	-1.42599600
C	-4.16724300	-1.22873800	0.34387800
H	-4.08259300	-0.95671900	1.40570700
H	-4.57255100	-2.24658800	0.26546600
O	-5.13120400	-0.39214500	-0.29230900
C	-5.31305700	0.85346500	0.20553100
O	-4.65433000	1.30850400	1.11159900
C	-6.43034100	1.54938500	-0.50237800
H	-7.38539200	1.10184200	-0.20039900
H	-6.43432600	2.60875000	-0.23606500
H	-6.34512200	1.42563500	-1.58721500
H	-2.27916500	0.63235700	0.81873100
Pt	-0.13556200	-0.57622700	-0.07018400

13_Pt

E = -1075.863490 au

H = -1075.506167 au

G = -1075.579087 au

N	1.26672700	-1.29272900	0.05856300
C	2.39867900	-0.57076000	0.28493500
C	3.60301300	-1.16989000	0.69912100
C	3.60465700	-2.56788100	0.87512200
C	2.45085300	-3.28484000	0.64228700
C	1.29278300	-2.61110000	0.23275300
H	4.51799500	-3.06913200	1.19351300
H	2.41961700	-4.36366800	0.76899600
H	0.36516800	-3.14489800	0.03996300
N	1.14008900	1.35754700	-0.31085900
C	1.04409700	2.66706400	-0.49866400
C	2.12623700	3.53818400	-0.29780800
C	3.33889600	3.02551400	0.10824100
C	3.47170000	1.63693700	0.31432400
C	2.33129800	0.84322000	0.08912500
H	0.07465500	3.04235600	-0.82159000
H	1.99179500	4.60363900	-0.46547300
H	4.19492000	3.67906800	0.27229700
C	4.68690400	1.00629800	0.73512500

C	4.74979800	-0.34039400	0.91916600
C	-2.93069600	-0.21244600	-2.73293500
H	-3.76358100	-0.88960400	-2.96417100
H	5.56358300	1.62917700	0.90687200
H	5.67746900	-0.81256900	1.23947800
H	-2.07000100	-0.51208400	-3.34105000
C	-1.90438100	-1.52992800	-0.81546000
H	-2.24072700	-1.97450500	0.12632000
C	-2.61149800	-0.30971200	-1.24997300
H	-3.22845000	0.80200400	-3.02519500
H	-1.82720300	0.67069000	-1.09459800
C	-3.77157600	0.15813800	-0.38985600
H	-4.61889500	-0.52630100	-0.54606000
H	-4.10767800	1.16412500	-0.67821900
O	-3.38178100	0.14806500	0.97365000
C	-4.36898100	0.48616100	1.85007200
O	-5.48401500	0.75784600	1.48370100
C	-3.86992100	0.49007000	3.25820700
H	-3.30743500	1.41431600	3.44113700
H	-4.72000600	0.45979200	3.94387900
H	-3.19582000	-0.35156300	3.44615900
H	-1.70724700	-2.26813700	-1.60054100
Pt	-0.38193200	-0.18950700	-0.54970700

14_Pt

E = -1075.872535 au

H = -1075.512121 au

G = -1075.583908 au

N	1.08970800	-1.32446800	0.24495100
C	2.25547400	-0.62543000	0.09785200
C	3.51538800	-1.24748000	0.20033200
C	3.54714500	-2.62200600	0.50478600
C	2.36430300	-3.30149700	0.69115000
C	1.14980200	-2.62077300	0.54846400
H	4.50629200	-3.13046200	0.59542900
H	2.35014200	-4.35921300	0.94002300
H	0.20185000	-3.13457200	0.68101100
N	0.93855200	1.33732000	-0.20968500
C	0.83571000	2.61941200	-0.52942800
C	1.94996000	3.42973800	-0.79531300
C	3.21042300	2.88047800	-0.71648900
C	3.35367800	1.51413000	-0.40083500
C	2.17428700	0.77663300	-0.17308700
H	-0.17255800	3.02895700	-0.58122200
H	1.80335400	4.47578300	-1.05187700
H	4.09690800	3.48493400	-0.90524600
C	4.62123700	0.85618900	-0.30855100
C	4.69833700	-0.46798900	-0.00971900
C	-4.10806700	-2.37081700	-1.25694400
H	-4.58172300	-2.63499800	-0.30077100
H	5.52456200	1.43963200	-0.48077600
H	5.66475000	-0.96390600	0.06895200
H	-3.68908500	-3.28739400	-1.68905300
C	-1.94034400	-1.80095800	-0.07287700

H	-2.37093500	-2.02487000	0.91888500
C	-3.01339100	-1.32653000	-1.04922900
H	-4.89157900	-2.01030500	-1.93669500
H	-2.53794000	-1.11798700	-2.02194000
C	-3.63035500	-0.05265200	-0.52700000
H	-4.31062500	-0.24554000	0.31293800
H	-4.16182800	0.53606300	-1.28130400
O	-2.53425700	0.78555900	0.00851400
C	-2.96994500	1.85749600	0.78378800
O	-4.12497900	2.16911600	0.76227300
C	-1.90692000	2.51191100	1.60189200
H	-1.73776200	3.52806100	1.22542800
H	-2.29601500	2.61969000	2.62028500
H	-0.96589900	1.95482900	1.62984000
H	-1.46104100	-2.71185200	-0.46036400
Pt	-0.62224500	-0.24658100	0.04834000

15_Pt

E = -1075.889444 au

H = -1075.528339 au

G = -1075.600122 au

N	1.10576400	-1.33140300	-0.02022400
C	2.30273000	-0.66600700	0.03031800
C	3.53390700	-1.34993200	0.07417000
C	3.50641300	-2.75782000	0.06878600
C	2.29538200	-3.40994200	0.01856300
C	1.11292600	-2.66251700	-0.02623900
H	4.44206200	-3.31467700	0.10259400
H	2.23397400	-4.49483700	0.01146000
H	0.14491400	-3.15491600	-0.07165400
N	1.08155700	1.38113700	-0.01009100
C	1.03226600	2.70356800	-0.02404800
C	2.18898300	3.49895100	0.00897100
C	3.42210300	2.88735700	0.05759800
C	3.50233600	1.47965200	0.07000000
C	2.28932800	0.76469400	0.03208100
H	0.03794300	3.14689700	-0.06656800
H	2.09662500	4.58187200	-0.00495800
H	4.33755300	3.47756300	0.08349700
C	4.73872900	0.76110600	0.11461800
C	4.75202800	-0.59845800	0.11809900
C	-4.15934800	-2.63657300	-0.21630500
H	-4.00030200	-3.19852100	0.71597800
H	5.66939600	1.32611600	0.14439600
H	5.69353000	-1.14481800	0.15178200
H	-3.87355100	-3.29060700	-1.04927100
C	-1.84526800	-1.68053400	-0.19309900
H	-1.65493300	-2.32474200	0.68646900
C	-3.33210700	-1.35094500	-0.22123000
H	-5.23372200	-2.42800100	-0.30585500
H	-3.56817200	-0.79798900	-1.14535100
C	-3.72907900	-0.46819600	0.96313100
H	-2.94739100	-0.42887100	1.73466500
H	-4.66198000	-0.79866600	1.42959900

O	-4.04414700	0.89443800	0.57722500
C	-3.15625000	1.68205900	0.03507300
O	-1.97364100	1.40134600	-0.20045900
C	-3.70345500	3.02660100	-0.30347300
H	-4.15905400	3.48089800	0.58354300
H	-2.91660900	3.67261800	-0.69867700
H	-4.49778300	2.91854600	-1.05178700
H	-1.58731900	-2.26060200	-1.09549100
Pt	-0.52863900	-0.11564200	-0.08459500

16_Pt

E = -1075.817396 au

H = -1075.460676 au

G = -1075.538612 au

N	0.87581100	1.31139300	-0.19327500
C	2.16326200	0.88137600	-0.20331400
C	3.25508100	1.76053100	-0.34285600
C	2.96575400	3.13326900	-0.48355000
C	1.65521800	3.55578000	-0.48246200
C	0.63296500	2.60600700	-0.33286800
Pt	-0.48996100	-0.39563000	0.05193100
H	3.78189900	3.84614100	-0.59555300
H	1.39949500	4.60608200	-0.59525000
H	-0.41353000	2.90890800	-0.33082600
N	1.31334200	-1.35407100	0.05290900
C	1.51049100	-2.66507100	0.17327400
C	2.79224700	-3.22802600	0.18270300
C	3.89257200	-2.40958000	0.06255400
C	3.71281200	-1.01876500	-0.06954300
C	2.39414500	-0.52360000	-0.06959200
H	0.62444900	-3.28747400	0.26320000
H	2.89355600	-4.30522200	0.28388700
H	4.90031100	-2.82312500	0.06636200
C	4.80425200	-0.10189200	-0.20493000
C	4.58534100	1.23353400	-0.33756800
C	-1.58440300	-2.11385700	0.23332500
H	-1.33037800	-2.62463700	1.17410400
H	5.81726900	-0.50147900	-0.20200100
H	5.41960200	1.92547600	-0.44324200
H	-1.38132000	-2.77696300	-0.61932100
H	-2.65995500	-1.88927200	0.24805400
C	-2.74986000	0.91930400	0.48852900
C	-2.37774400	0.85764000	1.92858700
H	-2.41462600	-0.12774900	2.39601500
H	-2.83223500	1.95687900	0.12664900
C	-2.07334500	1.94650400	2.63441900
H	-1.81820900	1.88610600	3.68959100
H	-2.07827600	2.94266200	2.18948700
O	-3.65499600	0.50847200	-1.92400100
C	-4.33439800	0.08211200	-1.02464100
C	-5.62692000	-0.65015100	-1.12614500
O	-3.94954100	0.22029200	0.28408400
H	-5.91222300	-0.74746600	-2.17555500
H	-6.40897200	-0.11712600	-0.57305800
H	-5.53068400	-1.64365400	-0.67121700

H	-2.03178500	0.50904500	-0.33555300

14TS_Pt

E = -1075.808854 au

H = -1075.455704 au

G = -1075.529823 au

N	0.79290200	1.31549100	-0.16274600
C	2.08829600	0.90602300	-0.16386900
C	3.16526500	1.81246100	-0.24217900
C	2.85414200	3.18417500	-0.33658200
C	1.53665300	3.58343100	-0.35601000
C	0.53034400	2.60996400	-0.26703800
Pt	-0.59133800	-0.40726700	-0.03749000
H	3.66014400	3.91430800	-0.40142500
H	1.26306600	4.63195800	-0.43943100
H	-0.52110300	2.89669900	-0.28905000
N	1.28979800	-1.36040600	-0.04696100
C	1.51699500	-2.66881400	0.01235100
C	2.81008400	-3.20624100	0.02938800
C	3.89102300	-2.35493900	-0.02103000
C	3.68086700	-0.96320300	-0.08729700
C	2.34981500	-0.50117400	-0.09456500
H	0.64133200	-3.31373800	0.04564600
H	2.93760300	-4.28421700	0.07959100
H	4.90898300	-2.74299700	-0.01251000
C	4.75465200	-0.01869200	-0.15208900
C	4.50707100	1.31576500	-0.22911800
C	-1.65260200	-2.16395500	-0.04197200
H	-1.43293600	-2.70876700	0.88923700
H	5.77657100	-0.39492600	-0.14395300
H	5.32647400	2.03091200	-0.28565100
H	-1.33610200	-2.76298600	-0.90711300
H	-2.73657400	-2.01482500	-0.10266100
C	-2.41870600	0.67764500	0.67285600
C	-2.10523400	0.38565000	2.09317600
H	-2.39829400	-0.60471400	2.44479600
H	-2.36155500	1.75165800	0.44434300
C	-1.54932900	1.28118200	2.91388800
H	-1.35060200	1.04653700	3.95670300
H	-1.27967100	2.28334500	2.57733500
O	-3.47887100	0.88784600	-1.71384600
C	-4.16961800	0.36484000	-0.86955200
C	-5.54268700	-0.18259700	-1.03670700
O	-3.70861100	0.18932000	0.40009000
H	-5.90846200	0.04082900	-2.04097200
H	-6.21816900	0.23954800	-0.28430400
H	-5.52705100	-1.26913400	-0.88408100
H	-1.88055200	0.35525800	-0.68620100

17_Pt

E = -1075.824556 au

H = -1075.469785 au

G = -1075.544017 au

N	0.59339100	1.29916500	0.11661300
C	1.92324500	1.05201700	-0.01832900
C	2.87640700	2.09256800	-0.03353400
C	2.40046700	3.41518100	0.06842800
C	1.04701100	3.64837600	0.15946700
C	0.16981600	2.55420400	0.17694400
H	3.11063200	4.24140700	0.05949900
H	0.64625900	4.65701700	0.21570300
H	-0.90838500	2.70870900	0.22404600
N	1.42145100	-1.29263300	-0.21785900
C	1.80581700	-2.55056400	-0.38211200
C	3.15294300	-2.91580500	-0.51526100
C	4.11636000	-1.93285900	-0.48029600
C	3.73556900	-0.58616600	-0.31296200
C	2.35868100	-0.30793500	-0.17776500
H	1.01738800	-3.30168000	-0.41144500
H	3.41382800	-3.96257700	-0.64740200
H	5.17196700	-2.18110600	-0.58577500
C	4.67998500	0.48899700	-0.29048400
C	4.26645300	1.77723900	-0.16175700
C	-1.57693200	-2.36293200	-0.37582400
H	-1.32947300	-3.05671600	0.44014000
H	5.73824000	0.25201100	-0.39132600
H	4.98639000	2.59443100	-0.15935700
H	-1.19415000	-2.75494800	-1.32488600
H	-2.66349700	-2.25564900	-0.45234300
C	-2.41217500	0.27309900	0.78545600
C	-2.08285700	-0.58341500	1.91420300
H	-2.64106300	-1.51464600	2.02501300
H	-2.22444900	1.34542100	0.90246700
C	-0.93587400	-0.37137000	2.62490300
H	-0.57946500	-1.10915700	3.33987100
H	-0.43385000	0.59618500	2.62566300
Pt	-0.65011500	-0.55812700	0.04570500
O	-3.63853800	0.03332200	0.18719800
C	-3.98097400	0.92260600	-0.79947000
O	-3.25999200	1.83926000	-1.10493800
C	-5.30347100	0.57800800	-1.39152300
H	-5.60518300	1.35709700	-2.09455800
H	-5.23540700	-0.38244300	-1.91721500
H	-6.05889500	0.46329000	-0.60609000
H	-0.86038800	-0.33660700	-1.49684900

15TS_Pt

E = -1075.808417 au

H = -1075.455211 au

G = -1075.530677 au

N	0.54518400	1.23141300	0.09569100
C	1.89303900	1.03873600	0.00571600
C	2.80355400	2.11468600	0.04393600
C	2.27512300	3.41729000	0.14673100
C	0.91193200	3.59721500	0.18159900
C	0.07544400	2.47313300	0.15154500
Pt	-0.61826100	-0.60974300	0.04073100

H	2.95319100	4.26948400	0.17927300
H	0.46900500	4.58831400	0.23092800
H	-1.00678200	2.59137300	0.14295800
N	1.49153400	-1.31132200	-0.25959200
C	1.93182200	-2.54921400	-0.43112900
C	3.29562700	-2.86314700	-0.52268600
C	4.21852800	-1.84562300	-0.43401800
C	3.78038100	-0.51777200	-0.25525900
C	2.39012800	-0.29646900	-0.16577300
H	1.17570500	-3.33034400	-0.50125100
H	3.60141800	-3.89649000	-0.66359400
H	5.28615100	-2.05153600	-0.50399100
C	4.68049700	0.59103400	-0.17547700
C	4.20900100	1.85811000	-0.03691400
C	-1.47278500	-2.55161700	0.10541400
H	-1.12671600	-2.81447200	1.11532200
H	5.75051700	0.39896600	-0.24032000
H	4.89281600	2.70453300	0.00799300
H	-1.05510400	-3.25659100	-0.62208400
H	-2.56446600	-2.60191400	0.06772000
C	-2.39050800	0.23139400	0.70527500
C	-2.61399200	-0.36487200	2.03814100
H	-3.22372000	-1.26950400	2.08213400
H	-2.18259300	1.30578000	0.77634100
C	-2.06072400	0.14178400	3.14627500
H	-2.19096200	-0.32499000	4.11977700
H	-1.46592500	1.05740500	3.11803500
O	-2.82819800	1.76967600	-1.38641100
C	-3.64273100	0.90331900	-1.16567700
C	-4.87481800	0.61973800	-1.95763500
O	-3.51953000	0.03887400	-0.12386200
H	-4.99512000	1.37567500	-2.73661600
H	-5.75529100	0.60749300	-1.30536700
H	-4.80244400	-0.37290300	-2.41892200
H	-1.46764100	-1.31569100	-1.07625100

18_Pt

E = -1075.834290 au

H = -1075.478475 au

G = -1075.554329 au

N	0.50540500	1.19496400	0.15090600
C	1.85853100	1.01313200	0.05091000
C	2.75911800	2.09441300	0.12308700
C	2.22462200	3.38926700	0.27435700
C	0.86092200	3.55560500	0.32030600
C	0.02643100	2.43177600	0.25215400
Pt	-0.58920000	-0.56648700	0.09888400
H	2.89698800	4.24432100	0.33364400
H	0.40874300	4.54007600	0.40564100
H	-1.05430600	2.54532200	0.24129100
N	1.46289700	-1.31772400	-0.28916700
C	1.90434600	-2.54699000	-0.51130800
C	3.26839000	-2.85435300	-0.62578500
C	4.19181400	-1.84022600	-0.50576400

C	3.75259300	-0.52084300	-0.27519300
C	2.36281100	-0.30856800	-0.16783200
H	1.15060800	-3.32781100	-0.60572600
H	3.57407300	-3.88116400	-0.80880700
H	5.25896700	-2.04242700	-0.59122100
C	4.64582000	0.59002800	-0.16104400
C	4.16556500	1.84789300	0.02550200
C	-1.68839200	-2.80506600	-0.13670000
H	-1.22806900	-2.66932900	0.85652000
H	5.71685200	0.40882200	-0.23880500
H	4.84382300	2.69691900	0.09687000
H	-1.20184400	-3.64584100	-0.63783900
H	-2.75615300	-2.98633300	0.00953400
C	-2.38728300	0.23933400	0.69935200
C	-2.80623600	-0.51580400	1.90121700
H	-3.49377400	-1.34921200	1.74117200
H	-2.24112100	1.30336700	0.92055500
C	-2.36799800	-0.22541700	3.13104300
H	-2.66808100	-0.80626000	3.99988400
H	-1.69439800	0.61465800	3.31143000
O	-2.63696700	1.97814500	-1.29744300
C	-3.41981200	1.05567500	-1.26802800
C	-4.53114500	0.81455600	-2.23464400
O	-3.38285100	0.09879000	-0.30887200
H	-4.48013900	1.54702800	-3.04300300
H	-5.49698700	0.90198700	-1.72252000
H	-4.47406600	-0.20099200	-2.64274300
H	-1.64370900	-1.94980600	-0.87028800

19_Pt

E = -1035.400627 au

H = -1035.093805 au

G = -1035.162987 au

N	-0.22431400	1.15623400	-0.06540200
C	-1.57983300	1.24813200	0.00825500
C	-2.25791300	2.48141100	0.02829400
C	-1.47461400	3.65131400	-0.04448800
C	-0.10572000	3.54554300	-0.14188300
C	0.48845100	2.27382800	-0.15033300
Pt	0.50718700	-0.86926200	-0.05288000
H	-1.96091400	4.62618900	-0.03175500
H	0.52701600	4.42605600	-0.21457000
H	1.56511600	2.15823200	-0.24880100
N	-1.62472100	-1.13446700	-0.00140400
C	-2.28956600	-2.28454700	0.02310100
C	-3.68813000	-2.34226600	0.09905800
C	-4.40890000	-1.16951000	0.14850600
C	-3.73055800	0.06534900	0.12125500
C	-2.32482900	0.02949700	0.04767200
H	-1.69406000	-3.19384200	-0.01806900
H	-4.18131700	-3.31057300	0.11680300
H	-5.49662400	-1.18432600	0.20656200
C	-4.39551400	1.33265900	0.15821400
C	-3.68713500	2.49305600	0.11181600

H	-5.48265500	1.34809900	0.21901100
H	-4.19711900	3.45517800	0.13404600
C	2.66054300	-0.81997900	-0.23804800
C	2.26689000	-2.03120900	0.37991800
H	2.48481800	-2.17097200	1.44019200
H	2.84682400	-0.73582300	-1.31213800
C	1.31266700	-2.82761300	-0.29505800
H	0.87139900	-3.66474800	0.24548500
H	1.37654500	-2.95851000	-1.37858200
O	3.58746400	1.52458200	-1.09378300
C	3.96694300	1.12517400	-0.02066200
C	4.99963000	1.74341500	0.85747900
O	3.46313600	-0.00996900	0.54884600
H	5.26133500	2.73425900	0.48011700
H	5.89775000	1.11293100	0.86265700
H	4.64524500	1.80544900	1.89221900

20_Pt

E = -1075.817012 au

H = -1075.459275 au

G = -1075.533222 au

C	-1.83244100	2.44300900	1.84909100
C	-0.57151700	1.75812300	2.26038200
H	-0.65101800	0.68477900	2.45285600
H	-2.63188800	2.29938000	2.58630800
H	-1.67757200	3.51430400	1.68393800
C	0.58868600	2.39262800	2.42367700
H	1.48381300	1.87199800	2.76445000
H	0.68339700	3.46717800	2.25636700
O	-3.26736000	0.17111200	1.59749300
C	-2.92867000	0.75485800	0.59851400
C	-3.22751200	0.28042100	-0.81097700
O	-2.29465800	1.93664900	0.57291000
H	-4.01641700	-0.47450600	-0.78958100
H	-3.51460600	1.13312900	-1.43929700
N	0.36818700	0.93494800	-0.97229500
C	1.62966100	0.67734900	-0.54541000
C	2.66457100	1.62992600	-0.61569500
C	2.34712100	2.88851500	-1.16669200
C	1.06525500	3.13446000	-1.60479200
C	0.09727100	2.12475900	-1.48644700
H	3.12074200	3.65192100	-1.24378200
H	0.78941600	4.09191800	-2.03922300
H	-0.92808300	2.29653400	-1.80985100
N	0.86702200	-1.52208000	0.07119500
C	1.09664200	-2.73389300	0.57241700
C	2.35709400	-3.11883800	1.04308800
C	3.39844600	-2.21955200	0.99905100
C	3.18353500	-0.93032200	0.47333000
C	1.89118600	-0.61610400	0.00792700
H	0.25351900	-3.41807600	0.60559600
H	2.48748800	-4.12158500	1.44107400
H	4.38789300	-2.49212900	1.36436500
C	4.21511300	0.05926900	0.39369200

C	3.96668300	1.28948700	-0.13013400
C	-1.94659300	-2.51244800	-0.07526500
H	-1.86071700	-2.68619800	1.00660300
H	5.20769400	-0.19905100	0.75966700
H	4.75698800	2.03639200	-0.19198700
H	-1.52944300	-3.35852500	-0.63892100
H	-3.01301500	-2.42867000	-0.31739200
Pt	-0.93662600	-0.79832100	-0.55293400
H	-2.40887700	-0.16181300	-1.49237200

16TS_Pt

E = -1075.803298 au

H = -1075.448843 au

G = -1075.520442 au

C	-1.21840700	2.70811700	2.01957400
C	-0.05193600	1.87229100	2.43336700
H	-0.27956500	0.86334000	2.78677000
H	-2.01033700	2.71223100	2.77796300
H	-0.91786200	3.73730100	1.79790100
C	1.20612700	2.31179200	2.40138200
H	2.03931400	1.69406000	2.73618100
H	1.45006800	3.32475900	2.07493700
O	-2.87453700	0.58059800	1.87583400
C	-2.52673600	1.11176300	0.84746400
C	-2.85550100	0.60117800	-0.53322500
O	-1.77527100	2.22137500	0.77465600
H	-3.80875500	0.06734300	-0.52117300
H	-2.86623600	1.40921000	-1.27249600
N	0.39528800	0.82068800	-1.10294300
C	1.62125600	0.45357900	-0.64981500
C	2.75146700	1.28613200	-0.77656200
C	2.56844000	2.53737600	-1.40003600
C	1.31923400	2.89660100	-1.85304100
C	0.25144100	2.00269100	-1.68160100
H	3.41933100	3.20768800	-1.51753200
H	1.14557400	3.85299900	-2.33949100
H	-0.75002500	2.26223100	-2.02131300
N	0.64212200	-1.60847400	0.11357500
C	0.74490100	-2.79427500	0.70594700
C	1.95868100	-3.27959000	1.20609900
C	3.08886000	-2.50114400	1.08949800
C	3.00942900	-1.23644300	0.47202200
C	1.75198000	-0.82358400	-0.01229100
H	-0.16942100	-3.37871200	0.78742600
H	1.98912600	-4.25765300	1.67855600
H	4.04766800	-2.85166600	1.47062400
C	4.14088000	-0.37244900	0.32312700
C	4.01629600	0.84157700	-0.27650000
C	-2.36342100	-2.25325900	-0.04224500
H	-2.32794300	-2.31001400	1.05505900
H	5.10457700	-0.71130500	0.70070300
H	4.87912900	1.49676800	-0.38803200
H	-1.97421400	-3.17572300	-0.49557500
H	-3.40787100	-2.13339900	-0.34739800

Pt	-1.15210300	-0.69854900	-0.60473500
H	-2.23987500	-0.39806000	-1.71111600

21_Pt

E = -1075.815608 au

H = -1075.460400 au

G = -1075.536159 au

C	-4.29576800	0.85576800	1.37806900
C	-5.67916400	1.36977200	1.21683100
H	-5.81237200	2.19085900	0.50994800
H	-3.59846300	1.61748600	1.75153000
H	-4.24895100	-0.01328600	2.04584600
C	-6.71104300	0.89356000	1.91012900
H	-7.71007400	1.31093300	1.80586100
H	-6.59540200	0.07307500	2.61919700
O	-1.81595400	-0.09713700	0.92873900
C	-2.59796800	-0.00678100	-0.03029200
C	-2.09027600	-0.44778500	-1.36346300
O	-3.81939100	0.44589800	0.05823100
H	-2.66841700	-1.29102400	-1.75859700
H	-2.11171600	0.35644100	-2.11048200
N	0.66423000	1.15604900	-0.68245500
C	1.88590000	1.22316100	-0.09270700
C	2.60113400	2.43551300	0.00869600
C	2.00167500	3.59239900	-0.52815000
C	0.76151300	3.50716100	-1.12003000
C	0.12393500	2.25961200	-1.17661600
H	2.52763100	4.54474600	-0.46798800
H	0.27371600	4.38112500	-1.54374700
H	-0.85636800	2.15771700	-1.64221800
N	1.74743700	-1.13925900	0.34021300
C	2.25935400	-2.25560200	0.83803600
C	3.50970500	-2.29959300	1.47085000
C	4.23997800	-1.13850100	1.58210900
C	3.72068500	0.06496500	1.06467800
C	2.45438000	0.01821800	0.44415600
H	1.65803800	-3.15756200	0.73691800
H	3.88052500	-3.24403900	1.86038600
H	5.21562400	-1.13586800	2.06704000
C	4.42249000	1.30948600	1.14925000
C	3.88453000	2.44965900	0.64170200
C	-0.88522000	-2.83746900	-0.54426500
H	-1.62970400	-2.87420300	0.26320300
H	5.39887100	1.32250200	1.63160300
H	4.42036900	3.39549300	0.70857600
H	-0.04939400	-3.50483800	-0.30077600
H	-1.33969200	-3.18408800	-1.47790200
Pt	-0.21279800	-0.90317500	-0.65772100
H	0.41007700	-1.36671800	-1.99011100

17TS_Pt

E = -1075.805222 au

H = -1075.451066 au

G = -1075.525973 au

C	-4.37362100	1.00352500	0.60815300
C	-3.50577000	1.88305000	1.44238800
H	-2.75803000	1.37367700	2.05646600
H	-4.91742300	0.27080300	1.21619900
H	-5.08469300	1.58398800	0.01148100
C	-3.63071900	3.20926500	1.48159900
H	-3.00704200	3.82667300	2.12584800
H	-4.38938400	3.72856400	0.89363400
O	-3.11529300	-1.28805100	1.18534700
C	-2.97611300	-0.84462300	0.06519100
C	-2.10304400	-1.44116200	-0.99275400
O	-3.57375800	0.28536700	-0.36219300
H	-2.36451500	-2.49843000	-1.10998400
H	-2.21911100	-0.93488700	-1.95886400
N	0.06719900	0.89829800	-0.58103900
C	1.31554100	1.35343900	-0.26299400
C	1.65305400	2.71837000	-0.33850500
C	0.64999300	3.61720100	-0.75894000
C	-0.60144700	3.14331200	-1.07592900
C	-0.85797600	1.76829000	-0.97553600
H	0.87978400	4.68018300	-0.82664600
H	-1.39798400	3.80866900	-1.39808900
H	-1.84480000	1.36819800	-1.20434100
N	1.95422000	-0.90833300	0.20645900
C	2.86113400	-1.80550600	0.56779400
C	4.17538900	-1.45629100	0.90911400
C	4.54563700	-0.13098200	0.86608900
C	3.60567300	0.84526600	0.47593000
C	2.30630500	0.40399400	0.14997200
H	2.54044800	-2.84628800	0.58621100
H	4.87766700	-2.23288000	1.20020000
H	5.55869300	0.17381300	1.12653900
C	3.91703800	2.23885600	0.39595100
C	2.97702400	3.13957600	0.00384500
C	-0.44602200	-3.01043200	0.75069600
H	-1.10596000	-2.56744000	1.50858700
H	4.92444500	2.56214800	0.65391900
H	3.21602200	4.20024700	-0.05837400
H	0.50829500	-3.34691100	1.16665200
H	-0.96511700	-3.84604100	0.27305300
Pt	-0.13092200	-1.26080000	-0.37320500
H	0.05064100	-2.68084500	-0.98803700

22_Pt

E = -1075.830042 au

H = -1075.473026 au

G = -1075.545213 au

C	-4.00391400	1.50545500	0.90696100
C	-2.98327700	1.85444100	1.93667100
H	-2.48386000	1.01142400	2.42136600
H	-4.77051700	0.82798400	1.30156900
H	-4.48241600	2.39827200	0.49144900
C	-2.69149500	3.10810600	2.28229300

H	-1.96229600	3.33578800	3.05775400
H	-3.19828200	3.95887300	1.82351900
O	-3.46358100	-1.12260300	0.84664100
C	-3.09715900	-0.45239100	-0.09632200
C	-2.23474900	-0.94395200	-1.20567500
O	-3.36624300	0.86355400	-0.22255500
H	-2.55490300	-1.94918800	-1.50420600
H	-2.24464000	-0.28929600	-2.08376900
N	0.19414700	0.86920400	-0.70519700
C	1.48674200	1.16051300	-0.35873700
C	2.02274200	2.45406300	-0.49907700
C	1.17782900	3.46382700	-1.00238900
C	-0.12480500	3.15799100	-1.31975100
C	-0.58917500	1.84559400	-1.15892700
H	1.56389000	4.47501000	-1.12592200
H	-0.81029800	3.91148700	-1.69828200
H	-1.62336900	1.59337200	-1.37589000
N	1.72377200	-1.10959600	0.32248600
C	2.44445200	-2.09929300	0.83066300
C	3.78001800	-1.93300000	1.22721100
C	4.37186600	-0.69729000	1.08755600
C	3.62903800	0.37513500	0.55228100
C	2.29625900	0.11390800	0.17862200
H	1.95019300	-3.06434300	0.93245300
H	4.32455200	-2.77859500	1.63901800
H	5.40662500	-0.53659900	1.38805700
C	4.15715300	1.69348200	0.38226200
C	3.38324400	2.69181300	-0.12177400
C	-0.97131900	-3.33811900	0.25142300
H	-1.33617400	-2.60133700	0.98598100
H	5.19048800	1.88268000	0.66924700
H	3.78528800	3.69632300	-0.24534500
H	-0.26506400	-4.01688500	0.73510300
H	-1.85823100	-3.86120200	-0.11784500
Pt	-0.32406700	-1.08978700	-0.41207900
H	-0.46130600	-2.99696300	-0.70553000

23_Pt

E = -1035.367579 au

H = -1035.060194 au

G = -1035.128673 au

N	0.88507800	1.36009300	-0.11447100
C	2.17727700	0.95941800	-0.01281700
C	3.25726900	1.85977500	0.00215400
C	2.94711400	3.23222900	-0.09260300
C	1.63048600	3.62788400	-0.19133600
C	0.61746100	2.65498300	-0.19960800
Pt	-0.46959500	-0.32119600	-0.10422500
H	3.75095700	3.96751700	-0.08444600
H	1.36223600	4.67873100	-0.26207900
H	-0.43494200	2.92648200	-0.27571500
N	1.32390000	-1.26780700	0.07024200
C	1.50897200	-2.58224100	0.16721200
C	2.78585600	-3.14585000	0.28675100

C	3.89388600	-2.32644100	0.30478400
C	3.72664600	-0.93117700	0.20268100
C	2.41256500	-0.44350600	0.08683000
H	0.61414000	-3.19979200	0.15064000
H	2.88085500	-4.22565800	0.36380600
H	4.89526800	-2.74500500	0.39841400
C	4.81231700	0.00394600	0.21276100
C	4.58797700	1.34300400	0.11586700
H	5.82645700	-0.38291700	0.30158100
H	5.42050700	2.04506000	0.12561500
C	-5.13503600	0.11839500	-0.55755300
C	-5.55058200	0.60891000	0.78357000
H	-6.08572700	-0.10068500	1.41688800
C	-5.31969900	1.85454200	1.19444500
H	-5.66261200	2.21076600	2.16354900
H	-4.78766200	2.57082800	0.56697000
O	-2.44790900	0.41093000	-0.28493400
C	-2.93681500	-0.75113400	-0.27378200
C	-1.90424700	-1.80095800	-0.10240500
O	-4.19520100	-1.00462100	-0.41789100
H	-1.89531400	-2.51459100	-0.93540100
H	-2.02533700	-2.33723700	0.84758300
H	-5.96038900	-0.32767100	-1.12007600
H	-4.65668400	0.90028700	-1.15726900

14TS_Pd

E = -1084.330835 au

H = -1083.978732 au

G = -1084.053405 au

N	0.64275400	1.26853500	-0.15140400
C	1.94566700	0.88539500	-0.14052000
C	3.00244200	1.82115500	-0.16470900
C	2.66138000	3.18789100	-0.22087300
C	1.33642100	3.55947900	-0.25996400
C	0.35352400	2.55872100	-0.22408800
Pd	-0.73787800	-0.47330300	-0.12480700
H	3.45267400	3.93661500	-0.24224800
H	1.04075400	4.60376600	-0.31796100
H	-0.70472600	2.82162700	-0.26413600
N	1.21819700	-1.41157800	-0.13619200
C	1.48705400	-2.71002100	-0.12875600
C	2.79455000	-3.21444400	-0.10366200
C	3.84694800	-2.32726300	-0.09165100
C	3.59380100	-0.94078100	-0.10335000
C	2.24711100	-0.52036000	-0.12082500
H	0.63134500	-3.38386200	-0.14624900
H	2.95630600	-4.28909500	-0.09789300
H	4.87709900	-2.68197000	-0.07679800
C	4.64191600	0.03400000	-0.10698400
C	4.35754800	1.36253300	-0.13990900
C	-1.77573800	-2.21438400	-0.36611300
H	-1.55207000	-2.81832000	0.52498300
H	5.67400800	-0.31343600	-0.09080200
H	5.15665300	2.10247600	-0.15230200

H	-1.37882800	-2.68373100	-1.27489900
H	-2.85764800	-2.08037800	-0.45654000
C	-2.43929400	0.43574700	0.79319300
C	-2.07945700	-0.06362600	2.13025600
H	-2.49344100	-1.03812200	2.39619700
H	-2.30702000	1.51632100	0.65096000
C	-1.30319900	0.61541300	2.98436100
H	-1.05764100	0.21690500	3.96570200
H	-0.90544600	1.60188200	2.74219600
O	-3.55726000	1.01496100	-1.52411800
C	-4.24109100	0.41641500	-0.72344900
C	-5.64598200	-0.03847900	-0.90348000
O	-3.74370800	0.04707100	0.48720700
H	-6.04552400	0.35938800	-1.83863600
H	-6.26463700	0.28158800	-0.05782200
H	-5.67735200	-1.13519500	-0.93011400
H	-1.92263200	0.17620500	-0.94093600

19_Pd

E = -1043.937834 au

H = -1043.631393 au

G = -1043.700624 au

N	0.11058100	1.02869200	0.06055600
C	1.46489700	1.13618000	-0.00462900
C	2.12253200	2.38335000	-0.02822300
C	1.32152200	3.54193600	0.03278900
C	-0.04612300	3.41872900	0.12003600
C	-0.61590400	2.13577600	0.13076000
H	1.79517300	4.52309300	0.01759600
H	-0.69204400	4.29056400	0.18203800
H	-1.69233200	2.00475700	0.21735900
N	1.57636100	-1.25700100	0.01531600
C	2.27691200	-2.38359300	-0.00325200
C	3.67724100	-2.40569500	-0.07407500
C	4.36084100	-1.21192300	-0.12495200
C	3.64554900	0.00188600	-0.10413300
C	2.23877100	-0.07079400	-0.03514300
H	1.71195400	-3.31281100	0.03982500
H	4.19886900	-3.35913500	-0.08653000
H	5.44878500	-1.19168300	-0.17924700
C	4.28383700	1.28239800	-0.14361000
C	3.55112200	2.42686100	-0.10500600
H	5.37077100	1.32029400	-0.20004800
H	4.03941200	3.40021100	-0.12945500
C	-2.74259700	-1.03733900	0.23104900
C	-2.31573700	-2.23299300	-0.37037900
H	-2.53425200	-2.39097300	-1.42776000
H	-2.85279100	-0.91142800	1.31185500
C	-1.34333500	-2.99289900	0.30062400
H	-0.87528600	-3.82777400	-0.21965000
H	-1.35441500	-3.06469800	1.39158900
O	-3.72826300	1.26295400	1.13775900
C	-4.09042500	0.88182300	0.05501800
C	-5.12368000	1.48907700	-0.82746400

O	-3.55073900	-0.23715900	-0.53648800
H	-5.45247900	2.44345100	-0.41101900
H	-5.98321100	0.81150800	-0.90471300
H	-4.73241100	1.62608400	-1.84190200
Pd	-0.56445400	-1.02492100	0.05657200

14TS_Ni

E = -1127.400611 au

H = -1127.047554 au

G = -1127.119721 au

N	0.31516400	1.15946000	-0.06174200
C	1.65367100	0.93550800	-0.07797400
C	2.60570000	1.97246400	-0.04701900
C	2.11513300	3.29379500	-0.03396700
C	0.75553400	3.51368200	-0.06975200
C	-0.11653100	2.41352200	-0.08289000
Ni	-0.72833900	-0.58653600	-0.14619600
H	2.81537700	4.12818800	-0.01099400
H	0.34603200	4.52032400	-0.08687000
H	-1.19676300	2.56127200	-0.12517900
N	1.11290600	-1.37543100	-0.26401900
C	1.48554400	-2.64453500	-0.36156900
C	2.83046000	-3.04331900	-0.35667400
C	3.81680300	-2.08674200	-0.25874300
C	3.45677600	-0.72744500	-0.16496700
C	2.08125800	-0.42547400	-0.16119500
H	0.69136300	-3.38356300	-0.45469700
H	3.07344700	-4.09962300	-0.43706000
H	4.86968100	-2.36716400	-0.26053500
C	4.40648700	0.34246200	-0.09166700
C	3.99853300	1.63976600	-0.04261500
C	-1.59810500	-2.16467100	-0.80430500
H	-1.38426500	-2.93228000	-0.04629900
H	5.46717800	0.09501800	-0.09081000
H	4.72720700	2.44831400	-0.00356900
H	-1.11250800	-2.40391500	-1.75812400
H	-2.68011000	-2.08576500	-0.94351000
C	-2.31340700	0.04186800	0.82477300
C	-1.81274400	-0.80353100	1.90520000
H	-2.30589400	-1.76955700	2.02710900
H	-2.16466900	1.12140800	0.92876200
C	-0.74230900	-0.47485800	2.65297600
H	-0.35160200	-1.15379000	3.40757000
H	-0.25739100	0.49750600	2.56493100
O	-3.56962000	1.36343400	-1.04978000
C	-4.19283500	0.49376200	-0.49101000
C	-5.59919600	0.07961200	-0.74661400
O	-3.62024600	-0.27006100	0.48977800
H	-5.61956300	-0.94748100	-1.13213800
H	-6.05321300	0.75328700	-1.47613400
H	-6.17608400	0.08559400	0.18508500
H	-1.75690100	-0.01514200	-0.98564700

19_Ni

E = -1087.005884 au

H = -1086.698774 au

G = -1086.766316 au

N	0.09799600	0.81234000	-0.15803400
C	-1.23195700	1.06846600	-0.02488600
C	-1.77077600	2.36585400	0.01937900
C	-0.86660100	3.44025400	-0.10659900
C	0.47349500	3.17651800	-0.27982500
C	0.92070700	1.84567800	-0.29950400
H	-1.23713800	4.46449500	-0.08035200
H	1.19659800	3.97816800	-0.40507500
H	1.97201200	1.62089600	-0.45879700
N	-1.49956400	-1.28390100	-0.05034700
C	-2.27498200	-2.36142800	-0.01627500
C	-3.67028000	-2.28710600	0.11348000
C	-4.27630300	-1.05356700	0.21211500
C	-3.48407500	0.11156000	0.17371100
C	-2.09489800	-0.06481700	0.04182000
H	-1.78017400	-3.32631900	-0.09759500
H	-4.25222000	-3.20486000	0.13268500
H	-5.35775300	-0.96866400	0.31333100
C	-4.00896400	1.44231400	0.24747900
C	-3.18650000	2.52427800	0.17044400
H	-5.08487400	1.57147200	0.35652400
H	-3.59451600	3.53306600	0.21605600
C	2.46918700	-1.17559600	-0.23057500
C	1.95663300	-2.35932100	0.31454400
H	2.13088900	-2.55917500	1.37405500
H	2.64882300	-1.02747800	-1.30000600
C	0.93763700	-3.01041700	-0.38967000
H	0.40262800	-3.82723000	0.09313900
H	0.94682300	-3.03425800	-1.48424400
O	4.02255600	0.82118500	-1.10750400
C	4.12075200	0.48982300	0.04706800
C	5.09947300	0.99457500	1.04973800
O	3.28976600	-0.44585700	0.60802300
H	5.58146900	1.89879600	0.67148700
H	5.86728100	0.22930300	1.22163900
H	4.61377000	1.18639500	2.01244300
Ni	0.44941100	-1.11138200	-0.12019500