

Supporting Information for

Theoretical Insight into C-H and C-C Scission Mechanism of Ethane on Tetrahedral Pt₄ Subnanocluster

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Species	BPW91/Lanl2tz, 6-311++G(d, p)			BPW91/Lanl2tz, aug-cc-pvtz// BPW91/Lanl2tz, 6-311++G(d, p)	
	ZPE	E_c	E_r	E_c	E_r
³ Pt ₄ +C ₂ H ₆	0.07450	-556.67429	0.0	-556.68168	0.0
³ 1-IM1	0.07350	-556.69145	-45.0	-556.70552	-62.6
³ 1-TS1	0.07098	-556.69046	-42.4	-556.70441	-59.7
³ 1-IM2	0.07243	-556.71522	-107.5	-556.73164	-131.2
³ 1-TS2	0.07022	-556.70613	-83.6	-556.72032	-101.4
³ 1-IM3	0.07006	-556.72495	-133.0	-556.74491	-166.0
³ 1-TS3	0.06823	-556.72537	-134.1	-556.74553	-167.6
³ 1-IM4	0.06942	-556.74043	-173.7	-556.76006	-205.8
³ 1-TS4	0.06758	-556.73930	-170.7	-556.75938	-204.0
³ 1-IM5	0.06848	-556.74503	-185.7	-556.76508	-219.0
³ 1-TS5	0.06721	-556.69705	-59.8	-556.71795	-95.2
³ 1-IM8	0.06860	-556.73354	-155.6	-556.75363	-188.9
³ 1-TS6	0.06557	-556.71282	-101.2	-556.73342	-135.9
³ 1-IM9	0.06771	-556.73186	-151.1	-556.75266	-186.4
³ 1-IM6+H ₂	0.06371	-556.70116	-70.5	-556.71584	-89.7
³ 1-IM7+C ₂ H ₄	0.06583	-556.67501	-1.9	-556.68875	-18.6
³ 1-IM10+H ₂	0.06333	-556.68088	-17.3	-556.69473	-34.3
¹ Pt ₄ +C ₂ H ₆	0.07444	-556.65593	48.2	-556.66333	48.2
¹ 1-IM1	0.07354	-556.674791	-1.3	-556.68435	-7.0
¹ 1-TS1	0.07074	-556.673711	1.5	-556.67778	10.2
¹ 1-IM2	0.072321	-556.69582	-56.5	-556.79589	-110.0
¹ 1-TS2	0.06998	-556.68877	-38.0	-556.70296	-55.9
¹ 1-IM3	0.07002	-556.71630	-110.3	-556.80590	-142.3
¹ 1-TS3	0.06822	-556.71758	-113.6	-556.80573	-146.6
¹ 1-IM4	0.06956	-556.73985	-172.1	-556.75897	-202.9
¹ 1-TS4	0.06740	-556.73456	-158.2	-556.82135	-189.7
¹ 1-IM5	0.06858	-556.74370	-182.2	-556.83230	-215.4
¹ 1-TS5	0.06720	-556.693478	-50.4	-556.71321	-82.8
¹ 1-IM8	0.06869	-556.72658	-137.3	-556.81508	-169.9
¹ 1-TS6	0.066454	-556.707262	-86.6	-556.72716	-119.4
¹ 1-IM9	0.06776	-556.72937	-144.6	-556.81751	-178.7

¹¹ I-M6+H ₂	0.06350	-556.68250	-21.6	-556.76079	-41.0
⁵ Pt ₄ +C ₂ H ₆	0.07457	-556.67239	5.0	-556.67978	5.0
⁵¹ I-M1	0.07439	-556.68825	-42.2	-556.70217	-53.8
⁵¹ -TS1	0.07087	-556.68339	-29.4	-556.69873	-44.8
⁵¹ -IM2	0.07243	-556.69257	-53.5	-556.70716	-66.9

Table S2: Zero-point energies (ZPE) (hartree), total energies (E_c) (hartree) corrected by ZPE, and relative energies (E_r) (kJ mol⁻¹) of various species plus H₂ with respect to the reactants [Pt₄ + C₂H₄] in the C-H activation of C₂H₄ by Pt₄ clusters calculated at the BPW91/Lanl2tz, 6-311++G(d, p) and BPW91/Lanl2tz, aug-cc-pvtz//BPW91/Lanl2tz, 6-311++G(d, p) levels of theory.

Species	BPW91/Lanl2tz, 6-311++G(d, p)			BPW91/Lanl2tz, aug-cc-pvtz// BPW91/Lanl2tz, 6-311++G(d, p)	
	ZPE	E_c	E_r	E_c	E_r
³ Pt ₄ + C ₂ H ₄	0.05134	-555.45968	0.0	-555.51879	0.0
³ 2-TS1	0.04844	-555.49393	-89.9	-555.55691	-107.7
³ 2-IM1	0.04969	-555.51097	-134.7	-555.57603	-154.6
³ 2-TS2	0.04767	-555.50146	-109.7	-555.56436	-129.3
³ 2-IM2	0.04884	-555.51296	-139.2	-555.57790	-161.8
³ 2-TS3	0.04320	-555.49583	-94.9	-555.55990	-129.3
³ 2-IM3	0.04475	-555.50734	-125.1	-555.57217	-157.4
³ 2-TS4	0.04326	-555.50307	-113.9	-555.56726	-148.5
³ 2-IM4	0.04449	-555.51905	-155.9	-555.58408	-189.4
³ 2-TS5	0.04860	-555.49629	-96.1	-555.56317	-123.7
³ 2-IM5	0.04012	-555.48516	-66.9	-555.54071	-87.0
³ 1-IM7+C ₂ H ₂	0.04240	-555.44284	44.2	-555.49874	29.2
³ 2-IM6	0.04771	-555.50432	-117.2	-555.56989	-143.7
³ 2-TS6	0.04579	-555.48924	-77.6	-555.55408	-107.2
³ 2-IM7	0.04947	-555.52090	-160.7	-555.58915	-189.7
³ 2-TS7	0.04393	-555.49649	-96.7	-555.56090	-130
³ 2-IM8	0.04613	-555.53045	-185.8	-555.59699	-219.0
³ 2-TS8	0.04313	-555.51114	-135.1	-555.57521	-169.7
³ 2-IM9	0.04519	-555.53374	-194.5	-555.59934	-227.6
³ 2-IM10+H ₂	0.4053	-555.47954	-52.1	-555.53716	-76.6
¹ Pt ₄ +C ₂ H ₄	0.06118	-555.60758	48.2	-555.67688	48.2
¹ 2-TS1	0.004804	-555.64392	-47.2	-555.71700	-65.7
¹ 2-IM1	0.04945	-555.49186	-84.5	-555.56987	-139.1
¹ 2-TS2	0.04741	-555.48339	-62.3	-555.73534	-115.4
¹ 2-IM2	0.04872	-555.50302	-113.8	-555.58155	-171.7
¹ 2-TS3	0.04325	-555.49064	-81.3	-555.55435	-114.6
¹ 2-IM3	0.04466	-555.50615	-122.0	-555.56956	-150.8
¹ 2-TS4	0.04303	-555.50375	-115.7	-555.56185	-134.9
¹ 2-IM4	0.04542	-555.53182	-189.4	-555.59825	-224.2
¹ 2-IM5	0.04016	-555.47014	-27.5	-555.52611	-48.6
¹ 2-IM6	0.05031	-555.51601	-147.9	-555.58432	-174.8
¹ 2-TS7	0.04387	-555.49782	-100.1	-555.73912	-134.7
¹ 2-TS5	0.04860	-555.48543	-67.6	-555.73634	-114.9

¹ 1-IM7+C ₂ H ₂	0.04262	-555.4366	60.6	-555.49690	34.6
¹ 2-TS6	0.04537	-555.47715	-45.9	-555.54206	-76.8
¹ 2-IM7	0.04944	-555.51385	-142.2	-555.58155	-169.8
¹ 2-IM8	0.04571	-555.52760	-178.3	-555.77023	-211.5
¹ 2-TS8	0.04335	-555.50588	-121.3	-555.56971	-154.7
¹ 2-IM9	0.04509	-555.52951	-183.3	-555.59454	-215.3
¹ 2-IM10+H ₂	0.04032	-555.46944	-25.6	-555.52517	-45.7

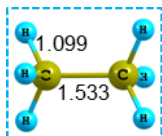
Table S3: Zero-point energies (ZPE) (hartree), total energies (E_c) (hartree) corrected by ZPE, and relative energies (E_r) (kJ mol⁻¹) various species with respect to the reactants [Pt₄+ C₂H₆] in the C-C bond activation of C₂H₆ by Pt₄ cluster calculated at the BPW91/Lanl2tz, aug-cc-pvtz//BPW91/Lanl2tz, 6-311++G(d, p) levels of theory

Species	BPW91/Lanl2tz, 6-311++G(d, p)			BPW91/ Lanl2tz, aug-cc-pvtz// BPW91/Lanl2tz, 6-311++G(d, p)	
	ZPE	E_c	E_r	E_c	E_r
³³ -TS1	0.07075	-556.65788	37.9	-556.74593	17.1
³³ -IM2	0.07194	-556.71663	-117.9	-556.80371	-131.5
³³ -TS2	0.06736	-556.67604	-10.2	-556.76215	-34.4
³³ -IM3	0.06801	-556.68177	-25.4	-556.76847	-49.3
³³ -TS3	0.06774	-556.66257	25.5	-556.74947	-0.1
³³ -IM4	0.06908	-556.68506	-34.2	-556.76753	-44.0
³³ -IM5+CH ₄	0.06871	-556.68522	-28.7	-556.69858	-44.4
³³ -TS4+CH ₄	0.06854	-556.66176	32.9	-556.67515	17.1
³³ -IM6+CH ₄	0.06974	-556.69624	-57.6	-556.71011	-74.6
³³ -TS5	0.06926	-556.68986	-40.9	-556.77699	-68.4
³³ -IM7	0.06913	-556.73419	-157.3	-556.82247	-188.2
³³ -TS6	0.06708	-556.70822	-89.1	-556.79533	-122.3
³³ -IM8	0.06880	-556.73432	-157.6	-556.82337	-188.8
³³ -TS7	0.06606	-556.69625	-57.7	-556.78355	-94.0
³³ -IM9	0.06602	-556.73633	-162.9	-556.82412	-200.6
³³ -TS8	0.06565	-556.69758	-61.2	-556.78474	-98.2
³³ -IM10	0.06867	-556.73311	-154.4	-556.82170	-187.3
³³ -TS9	0.06620	-556.71387	-103.9	-556.79981	-136.4
³³ -IM11	0.06928	-556.73520	-159.9	-556.82331	-190.0
³³ -TS10	0.06760	-556.71108	-96.6	-556.79765	-127.0
³³ -IM12	0.06929	-556.71040	-94.8	-556.79867	-125.2
³³ -TS11	0.065739	-556.65434	52.4	-556.73987	19.8
³³ -IM13	0.06689	-556.70791	-88.3	-556.79529	-122.7
³³ -TS12	0.06565	-556.70869	-90.3	-556.79428	-123.3
³³ -IM14	0.06663	-556.71274	-100.9	-556.79989	-135.4
³³ -TS13	0.06618	-556.69784	-61.8	-556.78337	-93.2
³³ -IM15	0.06902	-556.70054	-68.9	-556.78819	-98.4
¹³ -IM2	0.07182	-556.69661	-64.8	-556.79740	-115.3
¹³ -TS2	0.06772	-556.66681	14.3	-556.75369	-11.3
¹³ -IM3	0.06847	-556.67236	-0.5	-556.75978	-25.3
¹³ -TS3	0.06805	-556.65824	37.0	-556.74933	1.0
¹³ -IM4	0.06903	-556.680556	-22.2	-556.69356	-31.2
¹³ -IM5+CH ₄	0.06865	-556.68073	-16.7	-556.69406	-32.5
¹³ -TS4+CH ₄	0.06850	-556.65189	58.8	-556.66518	43.3
¹³ -IM6+CH ₄	0.06991	-556.68443	-26.6	-556.69799	-42.8
¹³ -TS5	0.06617	-556.65041	57.2	-556.73692	31.3

¹³ -IM7	0.06908	-556.72192	-125.1	-556.81024	-156.2
¹³ -TS6	0.06692	-556.71305	-101.8	-556.79997	-134.9
¹³ -IM8	0.06838	-556.72754	-139.8	-556.81632	-174.0
¹³ -TS7	0.06641	-556.68921	-39.2	-556.77614	-73.6
¹³ -IM9	0.06599	-556.73681	-164.1	-556.82419	-200.9
¹³ -TS8	0.06563	-556.69521	-54.9	-556.78214	-91.5
¹³ -IM10	0.06836	-556.72903	-143.7	-556.81693	-175.6
¹³ -TS9	0.06681	-556.71273	-100.9	-556.79881	132.1
¹³ -IM11	0.06902	-556.72342	-129.0	-556.81108	-158.5
¹³ -TS10	0.06775	-556.70852	-89.9	-556.79513	-120.0
¹³ -IM12	0.06986	-556.70755	-87.3	-556.79574	-116.0
¹³ -TS11	0.06617	-556.65041	57.2	-556.73592	31.3
¹³ -IM13	0.06710	-556.71393	-109.6	-556.73439	-138.4
¹³ -TS12	0.06534	-556.69849	-69.1	-556.78347	-95.7
¹³ -IM14	0.06660	-556.70805	-94.2	-556.79438	-121.0
¹³ -TS13	0.06600	-556.68506	-33.8	-556.77025	-59.3
¹³ -IM15	0.06856	-556.68593	-36.1	-556.77391	-60.3

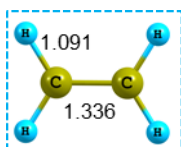
Table S4: Snapshot and standard orientation of all the species in the gas phase calculated at the BPW91/6-311++G(d, p), Lan12tz level. Distance lengths are reported in Å

C₂H₆



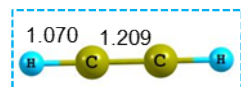
C	0.76641500	-0.00000100	-0.00000300
C	-0.76641300	-0.00000100	0.00000300
H	1.16844700	0.02235700	1.02295300
H	1.16837600	0.87474500	-0.53085700
H	1.16838200	-0.89709700	-0.49214400
H	-1.16837900	0.89711300	0.49211100
H	-1.16838500	-0.87472500	0.53088800
H	-1.16845100	-0.02238100	-1.02295200

C₂H₄



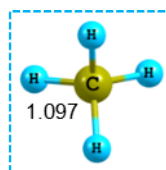
C	0.66808300	0.00000000	-0.00000400
C	-0.66808300	0.00000000	-0.00000400
H	1.24255700	-0.92781400	0.00012400
H	1.24254700	0.92782100	-0.00010200
H	-1.24254900	-0.92782000	-0.00010200
H	-1.24255500	0.92781500	0.00012400

C₂H₂



C	0.00000000	0.00000000	0.60457800
H	0.00000000	0.00000000	1.67420700
C	0.00000000	0.00000000	-0.60457800
H	0.00000000	0.00000000	-1.67420700

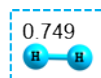
CH₄



H	-0.39414700	-1.02353800	0.00000000
H	-0.35112300	0.52694300	0.89556800

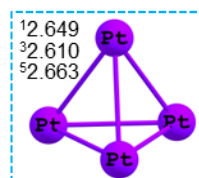
H	-0.35112300	0.52694300	-0.89556800
C	0.00000000	0.00000700	0.00000000
H	1.09639300	-0.03039000	0.00000000

H₂



H	0.00000000	0.00000000	0.37441600
H	0.00000000	0.00000000	-0.37441600

Pt₄



¹Pt₄

Pt	0.94377100	-0.94347900	-0.90000100
Pt	-0.94375600	0.94348500	-0.90000900
Pt	0.94378500	0.94345100	0.90001500
Pt	-0.94379900	-0.94345600	0.89999500

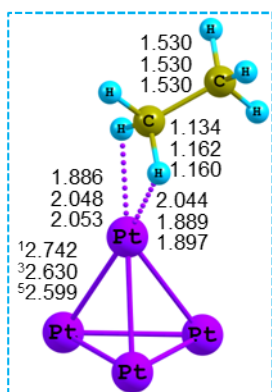
³Pt₄

Pt	1.35989600	-0.00796100	-0.90420300
Pt	-0.00205000	-1.29181400	0.91429200
Pt	-1.35861800	-0.00527900	-0.90592400
Pt	0.00077100	1.30505500	0.89583500

⁵Pt₄

Pt	0.98484400	0.50980400	1.15978900
Pt	-0.98503600	-1.15967700	0.50977600
Pt	0.98498900	-0.50990700	-1.15964100
Pt	-0.98479700	1.15978000	-0.50992300

1-IM1



¹I-IM1

Pt	-1.10360800	-0.03100800	1.32883200
Pt	-0.32191200	1.51127500	-0.59483400
Pt	-0.86459300	-1.05792800	-0.98750600
Pt	1.35933000	-0.41660200	0.18638900
C	3.65033800	-0.38975000	0.60363600
H	3.23384600	-1.17983400	-0.09590500
H	2.85409800	0.31366200	1.07579500
C	4.69231800	0.45848700	-0.12751700
H	5.50947400	-0.17409400	-0.50391900
H	4.24651700	0.98333000	-0.98135000
H	5.13050800	1.20871400	0.54605500
H	4.04971200	-0.93081200	1.47128500

³I-IM1

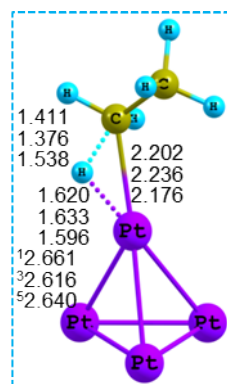
Pt	0.98943400	-0.89069600	-1.07131800
Pt	0.56653500	1.56477200	-0.30888800
Pt	0.77792000	-0.33465400	1.43491000
Pt	-1.37730700	-0.38993000	-0.04005000
C	-3.70395200	-0.40181500	-0.04983200
H	-3.02134500	-0.37090600	0.88992300
H	-3.16022000	-0.53640700	-1.03657800
C	-4.58353800	0.84906100	-0.08413700
H	-5.14320700	0.95824700	0.85566700
H	-3.98070300	1.75338300	-0.23000700
H	-5.31297500	0.78500700	-0.90459000
H	-4.26997000	-1.33320900	0.08646300

⁵I-IM1

Pt	1.23522200	-1.17135100	-0.46444100
Pt	0.18045900	1.23241500	-1.05085300
Pt	0.71153700	0.65391300	1.35979100
Pt	-1.19278700	-0.72571200	0.13863300
C	-3.63501200	-0.54898100	0.31493100
H	-2.74161900	-0.11125000	0.92772700
H	-3.36876800	-1.22855600	-0.51915400
C	-4.46306900	0.63699300	-0.18472500
H	-4.73080000	1.31174400	0.63986400

H	-3.90958700	1.21745500	-0.93324600
H	-5.39503400	0.28080300	-0.64747600
H	-4.15138400	-1.16101200	1.06690400

1-TS1



¹I-TS1

Pt	0.87419500	-0.30260000	1.41165500
Pt	-1.44551700	0.17639800	-0.02026200
Pt	0.61192000	-1.23915500	-0.93649200
Pt	0.88607700	1.36566300	-0.50708000
C	-3.60896000	0.60923200	0.05707600
H	-2.70672600	0.41157600	-1.01005500
H	-3.39459000	1.28930300	0.90104900
C	-4.41205100	-0.62823400	0.46615500
H	-4.55996800	-1.30906500	-0.38291700
H	-3.91790100	-1.19387000	1.26628000
H	-5.40821400	-0.32549600	0.82957000
H	-4.16724000	1.21771900	-0.67330600

³I-TS1

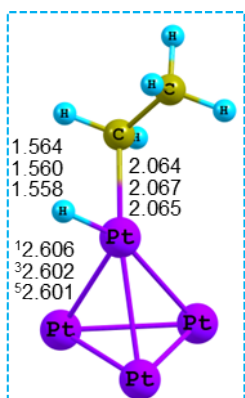
Pt	0.87058500	-0.47867100	1.40751200
Pt	-1.45671400	-0.05509800	-0.13779200
Pt	0.86328500	-0.93470600	-1.11088100
Pt	0.65050800	1.49280500	-0.23374600
C	-3.57746000	0.50737800	0.29565100
H	-2.80977600	0.52169600	-0.84609000
H	-3.23229200	0.89127000	1.26799000
C	-4.44624400	-0.74789000	0.41242900
H	-4.73925300	-1.13305100	-0.57378800
H	-3.93014200	-1.55561900	0.94862100
H	-5.36925100	-0.51532100	0.96834000
H	-4.13487600	1.33635300	-0.17080100

⁵I-TS1

Pt	-0.95721700	-0.00371300	1.37604900
Pt	1.37702900	-0.04888100	0.19010700
Pt	-0.62558400	1.39963300	-0.76366900
Pt	-0.71145700	-1.33043000	-0.79342800

C	3.43464800	-0.56436000	-0.26649100
H	2.42908700	0.39445300	-0.92537400
H	3.29254200	-1.44446900	0.39162100
C	4.51961100	0.37762000	0.25397400
H	4.67792600	1.23266100	-0.41753900
H	4.27926900	0.77151400	1.25041500
H	5.47447100	-0.16727100	0.33326100
H	3.66500900	-0.96198500	-1.26388700

1-IM2

¹1-IM2

Pt	0.42164900	1.51353000	-0.55884100
Pt	-1.39449400	-0.29654700	0.44686800
Pt	1.24743800	-0.16414700	1.18074700
Pt	0.57752500	-1.09016400	-1.06040500
C	-3.20688900	-0.15634600	-0.53164900
H	-2.02478600	-1.55730300	1.12477700
H	-2.98287500	0.37809100	-1.46886000
C	-4.20079600	0.61931400	0.33560100
H	-4.45672600	0.07937900	1.25821700
H	-3.82897400	1.61714000	0.61324800
H	-5.14178700	0.77443800	-0.22448500
H	-3.58398600	-1.15798600	-0.77939200

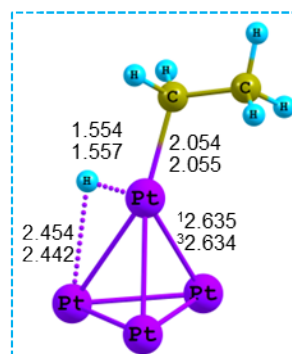
³1-IM2

Pt	0.51101700	1.35539000	-0.78117400
Pt	-1.41735100	-0.21441100	0.44453000
Pt	1.20266900	0.01931500	1.25898800
Pt	0.56067300	-1.22751500	-0.90910600
C	-3.24071800	-0.09079700	-0.52023000
H	-2.09706200	-1.36360500	1.25086700
H	-3.00873200	0.34435800	-1.50616900
C	-4.20430600	0.80012800	0.27043000
H	-4.47474700	0.35932800	1.24035800
H	-3.79327100	1.80394500	0.45516600
H	-5.14105600	0.93728800	-0.30003700
H	-3.66150000	-1.09406000	-0.67393300

⁵1-IM2

Pt	0.43289000	1.42735400	-0.71643300
Pt	-1.42461500	-0.25701900	0.45886700
Pt	1.33629600	-0.02579800	1.17425100
Pt	0.51477900	-1.21060600	-0.94157800
C	-3.28869300	-0.07678300	-0.40012600
H	-2.03344800	-1.47369100	1.21860200
H	-3.11069500	0.39629200	-1.37792800
C	-4.18640500	0.78748800	0.48993800
H	-4.38913800	0.31598200	1.46175800
H	-3.76424800	1.78641800	0.67267200
H	-5.16048000	0.93747500	-0.01030800
H	-3.72083400	-1.07333000	-0.56197300

1-TS2

¹1-TS2

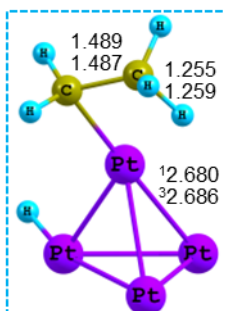
Pt	-0.85832800	-1.25814200	-0.75786500
Pt	1.41116400	-0.36873000	0.44261000
Pt	-1.28530600	0.33525200	1.16708500
Pt	-0.13205800	1.28348800	-0.91067400
C	3.40598600	-0.06702400	0.82812900
H	1.04945300	0.09444400	1.88091300
H	3.56067700	0.76047400	1.53505600
C	4.21881000	0.12606500	-0.45345700
H	4.05895500	-0.68709700	-1.17785700
H	3.97178200	1.07503700	-0.95077300
H	5.30055200	0.14596700	-0.22741600
H	3.69361600	-1.00100800	1.35406700

³1-TS2

Pt	-0.81218900	1.35978700	-0.57728600
Pt	1.42892200	-0.21962800	-0.49988400
Pt	-1.28899300	-1.15179700	-0.45231800
Pt	-0.19757800	0.05452500	1.55308100
C	3.43666900	-0.65236400	-0.44823100
H	1.06539900	-1.70463900	-0.79213900
H	3.61462700	-1.65212600	-0.02661200
C	4.24050000	0.42120400	0.29028900

H	4.05663400	1.43062300	-0.10811800
H	4.00941800	0.43492100	1.36497100
H	5.32441100	0.22933300	0.19007400
H	3.71385000	-0.69630200	-1.52074400

1-IM3



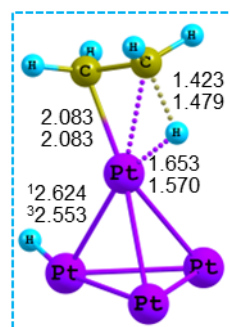
¹1-IM3

Pt	1.03809300	-0.16850900	1.31303600
Pt	-1.43676100	0.06350300	0.28507100
Pt	0.55577800	-1.27827500	-0.93274600
Pt	0.59422700	1.38391000	-0.66880100
C	-3.26062000	0.23074000	-0.65330700
H	0.46741600	2.84585000	-0.09334000
H	-3.59991700	1.26832200	-0.73887900
C	-3.62664900	-0.50260000	0.58882200
H	-2.62478900	-0.71928200	1.31870600
H	-4.24527200	0.04687400	1.30758700
H	-3.95781200	-1.53855300	0.45640600
H	-3.32029000	-0.32113700	-1.59532900

¹1-IM3

Pt	1.11526700	-0.26978600	1.24239500
Pt	-1.39239000	-0.04319000	0.30724200
Pt	0.60644300	-1.16548500	-1.05390800
Pt	0.41614400	1.53274200	-0.52582700
C	-3.34948900	0.26803800	-0.28980400
H	0.03473500	2.93982500	0.06834000
H	-3.78193000	1.16765700	0.15915400
C	-3.45744500	-0.99496900	0.48817100
H	-2.35101000	-1.36318300	0.96320200
H	-4.02137100	-0.93408200	1.42645100
H	-3.69274000	-1.89619700	-0.08823200
H	-3.49222800	0.21359900	-1.37142800

1-TS3



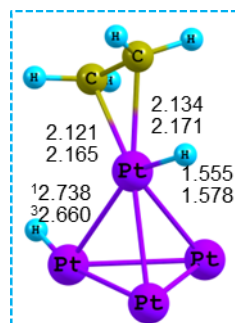
¹1-TS3

Pt	-1.44709400	0.04638700	0.28565000
Pt	0.59532900	1.36974000	-0.69667900
Pt	1.00224400	-0.12254900	1.32937200
Pt	0.59209200	-1.29522300	-0.90271700
C	-3.25354200	0.25608200	-0.72953600
H	0.44969400	2.84250500	-0.15391000
H	-3.56679700	1.30217100	-0.78987900
C	-3.58860600	-0.49804000	0.47811500
H	-4.17143000	0.01516300	1.24933200
H	-3.85779100	-1.55175600	0.35989300
H	-2.46384900	-0.75768300	1.31094000
H	-3.25745200	-0.27036300	-1.68672800

³1-TS3

Pt	0.74127100	-0.23944800	1.44428500
Pt	-1.39903900	-0.25195400	-0.16592000
Pt	1.00791800	-1.03917300	-0.93018800
Pt	0.39089200	1.57365800	-0.41120400
C	-3.33654000	0.43440900	0.27104500
H	-0.19855600	2.93308200	0.13236300
H	-3.37763100	0.98014400	1.21506200
C	-3.43646800	-1.02529300	0.29654600
H	-2.23240900	-1.68585300	-0.02090300
H	-3.57421400	-1.50736400	1.26872300
H	-4.00490500	-1.50309300	-0.50844600
H	-3.77549400	0.96793900	-0.57630200

1-IM4



¹1-IM4

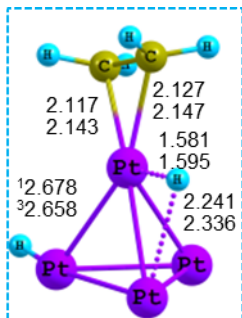
Pt	1.07727600	0.22287600	1.25263000
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Pt	-1.49877800	-0.38442400	0.17645300
Pt	0.80024000	-1.31792600	-0.67827800
Pt	0.33876300	1.37517500	-0.83453600
C	-3.14264500	0.67659900	1.02758900
H	0.06943700	2.85988500	-0.40649700
H	-3.49896400	0.19548500	1.94057300
C	-3.50509200	0.15563200	-0.25045200
H	-2.09037800	-1.74351400	0.64596900
H	-4.16045000	-0.71432300	-0.32193100
H	-3.52350600	0.81408000	-1.12281000
H	-2.87480700	1.73029000	1.13286700

³1-IM4

Pt	0.70092500	0.10353700	1.46636500
Pt	-1.36467700	-0.49498300	-0.12139400
Pt	1.06024500	-1.13800300	-0.73005600
Pt	0.31002900	1.49540600	-0.67560900
C	-3.09893700	0.76841300	0.16931300
H	-0.30387800	2.90629800	-0.35003400
H	-2.89443000	1.46194800	0.98552300
C	-3.46243900	-0.57418000	0.43208300
H	-1.61221600	-2.03158700	0.13757600
H	-3.56609800	-0.93199100	1.45695700
H	-4.01400300	-1.14608400	-0.31703200
H	-3.34982600	1.23136300	-0.78724300

1-TS4



¹1-TS4

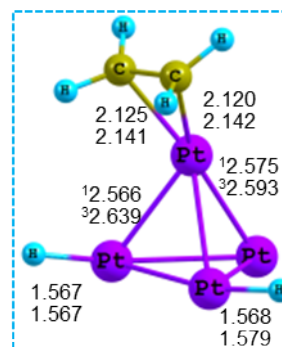
Pt	1.10411200	0.06098700	1.27022500
Pt	-1.54146100	-0.11419100	0.12467700
Pt	0.62957500	-1.38504700	-0.69833200
Pt	0.54050700	1.36692700	-0.79501200
C	-3.28530300	0.86912600	0.81296000
H	0.62395700	2.86187400	-0.34496500
H	-3.30011800	0.93463700	1.90336800
C	-3.65574200	-0.34243100	0.15699400
H	-1.43092500	-1.69171900	0.12874900
H	-3.96665500	-1.20684100	0.74658200
H	-4.04819100	-0.31834800	-0.86278100

H	-3.38491000	1.82354200	0.28776300
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³1-TS4

Pt	0.66587700	0.11095900	1.47296300
Pt	-1.42246800	-0.25334500	-0.15400100
Pt	0.90510600	-1.31969500	-0.64161100
Pt	0.56301300	1.41626900	-0.73282400
C	-3.21679300	0.84322400	0.26056800
H	0.26462900	2.93055600	-0.45070700
H	-3.09260100	1.43144400	1.17131900
C	-3.49110500	-0.55260200	0.33548100
H	-1.31887200	-1.84543300	-0.15507800
H	-3.59400700	-1.04716100	1.30243700
H	-4.00197700	-1.05148000	-0.49166700
H	-3.50903300	1.41173800	-0.62562100

1-IM5



¹1-IM5

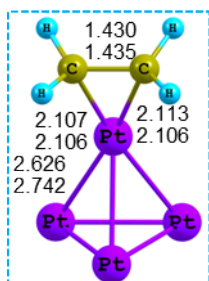
Pt	0.97783500	-0.29938200	1.30592300
Pt	-1.30727400	-0.64450800	0.14474300
Pt	1.20080900	-0.51888700	-1.16548400
Pt	-0.21815600	1.61990400	-0.15110200
C	-3.40669600	-0.40343400	0.07088000
H	-1.13385400	2.36148800	-1.18610300
H	-3.85459300	-0.90027900	0.93789300
C	-2.98122100	-1.18245200	-1.04581100
H	2.05122900	-1.82678400	-1.24260600
H	-3.09512600	-2.27191100	-1.02151100
H	-2.91308600	-0.74964000	-2.04503100
H	-3.67778000	0.64649600	-0.05128200

³1-IM5

Pt	-1.10025900	-0.54591500	-1.16713400
Pt	1.35819500	-0.34273300	-0.36680600
Pt	-0.67157600	-0.72199500	1.30781000
Pt	-0.26665400	1.67268400	0.14463300
C	3.35958800	0.33624800	-0.02618100
H	0.46840000	2.65033000	1.12339400
H	3.81866400	0.51455600	-1.00385300

C	3.22650300	-0.98810400	0.45950600
H	-0.81340900	-2.26679400	1.60124400
H	3.58594200	-1.82807500	-0.14304200
H	3.12657600	-1.18874100	1.52737800
H	3.36018600	1.19069100	0.65169500

1-IM6

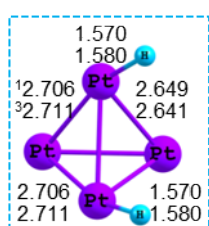
¹1-IM6

Pt	1.46416700	0.31247700	0.19180200
Pt	-0.83588000	1.31398800	-0.63429900
Pt	-1.04776500	-0.31856200	1.29200800
Pt	-0.28779300	-1.28696200	-0.93440200
C	3.30715900	-0.15364300	1.11422900
C	3.48395600	-0.03429000	-0.29933800
H	3.28409300	-1.13133000	1.60015600
H	3.60513000	0.67355800	1.76766300
H	3.60303400	-0.92424800	-0.92143500
H	3.92821100	0.87627900	-0.71413400

³1-IM6

Pt	-1.46293800	0.00087800	-0.38983300
Pt	0.95822900	1.27658800	-0.56095600
Pt	0.96163300	-1.26645600	-0.57959100
Pt	0.25828600	-0.01138900	1.56379400
C	-3.43095400	-0.71553900	-0.16917700
C	-3.42949000	0.71914100	-0.16550400
H	-3.56489100	-1.27239000	0.76111800
H	-3.74951500	-1.25620300	-1.06661100
H	-3.56243500	1.27156600	0.76757400
H	-3.74684500	1.26502000	-1.06023700

1-IM7

¹1-IM7

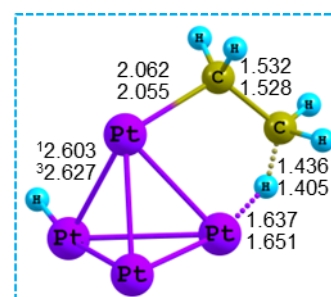
Pt	0.96752600	1.30301900	-0.15296900
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Pt	0.96753700	-1.30301200	-0.15297100
Pt	-1.21855000	-0.00000300	-1.07267400
Pt	-0.77303500	-0.00000400	1.36027000
H	2.20436000	-1.72751700	0.71540700
H	2.20434600	1.72753400	0.71540900

³1-IM7

Pt	-0.96819900	-1.26159900	-0.17948600
Pt	-0.96830000	1.26183700	-0.17742700
Pt	1.26457000	0.00093200	-1.05735000
Pt	0.73115100	-0.00115700	1.40027700
H	-2.30968900	1.67656500	0.54677100
H	-2.30954100	-1.67754300	0.54409100

1-TS5

¹1-TS5

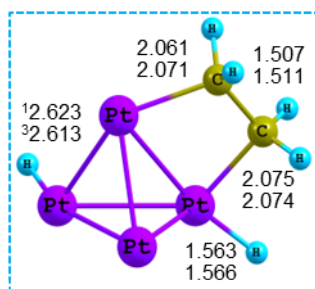
Pt	0.58646200	-1.15588500	-0.74745400
Pt	0.88507600	0.58140500	1.13575600
Pt	-1.52747700	-0.67111600	0.60489900
Pt	-0.56855200	1.27100400	-0.91065000
C	2.76811300	0.37702900	0.31961800
H	0.31645500	2.28057300	-1.75091600
H	3.05517200	1.33299800	-0.13688100
C	2.80869000	-0.78010700	-0.68320400
H	3.13957300	-1.73334300	-0.25198100
H	3.46161300	-0.54174900	-1.53900800
H	3.41381300	0.14902600	1.18787500
H	1.86285800	-1.05093400	-1.76653600

³1-TS5

Pt	0.75048900	-0.71400200	-1.08586100
Pt	0.73797400	0.35574300	1.29874200
Pt	-1.30604300	-1.08351100	0.40276800
Pt	-0.80739100	1.40394800	-0.57346000
C	2.70225300	0.27856600	0.67069000
H	-0.22562700	2.78212900	-1.08578900
H	3.02600300	1.32634500	0.77736900
C	2.92023000	-0.25275000	-0.74812300
H	3.31630000	-1.27560500	-0.77758500
H	3.60654200	0.39919900	-1.31475600

H	3.20228400	-0.37263600	1.40542500
H	2.08730600	-0.06418600	-1.83075400

1-IM8



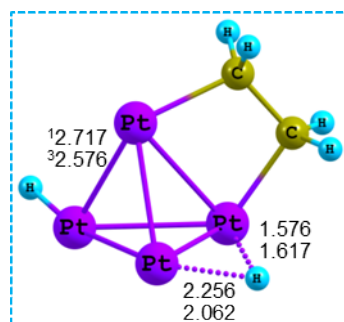
¹1-IM8

Pt	1.01691800	-1.19125000	-0.38953000
Pt	0.14399500	1.52644500	-0.43086400
Pt	-0.11363100	0.01356200	1.62111300
Pt	-1.56683100	-0.45866900	-0.61820600
C	2.15113500	1.37040200	-0.83810500
H	-1.99198700	-0.56142800	-2.11889700
H	2.17945000	1.69876600	-1.89302900
C	2.70919400	-0.01378700	-0.63788200
H	2.02463100	-2.30055600	0.05408600
H	3.23012800	-0.41278300	-1.52143300
H	3.33232200	-0.11332400	0.25741900
H	2.58828100	2.12284000	-0.15825900

³1-IM8

Pt	1.00049200	-1.15239600	-0.49718200
Pt	0.15081200	1.53344300	-0.33288900
Pt	-0.06512600	-0.11936200	1.61213600
Pt	-1.60539100	-0.38244200	-0.60450700
C	2.17915000	1.43349900	-0.73988500
H	-2.10264500	-0.37913300	-2.08663200
H	2.25783100	1.87686700	-1.74654200
C	2.70409000	0.01889500	-0.66672500
H	1.90018200	-2.40037900	-0.20615300
H	3.18791800	-0.32053500	-1.59524000
H	3.34990500	-0.17270800	0.19746200
H	2.60600800	2.10055700	0.02718900

1-TS6



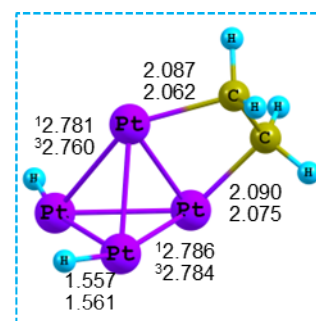
¹1-TS6

Pt	-0.78964900	-1.08438400	-0.77594500
Pt	-0.68587700	0.59377000	1.21924600
Pt	0.48214700	1.28065300	-0.96283900
Pt	1.57075700	-0.72583200	0.47899400
C	-2.70614600	0.27686000	0.80747300
H	1.86493800	-1.88516000	1.48353300
H	-3.04468700	-0.16764900	1.76164800
C	-2.82253600	-0.65523200	-0.36848800
H	-0.97109500	-0.10251400	-1.99515900
H	-3.25464600	-1.63860000	-0.12450200
H	-3.31151000	-0.21602400	-1.24386700
H	-3.14638300	1.27196500	0.64682700

³1-TS6

Pt	1.05518500	-0.74213200	-0.94621500
Pt	0.23895200	1.44318100	0.57353000
Pt	-0.28083700	-1.09021600	1.23362300
Pt	-1.53721400	0.19181200	-0.80983500
C	2.25558900	1.63029100	0.09761700
H	-2.07983200	1.22321200	-1.85260200
H	2.32467400	2.44307200	-0.63829700
C	2.76089200	0.30835200	-0.38382400
H	1.25255500	-1.92572800	0.13754600
H	3.28733400	0.34781000	-1.35670100
H	3.32920200	-0.26184700	0.35784400
H	2.65240700	1.93530400	1.08344100

1-IM9



¹1-IM9

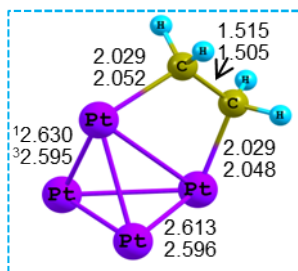
Pt	-0.71711300	1.34460300	-0.34958400
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Pt	-0.71892000	-1.33951100	-0.36629000
Pt	0.40703600	-0.01052900	1.58268200
Pt	1.57074600	0.00477300	-0.83086000
C	-2.68865300	-0.74990400	-0.32708500
H	3.07021400	0.00471500	-0.42542000
H	-3.10233700	-1.18551000	-1.25417100
C	-2.68802200	0.75806700	-0.31438600
H	-0.59846200	-0.01951500	2.79786100
H	-3.10354500	1.20974300	-1.23287600
H	-3.12935600	1.19974700	0.59041200
H	-3.13290900	-1.20632600	0.56904900

³1-IM9

Pt	-0.84621000	0.63694100	1.09462800
Pt	-0.67802200	-1.15441600	-0.80368600
Pt	1.47419300	-0.77041700	0.59306500
Pt	0.59449300	1.31983700	-0.88844100
C	-2.69446300	-0.77653800	-0.49174300
H	1.40692300	2.58820700	-0.47888100
H	-3.03566800	-0.57487200	-1.52179500
C	-2.78539800	0.40183600	0.43500600
H	1.60881900	-2.08307700	1.43919200
H	-3.11384900	1.33702700	-0.03472400
H	-3.33779100	0.19699300	1.37045400
H	-3.11663600	-1.70772600	-0.08800500

1-IM10



¹1-IM10

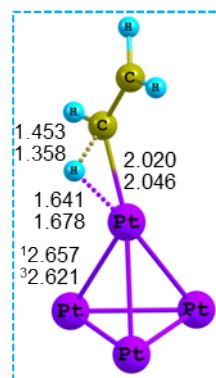
Pt	-1.59184700	-0.53914800	-0.39467500
Pt	1.59182500	-0.53923100	-0.39462900
Pt	-0.00002600	0.03176800	1.59746800
Pt	0.00005900	1.54351000	-0.61139100
C	0.75739300	-2.31032600	-0.92593500
H	1.17347500	-2.49904800	-1.93237400
C	-0.75750300	-2.31034600	-0.92578600
H	-1.17377400	-2.49926500	-1.93211100
H	-1.17369500	-3.01783400	-0.18656500
H	1.17374500	-3.01793900	-0.18692100

³1-IM10

Pt	-1.54323800	0.72759300	0.06029900
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Pt	1.57541800	0.65409500	-0.17778000
Pt	-0.16620200	-1.06793300	-1.21010400
Pt	0.12404100	-0.86406700	1.34824900
C	0.79693900	2.54511100	-0.07255700
H	1.20713500	2.94756600	0.86807900
C	-0.70624100	2.59211800	-0.12410300
H	-1.14705900	3.14241300	0.72640600
H	-1.09456500	2.98099900	-1.07888100
H	1.26877100	3.03000500	-0.94748600

2-TS1



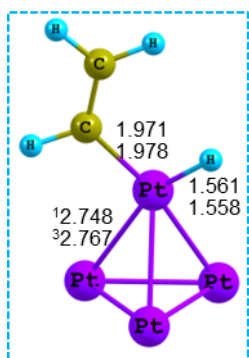
¹2-TS1

Pt	1.47198000	-0.14132400	0.21766200
Pt	-0.47969800	1.40184200	-0.71411200
Pt	-1.15479700	-0.02113800	1.28720400
Pt	-0.64549600	-1.26408800	-0.85744200
C	4.46136400	-0.26962700	0.49760200
C	3.39691900	0.44825900	0.05772700
H	5.45255100	-0.11284300	0.06413200
H	4.37175200	-1.04482400	1.26015700
H	3.55278600	1.29346500	-0.62108200
H	2.49805100	0.71962800	1.16646800

³2-TS1

Pt	1.46565900	-0.10539800	0.23999000
Pt	-0.49672500	1.42673800	-0.58076600
Pt	-1.09751000	-0.18849400	1.32880700
Pt	-0.68974900	-1.11929900	-1.01565600
C	4.49182000	-0.48159700	0.30327600
C	3.44459300	0.28083800	-0.10973800
H	5.45313400	-0.43299000	-0.21370600
H	4.41444400	-1.18048200	1.13746700
H	3.61059000	1.03325700	-0.88713700
H	2.73272500	0.72806000	0.95689000

2-IM1



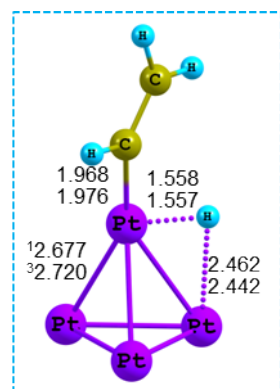
¹2-IM1

Pt	1.44692100	-0.16671000	-0.38876300
Pt	-0.48459100	-0.96758700	1.19711500
Pt	-1.16692500	-0.44247300	-1.15630400
Pt	-0.57617200	1.54226300	0.34450900
C	4.42015700	0.10923700	-0.18391800
C	3.19906500	0.39239900	0.32092100
H	5.30566000	0.64905000	0.16920600
H	4.57970800	-0.63155400	-0.96815500
H	3.11649200	1.10522100	1.15463500
H	2.18266700	-1.44099400	-0.90914900

³2-IM1

Pt	1.44853400	-0.22614400	-0.36388600
Pt	-0.41780100	-0.64594800	1.41338800
Pt	-1.15174800	-0.71280300	-1.05994300
Pt	-0.65841400	1.52428100	0.02618600
C	4.41652300	0.21294900	-0.26007200
C	3.18416500	0.56487700	0.16115100
H	5.28177600	0.84806100	-0.04105300
H	4.60872800	-0.68772300	-0.84448900
H	3.06893000	1.46191700	0.78745000
H	2.23190900	-1.56136500	-0.53647500

2-TS2



¹2-TS2

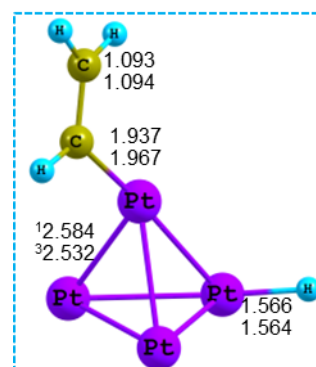
Pt	-1.51964300	-0.01754200	-0.11884900
Pt	0.72747200	-0.73178400	1.28613100

Pt	0.79477100	1.52877600	0.00067200
Pt	0.79298600	-0.80028800	-1.21612600
C	-4.46818400	0.30535700	-0.02915900
C	-3.36944200	-0.28373100	0.49736600
H	-5.47019500	-0.08735400	0.17705000
H	-4.41145100	1.16703900	-0.69678900
H	-3.49111300	-1.08085500	1.24661500
H	-1.65719900	1.49673600	0.22129800

³2-TS2

Pt	1.51591800	0.05769200	0.20863300
Pt	-0.48085900	-0.96991200	-1.19780400
Pt	-0.94170400	1.41076500	-0.31290800
Pt	-0.89065800	-0.56558800	1.31344000
C	4.43199500	0.69076900	0.08006900
C	3.44457100	-0.20720300	-0.13218400
H	5.48403100	0.38586600	0.05598200
H	4.23714700	1.74147200	0.30209700
H	3.71677000	-1.23550500	-0.41668500
H	1.49228300	1.43617600	-0.51485400

2-IM2



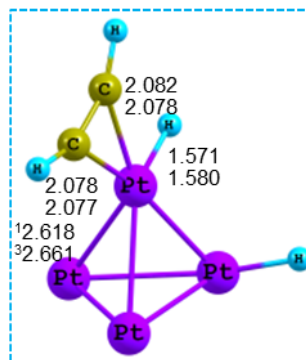
¹2-IM2

Pt	1.41399000	-0.49256800	0.13107900
Pt	-0.92789700	0.38240100	1.32192100
Pt	-1.12253300	-1.15145100	-0.63869600
Pt	-0.08641000	1.35150600	-0.87952100
C	4.23645700	-0.41108600	0.02414300
C	3.17529700	0.03283900	0.74008100
H	5.22430800	-0.52604200	0.48642400
H	4.15900700	-0.69980800	-1.02743100
H	3.29190400	0.46655300	1.74219900
H	-1.57978000	-2.51032500	-0.00838600

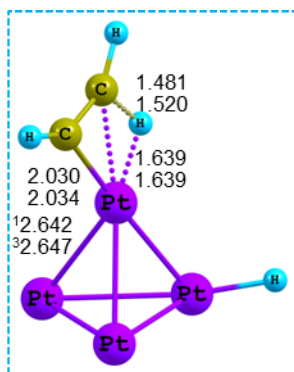
³2-IM2

Pt	1.33905700	-0.53070700	-0.06745000
Pt	-0.68887000	0.21933300	1.45797400
Pt	-1.27253300	-1.02059600	-0.68646400

Pt	-0.08467200	1.44918500	-0.74883000
C	4.20096800	-0.77535300	-0.02449900
C	3.16650700	-0.08301700	0.50529600
H	5.20465100	-0.72040900	0.41331500
H	4.09820800	-1.43204800	-0.89342500
H	3.32846500	0.62110000	1.32869100
H	-1.68882300	-2.46113500	-0.24125800



2-TS3



¹2-IM3

Pt	-1.47912100	-0.06929900	-0.13075400
Pt	0.59689800	-0.24311900	1.46443800
Pt	0.74533000	1.45224900	-0.49142900
Pt	0.79416700	-1.20604000	-0.85253400
C	-3.59005700	0.03894100	-0.48178400
C	-3.27352000	0.28541100	0.75010700
H	-4.39966400	-0.09235900	-1.19057200
H	-2.46617500	-0.07737700	-1.43967800
H	-3.67527800	0.50599500	1.73098600
H	0.45517100	2.88188900	0.09110200

³2-TS3

Pt	-1.43074100	0.22314000	0.02235700
Pt	0.67252200	-0.56243900	1.35956100
Pt	0.85877000	1.45414500	-0.29760800
Pt	0.54295000	-1.13782500	-1.10031000
C	-3.54285500	0.35765000	-0.26500400
C	-3.21123500	-0.63660100	0.49792100
H	-4.35706800	0.91096500	-0.71823900
H	-2.41458300	1.14947600	-0.90523200
H	-3.60345200	-1.45619700	1.08725400
H	0.70664800	2.86191400	0.38668900

2-IM3

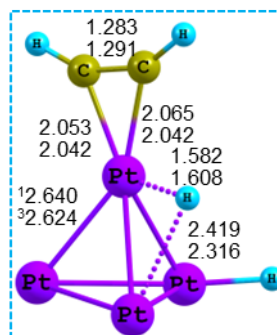
¹2-IM3

Pt	-1.46932900	0.00502600	-0.25931800
Pt	0.52777500	-0.25894300	1.49671600
Pt	0.80300000	1.42361300	-0.45637500
Pt	0.76666600	-1.22953500	-0.83233600
C	-3.54947800	0.08482300	-0.21846200
C	-3.12935400	0.14539500	0.98302700
H	-4.32980300	0.09305600	-0.96277900
H	-1.84449100	0.11991600	-1.78045800
H	-3.25314600	0.21388400	2.05266200
H	0.50771800	2.85918300	0.10559300

³2-IM3

Pt	-1.44573700	0.26784600	-0.05140700
Pt	0.62991300	-0.74721200	1.30182500
Pt	0.82847000	1.48202400	-0.08564400
Pt	0.60258200	-0.97748800	-1.20641100
C	-3.51284100	0.06531900	-0.10267200
C	-3.04215500	-0.89029700	0.60015600
H	-4.32131000	0.59352000	-0.58342500
H	-1.81998600	1.39339800	-1.09556600
H	-3.12845900	-1.79286000	1.18578800
H	0.61205200	2.79260700	0.75594300

2-TS4



¹2-TS4

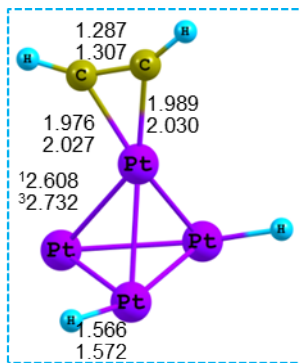
Pt	-1.48590600	0.04276700	0.19398900
Pt	0.88001100	-0.32578900	1.35134000
Pt	0.73005300	1.42524800	-0.55623800

Pt	0.51189000	-1.20940600	-0.99470100
C	-3.51633100	0.17121300	0.54691100
C	-3.32495600	0.08585100	-0.71833600
H	-4.16945500	0.29782600	1.39770700
H	-1.36346700	0.50932500	1.70088200
H	-3.68749900	0.04332200	-1.73648100
H	0.65642600	2.84709900	0.10401700

³2-TS4

Pt	1.44812100	-0.12108900	0.18306400
Pt	-0.93068000	-0.08770900	1.36436600
Pt	-0.67149100	-1.20436200	-0.93550200
Pt	-0.47277100	1.46941600	-0.63290000
C	3.42427600	-0.55027700	0.46579800
C	3.33721200	0.47533600	-0.31270500
H	4.03230600	-1.25249400	1.01946800
H	1.11898800	-1.16528500	1.36043600
H	3.80931000	1.25695700	-0.89350100
H	-0.63760800	-2.77751100	-0.76914800

2-IM4



¹2-IM4

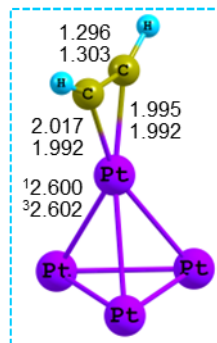
Pt	1.44098200	-0.28079200	-0.09977500
Pt	-0.71372100	-0.62325300	1.32934700
Pt	-1.11104900	-0.61225800	-1.14054000
Pt	-0.19693500	1.64645200	0.00807900
C	3.10662700	-0.93566200	-0.96682300
C	3.36676300	-0.54773300	0.25371100
H	3.44872800	-1.36596000	-1.90068100
H	0.36843900	2.65994300	-1.04326300
H	4.09456900	-0.42778800	1.04955400
H	-1.45575300	-2.11743000	-1.40157200

³2-IM4

Pt	-1.46455800	-0.09534600	0.16147300
Pt	0.77326800	-0.91705800	-1.17223900
Pt	0.87165800	-0.48972100	1.30896400
Pt	0.40886400	1.60915300	-0.29215100
C	-3.49332500	-0.15582800	0.17211900

C	-3.05700300	-1.12547400	-0.55262200
H	-4.30713900	0.41432500	0.60126600
H	-0.08467100	2.85677800	0.52524800
H	-3.19177000	-1.98025800	-1.20049600
H	0.92546300	-1.95123200	1.88529400

2-IM5



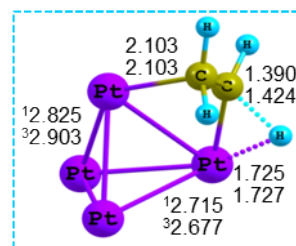
¹2-IM5

Pt	1.47738700	0.00200600	0.17478900
Pt	-1.04911400	-0.01873700	1.32203300
Pt	-0.51398300	-1.33211300	-0.81103400
Pt	-0.52506300	1.34875000	-0.78068400
C	3.43488000	0.01630000	-0.12919200
C	3.21092200	-0.01539800	1.15722800
H	4.16297300	0.03884300	-0.93367900
H	3.60249400	-0.03683700	2.16741800

³2-IM5

Pt	1.51159600	0.01236600	-0.12576300
Pt	-0.82533000	1.33611300	-0.54392500
Pt	-0.48196000	-0.16362500	1.53731100
Pt	-0.82646400	-1.19091900	-0.81311800
C	3.38768800	-0.61542500	-0.36023300
C	3.38587100	0.68034700	-0.22481400
H	3.94633000	-1.52801000	-0.53433400
H	3.94060900	1.61149400	-0.20673000

2-TS5



¹2-TS5

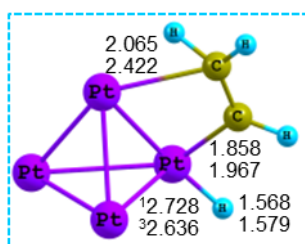
Pt	-1.16563000	-1.00636100	-0.59208700
Pt	-0.37752800	1.59794400	0.17987200
Pt	1.45678300	-0.01293300	-0.93368500

Pt	0.62196500	-0.65542200	1.31848600
C	-2.21518300	0.89338100	-0.20017000
H	-1.98884500	1.92553700	0.70246400
C	-2.87144000	-0.26646700	0.39029400
H	-2.79149800	-0.44104400	1.46578300
H	-3.83316700	-0.56009100	-0.04444600
H	-2.64278100	1.30232300	-1.12625900

³2-TS5

Pt	-1.27000400	-0.82869600	-0.69059700
Pt	-0.22192000	1.55125700	0.32106800
Pt	1.50414800	-0.00286100	-0.90977500
Pt	0.51847300	-0.84751000	1.24921600
C	-2.13294400	1.12286800	-0.12769400
H	-1.77330200	2.05506600	0.88709600
C	-2.91883500	-0.01234900	0.32888900
H	-2.89809800	-0.30180800	1.38224600
H	-3.88828700	-0.15639700	-0.16039300
H	-2.52404400	1.70914800	-0.96921000

2-IM6



¹2-IM6

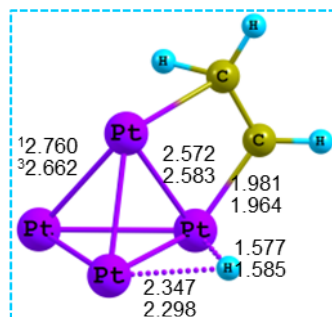
Pt	1.28584700	-0.73415200	-0.70352200
Pt	0.04027300	1.63485900	0.38425400
Pt	-0.37471800	-0.95748800	1.26727400
Pt	-1.41931000	-0.13543000	-0.94224400
C	1.83134200	1.21509900	-0.35914900
H	0.04329900	3.08941600	-0.21004800
C	2.80260600	0.38085500	0.31104200
H	2.71765100	0.16934200	1.37941300
H	3.82541600	0.36208000	-0.08179600
H	2.10677100	1.79588400	-1.24824100

³2-IM6

Pt	0.35198600	1.43635700	0.32397900
Pt	1.15754900	-0.77787900	-0.84388800
Pt	-1.60788100	0.16221000	-0.76966400
Pt	-0.46556200	-0.90110700	1.22903000
C	2.76325600	-0.15047300	0.10286500
H	1.79065400	-2.14527400	-1.31622800
C	2.73674900	1.11617400	0.60047800

H	2.17712200	1.98887800	0.09983800
H	3.45275200	1.48013100	1.34354200
H	3.56427500	-0.84527400	0.37524800

2-TS6



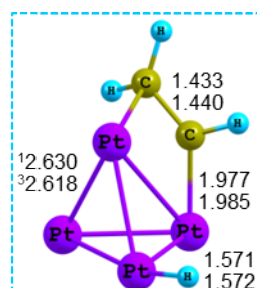
¹2-TS6

Pt	0.73595200	1.11193900	-0.71308600
Pt	1.04162100	-1.04355400	0.65690000
Pt	-1.18306100	-0.85998400	-0.93155100
Pt	-1.16866400	0.75016000	1.00503100
C	2.85790000	-0.32416400	0.32907600
H	0.77245200	-0.17468100	1.94505500
C	2.86323500	0.66701300	-0.62837500
H	2.23853100	0.54463000	-1.64294900
H	3.72077300	1.31773500	-0.82713300
H	3.72531900	-0.51253100	0.97190800

³2-TS6

Pt	-0.68198600	1.33174900	-0.14602800
Pt	-1.05434800	-1.21275700	0.09182500
Pt	1.13015200	0.01607500	1.29249000
Pt	1.18077100	-0.18336300	-1.23245500
C	-2.85072600	-0.43022100	-0.04564400
H	-0.77655200	-1.36486000	-1.46141900
C	-2.86623300	0.94759700	0.14532600
H	-2.30582400	1.41279500	1.03435600
H	-3.71782100	1.56713300	-0.15425500
H	-3.71595200	-0.95224000	-0.47165700

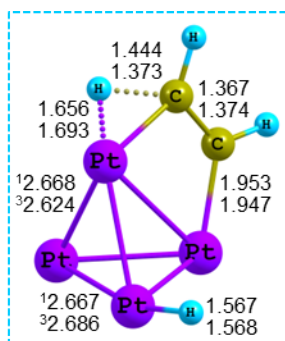
2-IM7



¹ 2-IM7			
Pt	1.48838000	-0.59086300	-0.41462800
Pt	-0.53070100	1.56373000	-0.25066600
Pt	-0.14810200	-0.26897700	1.61907800
Pt	-1.17221400	-0.95360900	-0.77945300
C	1.25032200	1.30980300	-1.07060100
H	-1.47207100	-1.10142500	-2.31465200
C	2.51238400	1.35906600	-0.39413000
H	2.57868100	1.64013800	0.65854200
H	3.41864400	1.52091700	-0.98589700
H	1.18422000	1.40521900	-2.16748100

³ 2-IM7			
Pt	1.28030900	-0.98628600	-0.30132200
Pt	-0.32436600	1.45497800	-0.75111300
Pt	0.06852000	0.40072300	1.55990900
Pt	-1.41104100	-0.97997900	-0.27741100
C	1.39926400	0.71637000	-1.40349900
H	-1.97773900	-1.70043000	-1.55410500
C	2.66705500	0.64109500	-0.72530300
H	2.84249600	1.18958400	0.20064600
H	3.55949400	0.43596100	-1.32522700
H	1.33097200	0.55406400	-2.49340700

2-TS7

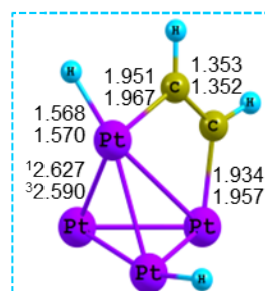


¹ 2-TS7			
Pt	-0.93490500	0.67854200	1.06955900
Pt	0.56761300	1.22928700	-0.98085800
Pt	-0.61293600	-1.15355600	-0.76378500
Pt	1.48605600	-0.64581300	0.67862800
C	-2.64734200	-0.88969300	-0.49936100
C	-2.69143700	0.09720100	0.44505900
H	-3.50775700	-1.46868600	-0.84725600
H	-1.90855800	-0.81557300	-1.73763800
H	-3.60292700	0.43042900	0.96083800
H	1.59728200	-1.85107500	1.67344100

³ 2-TS7			
Pt	-1.36568200	-0.73239700	-0.57608000

Pt	-0.05093100	-0.33309200	1.57776100
Pt	0.41732700	1.57947700	-0.15600900
Pt	1.33225300	-0.83025800	-0.67083000
C	-1.46270000	2.14330800	-0.70275200
C	-2.20242200	0.99910000	-0.88003200
H	-1.78506500	3.10749700	-1.11211300
H	-0.83444000	2.54424000	0.45078000
H	-3.20702200	1.00849000	-1.32737600
H	1.84581900	-0.84560300	-2.15226500

2-IM8



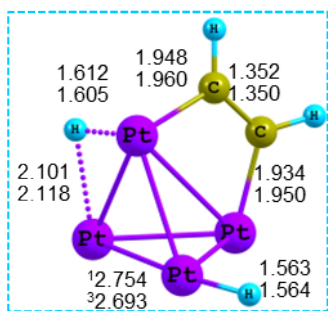
¹2-IM8

Pt	1.30376900	-0.96380900	-0.40220700
Pt	0.03742900	0.02549000	1.61914300
Pt	-1.65836200	-0.16710500	-0.37790100
Pt	0.46764100	1.48552100	-0.60588000
C	-1.29809200	-1.95331500	-1.07375700
C	0.02539900	-2.23510300	-1.10132100
H	-2.08720700	-2.65399600	-1.35777700
H	-3.12788900	-0.65701500	-0.13730300
H	0.48942800	-3.13400800	-1.53960200
H	0.62462400	1.92800100	-2.10090900

³2-IM8

Pt	1.51228200	-0.62004700	-0.52609200
Pt	-0.02233400	-0.40448600	1.53456800
Pt	-1.63087600	-0.26510200	-0.49082300
Pt	0.22164200	1.62829300	-0.21586200
C	-0.92172600	-1.81829900	-1.46815800
C	0.42499900	-1.93190400	-1.48963400
H	-1.60905300	-2.53651100	-1.92344200
H	-2.96065100	-1.08407300	-0.33003100
H	0.94850200	-2.75270900	-1.99961900
H	0.30591000	2.45912800	-1.53986700

2-TS8



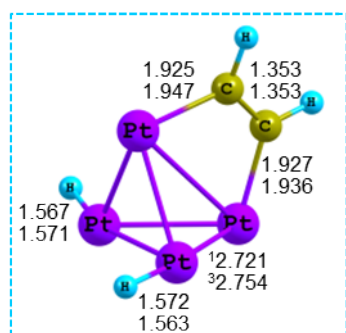
¹²-TS8

Pt	1.40443600	-0.85840900	-0.46195600
Pt	0.62801900	1.54536100	-0.11122600
Pt	-0.29462200	-0.45554200	1.54112800
Pt	-1.64408600	0.05956800	-0.64540400
C	-1.11787800	-1.50264000	-1.68286000
C	0.20740500	-1.77439100	-1.67408300
H	-1.88654100	-2.13807000	-2.13897400
H	1.45442300	2.42834200	-1.10126000
H	0.70805900	-2.46910200	-2.36784000
H	-2.12538600	-0.85527400	0.59144700

³²-TS8

Pt	-1.32423200	0.99927900	0.31056400
Pt	-0.68950100	-1.01891700	-1.11693600
Pt	0.30118400	-0.82613400	1.38007800
Pt	1.61850900	0.39996700	-0.50170900
C	1.11608100	2.29066500	-0.37796800
C	-0.20061700	2.52026200	-0.18554000
H	1.90746500	3.04903300	-0.42453200
H	-1.48898600	-0.81952000	-2.44655700
H	-0.69540100	3.48336800	-0.37315800
H	2.11931100	0.19440000	1.00957500

2-IM9



¹²-IM9

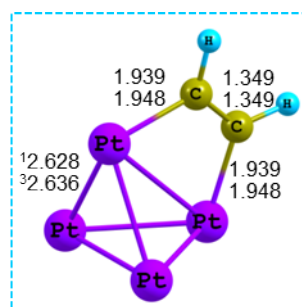
Pt	-0.26961600	-0.96466500	-1.23914200
Pt	-1.69962500	0.09417200	0.64463000
Pt	0.37913100	1.51830900	-0.38158100
Pt	1.61115000	-0.47095200	0.61083100

C	0.50947900	-0.99586700	2.09930500
C	-0.83124700	-0.81306000	2.10637200
H	1.07918800	-1.44252500	2.93148800
H	-0.78460200	-2.44436000	-1.27361400
H	-1.48377900	-1.25328600	2.87507300
H	1.47864400	2.19834400	-1.27658100

³²-IM9

Pt	0.30936400	1.53788200	-0.28984600
Pt	1.67845500	-0.52033200	0.40093000
Pt	-0.45674600	-0.82622600	-1.31107200
Pt	-1.54444800	-0.00936700	0.82863800
C	-0.54121400	-1.02459500	2.15361300
C	0.79558900	-1.16236100	1.99983800
H	-1.11828400	-1.52902900	2.94162900
H	0.82022800	2.68915400	0.64851700
H	1.45039600	-1.58612400	2.77649700
H	-1.63529200	-0.64487900	-2.32208400

2-IM10



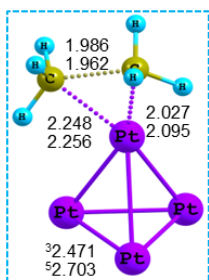
¹²-IM10

Pt	-1.64035800	-0.45202800	-0.50575100
Pt	1.64035900	-0.45202600	-0.50575100
Pt	0.00000000	-0.32789000	1.55067200
Pt	-0.00000100	1.59570700	-0.28945400
C	0.67490400	-1.90952100	-1.33510000
C	-0.67490100	-1.90952100	-1.33510000
H	-1.29612000	-2.72966100	-1.72830100
H	1.29612300	-2.72966000	-1.72830000

³²-IM10

Pt	1.61071300	0.67334300	-0.18066300
Pt	-1.61072300	0.67331700	-0.18069300
Pt	-0.00001600	-0.56349500	1.47514000
Pt	0.00003000	-1.23066200	-1.03480000
C	-0.67467800	2.36452000	-0.42550900
C	0.67464300	2.36452800	-0.42547200
H	1.29744900	3.26524100	-0.52744600
H	-1.29748800	3.26523100	-0.52747700

3-TS1



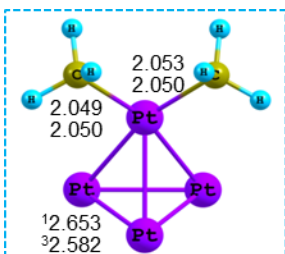
¹³-TS1

Pt	-1.61106700	0.26248100	0.19247700
Pt	0.48643800	1.53325100	-0.46566400
Pt	0.06936600	-1.48934200	-0.54922700
Pt	1.83302700	-0.23530900	0.64377800
C	-3.21668400	-1.27233100	0.53854000
H	-2.35491300	-1.97041800	0.61073900
H	-3.78120900	-1.41970100	-0.38458400
C	-3.43746100	0.65116300	0.97942200
H	-2.82727900	1.62492900	0.66260800
H	-4.38822800	0.73752600	0.44362900
H	-3.55809000	0.66715700	2.06693700
H	-3.83109800	-1.45680600	1.42649100

³³-TS1

Pt	1.48445300	-0.29608700	0.11411700
Pt	-0.78660700	-1.25150200	-0.75271200
Pt	-0.33805500	1.31492100	-0.84494200
Pt	-1.12539400	0.19515900	1.34339200
C	3.25097100	1.07711000	0.23747200
H	2.45970600	1.85008900	0.17851600
H	3.81335200	1.02339200	-0.69745300
C	3.29767400	-0.74568500	0.95124400
H	2.60504300	-1.68657500	0.75997000
H	4.23905700	-0.98464300	0.44720700
H	3.41595200	-0.62654500	2.03196400
H	3.89210200	1.36147400	1.07875200

3-IM2



¹³-IM2

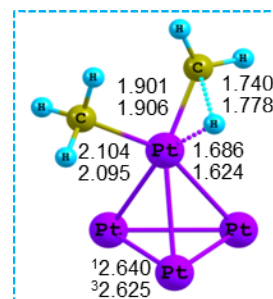
Pt	1.47816300	0.09517700	-0.34678800
Pt	-0.98625800	-1.02071700	-0.88590900
Pt	-0.91141800	1.43946000	-0.19756100

Pt	-0.27709600	-0.52112000	1.47378700
C	2.92986100	1.35743100	0.35864500
H	2.43679500	2.15275500	0.93538600
H	3.43086900	1.79266100	-0.52343000
C	2.93982300	-1.29267700	-0.73823000
H	2.46931200	-2.28404200	-0.80203900
H	3.36631200	-1.02461100	-1.72172000
H	3.74225200	-1.30481400	0.01158800
H	3.67184300	0.84107100	0.98248800

³³-IM2

Pt	-1.48430300	0.00002100	-0.36231500
Pt	0.95928300	1.26811700	-0.57536200
Pt	0.95929100	-1.26802900	-0.57554400
Pt	0.26393200	-0.00011200	1.56380500
C	-2.94176500	-1.43451800	-0.21971100
H	-2.46353200	-2.37979000	0.07424500
H	-3.38352700	-1.54021700	-1.22607900
C	-2.94176700	1.43455300	-0.21968400
H	-2.46362500	2.37970100	0.07481700
H	-3.38309800	1.54064300	-1.22620300
H	-3.73263000	1.17483100	0.49680600
H	-3.73231600	-1.17503300	0.49721000

3-TS2



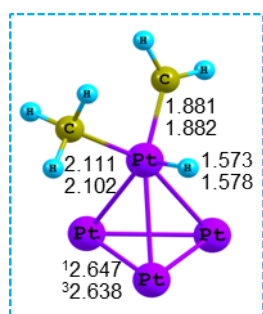
¹³-TS2

Pt	1.39911600	0.31966000	-0.18102800
Pt	-0.69439300	-0.92884500	-1.19876800
Pt	-1.07910500	1.33014200	0.04394500
Pt	-0.28743400	-0.77138400	1.40445100
C	2.71271000	1.69338900	-0.14200900
H	2.40386300	2.74689600	-0.14026800
H	2.05290400	0.91294900	-1.55080900
C	2.91978600	-1.13378400	-0.13020600
H	2.57529700	-1.96533900	-0.75734800
H	3.87454600	-0.74458200	-0.50793700
H	3.03165800	-1.45754900	0.91235300
H	3.78814300	1.52210400	-0.28313800

³³-TS2

Pt	-1.45233000	0.30139100	0.13477200
Pt	0.77767600	-0.57096800	1.35037700
Pt	1.02653200	1.29485400	-0.34368100
Pt	0.31943100	-1.06934400	-1.18603200
C	-2.81728700	1.57701200	-0.24052900
H	-2.53157400	2.58126400	-0.57795200
H	-2.08660400	1.19416600	1.33424500
C	-2.91885100	-1.16241000	0.44546900
H	-2.49133500	-1.86272500	1.17430200
H	-3.84888300	-0.72986700	0.83597300
H	-3.10708000	-1.66592600	-0.51036700
H	-3.87977700	1.43263200	-0.00985400

3-IM3



¹³3-IM3

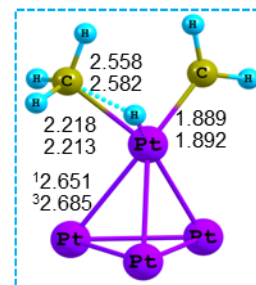
Pt	1.40701500	0.23093800	-0.31043700
Pt	-0.75959500	-1.17229700	-0.93893800
Pt	-1.03558900	1.32866100	-0.24808900
Pt	-0.26728300	-0.41665900	1.54944700
C	2.69206100	1.60380300	-0.29464300
H	2.36984700	2.65398900	-0.32583900
H	1.62200800	-0.05116400	-1.84296600
C	2.94264000	-1.18261400	0.00445900
H	2.52686200	-2.15663500	-0.27927700
H	3.82821200	-0.95432200	-0.60143500
H	3.19229900	-1.16724400	1.07245200
H	3.77782400	1.43813100	-0.33649100

³³3-IM3

Pt	1.45165600	0.16427900	-0.33032700
Pt	-0.79480000	-1.23976800	-0.78589100
Pt	-1.02028600	1.26597500	-0.42519000
Pt	-0.30097300	-0.20068300	1.58783200
C	2.76680800	1.51094900	-0.32004000
H	2.46298800	2.55660900	-0.46699600
H	1.55647900	-0.25210100	-1.84893500
C	2.96138600	-1.24123000	0.07347600
H	2.49866300	-2.22483100	-0.07307200
H	3.81075100	-1.11520500	-0.60838800

H	3.27742800	-1.11481400	1.11548200
H	3.84796000	1.32737600	-0.25973400

3-TS3



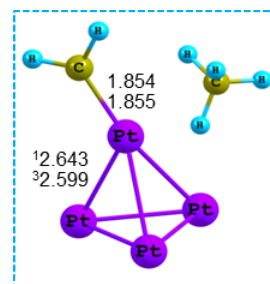
¹³3-TS3

Pt	-1.43585700	0.07509500	0.13992500
Pt	0.83910800	-0.65826500	1.30059800
Pt	0.67114600	1.52463100	-0.17849800
Pt	0.59477700	-0.88341200	-1.26846900
C	-2.83280400	1.34091900	0.01193700
H	-2.61117300	2.39418600	-0.19928800
H	-2.35687200	-0.74109100	1.14881400
C	-2.86039500	-1.61593600	-0.03745900
H	-2.43737200	-2.54359200	0.36044600
H	-3.88897600	-1.46150100	0.31345400
H	-2.84790700	-1.62783800	-1.13247500
H	-3.89411100	1.10214100	0.16489400

³³3-TS3

Pt	1.46371500	-0.02058600	-0.07737900
Pt	-0.80793600	-0.87395800	-1.18846900
Pt	-0.56919900	1.57446900	-0.09062300
Pt	-0.75656300	-0.58853500	1.32063000
C	2.93952700	1.16084700	-0.15433400
H	2.79911600	2.23960400	-0.28770000
H	2.26315700	-1.12756000	-0.88910200
C	2.78002600	-1.70169000	0.50350900
H	2.40518700	-2.69202400	0.22533800
H	3.83365000	-1.58212900	0.22497700
H	2.65478900	-1.54397000	1.58057100
H	3.98537100	0.82270000	-0.15353200

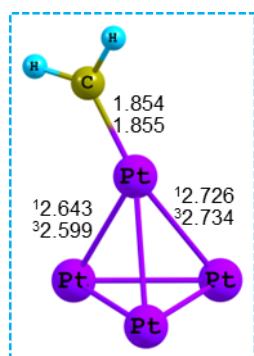
3-IM4



¹ 3-IM4			
Pt	0.17369200	1.58879700	0.02369900
Pt	-0.46019500	-0.72566900	1.31359100
Pt	1.67399600	-0.58260100	-0.11907300
Pt	-0.65071000	-0.69653800	-1.21646600
C	0.96803000	3.26377000	-0.00124300
H	2.04694400	3.45988600	-0.07000100
H	-6.14306000	1.35212500	-0.59082800
C	-6.56731600	0.52302700	-0.01173100
H	-7.65850600	0.62575000	0.02935900
H	-6.30748300	-0.42870100	-0.49093300
H	-6.15943800	0.54289600	1.00611600
H	0.34816600	4.17619600	0.05765000

³ 3-IM4			
Pt	0.17391500	1.57507500	0.03035500
Pt	-0.47578900	-0.75786500	1.29703100
Pt	1.69009400	-0.53102800	-0.10881300
Pt	-0.64538900	-0.71727900	-1.21828000
C	0.96887000	3.25142800	0.01198600
H	2.04554600	3.45792500	-0.05240500
H	-6.17941100	1.45389800	-0.61756100
C	-6.61422800	0.65004500	-0.01144200
H	-7.70312100	0.77324700	0.03365000
H	-6.37415700	-0.31977000	-0.46395300
H	-6.19903900	0.69224800	1.00277900
H	0.34147600	4.15912100	0.07140000

3-IM5

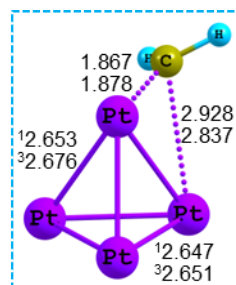


¹ 3-IM5			
Pt	0.86157500	-0.56406800	1.27007600
Pt	-1.54780800	-0.42761000	0.00136300
Pt	0.86075400	-0.56982800	-1.26796800
Pt	0.18620800	1.56736200	-0.00349800
C	-3.36847200	-0.07769200	0.00035200
H	-3.83084600	0.91902300	-0.00200200
H	-4.09516000	-0.90968600	0.00195900

³3-IM5

Pt	0.91977100	-0.50702600	1.26115400
Pt	-1.50710900	-0.52522800	0.00152900
Pt	0.91862400	-0.51167400	-1.25994700
Pt	0.02743300	1.57267700	-0.00278600
C	-3.34757600	-0.29005800	0.00056500
H	-3.88102900	0.66986800	-0.00170700
H	-4.01364500	-1.17193700	0.00219900

3-TS4



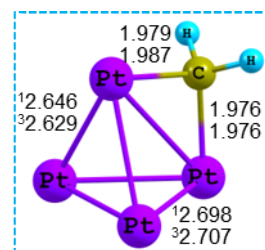
¹3-TS4

Pt	1.13689700	-1.03058600	-0.27092800
Pt	-1.28499800	-0.39368100	-0.96697500
Pt	0.41557600	1.53250100	-0.33234300
Pt	-0.55865000	-0.09840700	1.54465800
C	2.72442500	-0.18140500	0.22178500
H	2.86128400	0.30301100	1.19717600
H	3.50384700	0.01886400	-0.53207500

³3-TS4

Pt	1.20570100	-1.03937700	-0.11930400
Pt	-1.21003100	-0.42457700	-1.03511400
Pt	0.44804300	1.51658300	-0.32048900
Pt	-0.73572600	-0.05805000	1.43962800
C	2.73391900	-0.03829800	0.31714800
H	2.85185300	0.48767500	1.27353700
H	3.52153300	0.16493300	-0.42459700

3-IM6



¹3-IM6

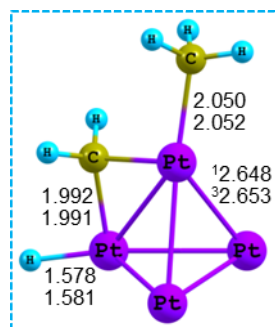
Pt	1.53720200	-0.00040200	0.78163500
Pt	-0.00032300	1.36815600	-0.89300600
Pt	-1.53683000	-0.00062000	0.78209600
Pt	-0.00007600	-1.36727700	-0.89394000
C	0.00021400	0.00135800	2.02620700

H	0.00031900	-0.92926300	2.62710400
H	0.00049800	0.93230900	2.62646000

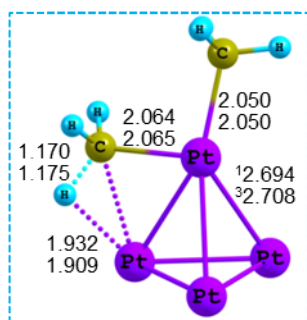
³³-IM6

Pt	-1.49312400	-0.76453000	-0.42088800
Pt	-0.06586900	1.48905700	-0.65218400
Pt	1.57607900	-0.64666700	-0.39127200
Pt	-0.02766300	0.12128400	1.57348500
C	0.09669000	-1.81019400	-0.99306800
H	0.13189800	-2.77785000	-0.45693000
H	0.11289600	-1.89421800	-2.09771500

3-IM7



3-TS5



¹³-TS5

Pt	1.51961900	-0.26620500	0.33711800
Pt	-1.12727600	-0.30619500	1.25206100
Pt	-0.61170800	-1.03811600	-1.11794000
Pt	-0.41594000	1.49832600	-0.48228700
C	3.44228700	-0.87555300	-0.02695100
H	3.43158600	-1.96857400	-0.17151000
H	4.06407500	-0.63230600	0.85148200
C	1.91410500	1.74922000	0.13106700
H	1.06229100	2.55089800	0.15229000
H	2.44380000	1.99932200	1.06686300
H	2.53974700	1.95515800	-0.74478300
H	3.87396400	-0.39569700	-0.91729500

³³-TS5

Pt	1.52167900	-0.28900000	0.29506900
Pt	-1.08469300	-0.33176500	1.27628900
Pt	-0.66333800	-0.99531500	-1.13941600
Pt	-0.41010500	1.50734100	-0.43820400
C	3.45004400	-0.88921600	-0.05695300
H	3.43303900	-1.95569300	-0.33473600
H	4.02337200	-0.76485100	0.87812800
C	1.91444200	1.73053600	0.11673600
H	1.07404900	2.55070400	0.15718000
H	2.45715000	1.96732300	1.04816600
H	2.52975800	1.94928200	-0.76346000
H	3.93934700	-0.31302100	-0.85551700

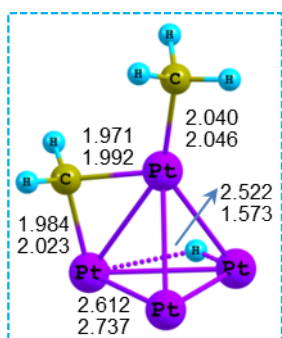
¹³-IM7

Pt	-1.57047200	0.03568100	-0.37577600
Pt	0.97871600	-0.67532400	-1.18844200
Pt	0.23904700	-1.09409900	1.19372100
Pt	0.87091500	1.45601900	0.37007500
C	-3.55998600	0.24928700	0.07162700
H	-3.99120300	-0.76267400	0.15489900
H	-4.05601800	0.78713900	-0.75417200
C	-1.01189700	1.93165300	-0.07306400
H	1.41031300	2.84000900	-0.16186900
H	-1.12653800	2.51034300	-1.00287500
H	-1.49586200	2.40916600	0.79452100
H	-3.72948300	0.79276600	1.01105000

³³-IM7

Pt	1.57384000	0.00162200	0.33105900
Pt	-0.96239200	-0.66053300	1.20898200
Pt	-0.30059700	-1.08475400	-1.19485900
Pt	-0.83910900	1.47504700	-0.34892600
C	3.58822500	0.18447000	-0.01202400
H	4.00097000	-0.83360200	-0.11066300
H	4.05121000	0.68064900	0.85794200
C	1.06323300	1.91212700	0.04415600
H	-1.32784200	2.89746400	0.13926500
H	1.22018200	2.48870100	0.96906100
H	1.53146900	2.38026700	-0.83732600
H	3.81942300	0.75905800	-0.91902800

3-TS6



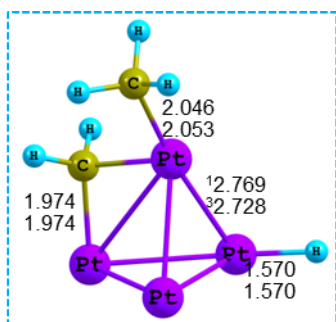
¹³-TS6

Pt	1.56139200	-0.18994200	-0.01506400
Pt	-0.73378600	-0.07409900	1.48954200
Pt	-0.82128700	-1.32062000	-0.83596300
Pt	-0.56720900	1.48397700	-0.59989400
C	3.51454100	-0.66344600	0.33641200
H	3.52097900	-1.71621100	0.67086000
H	3.94832400	-0.03200600	1.12478300
C	1.40031400	1.71571500	-0.49007600
H	-0.83578600	-0.49090000	-2.14480300
H	1.68677300	2.39942000	0.32607700
H	1.83413700	1.95016400	-1.48011200
H	4.10587500	-0.57074700	-0.58726500

³³-TS6

Pt	1.47443100	-0.41144000	0.06448300
Pt	-0.97087700	-0.55122200	1.27662600
Pt	-0.86301400	-0.77262800	-1.24254300
Pt	-0.22597600	1.70389900	-0.08375900
C	3.31629500	-1.29313200	0.19001500
H	3.14828100	-2.37940300	0.28097200
H	3.85418800	-0.92927500	1.07811000
C	1.78891200	1.54333500	-0.15414900
H	-0.38764000	1.49775200	-1.63505300
H	2.24650800	2.02692900	0.72553700
H	2.26038200	1.81552800	-1.10842800
H	3.91106100	-1.08423200	-0.71124700

3-IM8



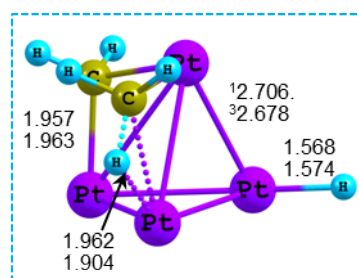
¹³-IM8

Pt	-0.97614500	1.47955800	-0.18124700
Pt	1.62749700	-0.05341000	-0.28073500
Pt	-0.83162400	-1.14430600	-0.93471300
Pt	-0.33929200	-0.49547100	1.46363700
C	3.57323900	0.43376500	0.12521700
H	4.04871500	-0.44557200	0.59173800
H	3.66243700	1.29609600	0.80027200
C	0.91964100	1.78428100	-0.64024800
H	1.37906600	2.55855800	-0.00497300
H	-0.63902800	-2.70176900	-0.96972800
H	1.03215800	1.98662900	-1.72329800
H	4.08540300	0.66074400	-0.82529500

³³-IM8

Pt	-1.14151400	1.33574400	-0.39114500
Pt	1.62414100	0.00320800	-0.28952700
Pt	-0.69145300	-1.36781900	-0.73771500
Pt	-0.28245300	-0.21819100	1.52392300
C	3.47685400	0.82303400	0.04069000
H	4.03761100	0.14075300	0.70137800
H	3.43548000	1.81931900	0.50152000
C	0.72369500	1.67945200	-0.93680900
H	1.13186500	2.58847500	-0.46827600
H	-0.28137600	-2.87882500	-0.61753300
H	0.79504000	1.68944500	-2.04222500
H	3.99788800	0.89651800	-0.92997800

3-TS7

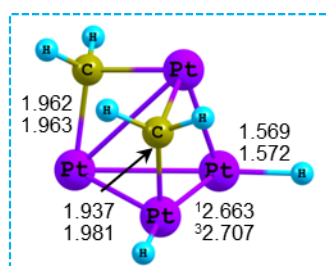


¹³-TS7

Pt	-1.53579400	-0.36243800	-0.91641100
Pt	1.65727300	-0.46793800	-0.55610300
Pt	-0.18877700	-0.80740900	1.39251700
Pt	-0.20154800	1.55089800	0.31915200
C	2.06249300	1.53342500	-0.63664300
H	3.13675800	1.52333600	-0.36156000
H	1.62551100	2.24880800	0.16484900
C	0.12437700	-0.85944200	-1.82463300
H	0.26043300	-0.30621600	-2.76912200
H	0.72955500	-0.73092800	2.66058900
H	0.17927100	-1.96333800	-1.94547100

H	1.91721400	1.96161100	-1.63570900
³³ -TS7			
Pt	-1.07167200	1.49525900	-0.48981200
Pt	1.67474600	0.08123800	-0.10868100
Pt	-0.62175400	-1.20702200	-0.59531900
Pt	-0.48828800	0.11589100	1.67050300
C	1.73593300	0.77750100	1.87937900
H	2.52514500	0.13465800	2.30261600
H	0.93670000	0.79175700	2.73693200
C	0.81509200	1.67574400	-1.00239000
H	1.26481500	2.61789600	-0.64558700
H	-0.27215000	-2.73306300	-0.42948100
H	0.92891300	1.51531200	-2.09329300
H	2.04878000	1.82870200	1.82906000

3-IM9

¹³-IM9

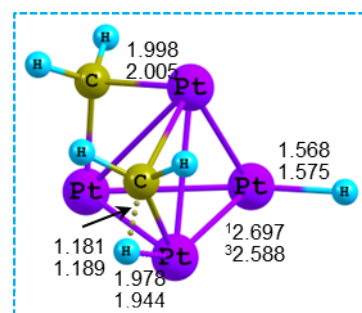
Pt	-1.07204400	1.57378100	-0.65046200
Pt	1.79382400	0.25498700	-0.21615400
Pt	-0.55785800	-1.07032000	-0.40058900
Pt	-0.53651800	0.51553300	1.77982900
C	1.42576900	0.61521600	1.71620800
H	1.91774400	-0.20848400	2.26316400
H	-0.50689900	-0.15224900	3.21116800
C	0.79358200	1.72464800	-1.18489600
H	1.24446700	2.70128000	-0.93609200
H	-0.16768100	-2.52475400	0.04064900
H	0.89703900	1.44687900	-2.25521900
H	1.76090000	1.62798000	2.00629600

³³-IM9

Pt	-1.18898300	-1.21433700	-0.49826000
Pt	1.73545200	-0.05569900	-0.61446300
Pt	0.24019000	-0.18920400	1.60994500
Pt	-0.92519900	1.41360400	-0.23414200
C	0.78229500	1.60334100	-1.21951000
H	1.33063100	2.45208900	-0.76359600
H	-1.72460300	2.22984300	-1.32643100
C	0.55301500	-1.52405000	-1.34833000
H	0.51321700	-1.48663500	-2.44957800

H	0.98251200	0.67704700	2.69079100
H	1.00171400	-2.45752000	-0.95226400
H	0.69079600	1.66906900	-2.31206000

3-TS8

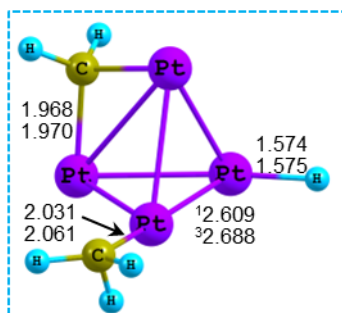
¹³-TS8

Pt	-1.55887700	-0.63403300	-0.67083300
Pt	1.59894700	-0.34222700	-0.72460400
Pt	0.17514500	-0.72294800	1.42800500
Pt	-0.40753200	1.59583000	0.17942900
C	1.39040900	2.03066600	-0.57236800
H	2.35500800	1.87638900	-0.05098700
H	0.97087900	2.99712100	-0.03789200
C	0.05573700	-1.23734800	-1.62349900
H	0.04046900	-0.94629400	-2.69070100
H	1.30323900	-0.56019600	2.50555100
H	0.14028000	-2.33007000	-1.44793200
H	1.51394900	2.26659400	-1.63852200

³³-TS8

Pt	1.46576700	-0.46684700	-0.90011700
Pt	-1.59126600	-0.01715000	-0.74602700
Pt	0.23893100	1.57971600	0.43799300
Pt	0.08269700	-0.83898400	1.34420300
C	-1.46793700	-1.95886600	0.57780600
H	-2.48988300	-1.86146800	0.97066900
H	-0.87216700	-2.52936200	1.43480000
C	-0.13363400	-0.45653800	-2.05042700
H	-0.31210100	-1.43618900	-2.52933500
H	-0.54371400	2.56571900	1.38471000
H	-0.06594800	0.38315500	-2.77024000
H	-1.40478400	-2.65470300	-0.26696000

3-IM10



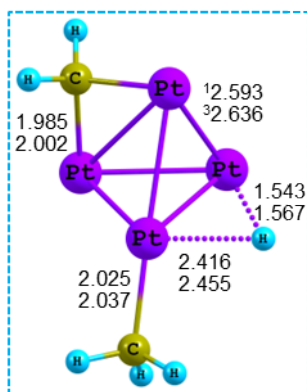
¹3-IM10

Pt	1.30506100	-0.70069900	-0.83743300
Pt	-1.57034000	0.37158800	-0.50076900
Pt	0.46292300	1.67417100	0.26647700
Pt	0.11368600	-0.78030000	1.42916100
C	-0.05179600	-2.69029000	2.07524900
H	-0.68757300	-3.31506500	1.43234300
H	-0.53483400	-2.59047800	3.07069300
C	-0.39150400	-0.49931800	-1.83349200
H	-0.83829100	-1.47203500	-2.11631500
H	-0.24132500	2.83816700	1.03632400
H	-0.19956000	0.17491200	-2.69166800
H	0.93566800	-3.16467400	2.18641700

³3-IM10

Pt	-0.62859600	1.52753700	0.61976000
Pt	0.81390500	-1.20197600	0.91021100
Pt	1.30726800	0.47172100	-0.98623700
Pt	-1.18227000	-0.65859500	-0.70228800
C	-3.02004600	-1.45437300	-0.33056000
H	-3.01310200	-2.50073400	-0.68466000
H	-3.75781900	-0.87309900	-0.91258200
C	0.20182700	0.37038200	1.99237100
H	-0.55077500	0.03370000	2.72760300
H	2.23429500	-0.39858100	-1.89486100
H	1.09285600	0.85656200	2.43026800
H	-3.30014200	-1.43152900	0.73067300

3-TS9



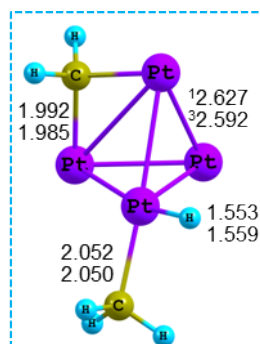
¹3-TS9

Pt	-1.39703300	-0.08682300	-1.11659800
Pt	0.88585800	1.46393800	0.21426500
Pt	1.14397800	-0.97625800	-0.39511500
Pt	-0.94789000	-0.36810300	1.42184800
C	3.04084000	-1.56127000	0.00519500
H	3.78151200	-0.94164200	-0.52213700
H	3.07408200	-2.59704700	-0.39639000
C	-0.40583900	1.60944400	-1.28569300
H	-1.03612800	2.50759200	-1.13526700
H	-0.45361900	-1.81464600	1.21163100
H	0.12791900	1.59011500	-2.25708700
H	3.27296100	-1.58821200	1.07901900

³3-TS9

Pt	-1.50874300	-0.68686400	-0.70234100
Pt	0.42713600	1.61931900	-0.37939400
Pt	1.21871900	-0.91399800	-0.36317100
Pt	-0.40175300	0.00536600	1.58770600
C	3.22401700	-1.13083200	-0.08153700
H	3.72490400	-0.88036700	-1.03312200
H	3.41135700	-2.18812600	0.17803900
C	-1.18732500	1.12334600	-1.45348300
H	-2.02676100	1.81650400	-1.27176900
H	0.60993600	-1.11549300	2.00654700
H	-0.92220500	1.04559700	-2.52468500
H	3.62464900	-0.49143900	0.71669600

3-IM11



¹3-IM11

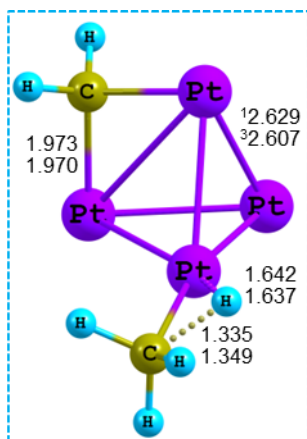
Pt	-1.14543600	-0.81822300	-0.95333100
Pt	0.28532800	1.66113700	0.19875200
Pt	1.06949100	-1.00635700	0.48041600
Pt	-1.22222200	0.10343600	1.53493000
C	2.86200900	-1.40493300	-0.43285800
H	2.88689900	-2.37724200	-0.94194100
H	3.63040400	-1.39963500	0.36090600
C	-0.64111300	1.03652400	-1.43550000

H	-1.55135000	1.62473300	-1.65122800
H	1.13821200	-2.51921500	0.83339000
H	0.09328900	1.02809100	-2.26695900
H	3.06772500	-0.60042800	-1.15501300

³³-IM11

Pt	-1.63069500	-0.61500600	-0.54684000
Pt	0.61061600	1.59537200	-0.52907300
Pt	1.05147400	-1.15116300	-0.25214600
Pt	-0.29921000	0.25475100	1.49937500
C	3.07967600	-1.40253100	-0.08663700
H	3.41171200	-1.89642200	-1.01718600
H	3.35982500	-2.02994800	0.76923400
C	-1.04996900	1.04405600	-1.46593200
H	-1.82076200	1.83041800	-1.37861000
H	0.98938300	-2.66984600	0.09432000
H	-0.78637100	0.78349900	-2.51194200
H	3.55755800	-0.41529400	-0.00300000

3-TS10



¹³-TS10

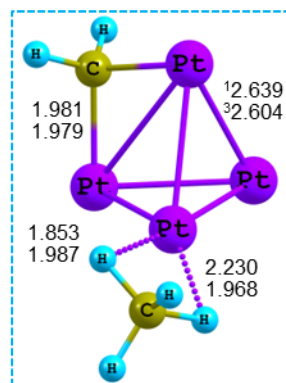
Pt	-1.44130900	-0.62588700	0.21581700
Pt	-0.26747700	1.59386200	-0.62294500
Pt	1.26211500	-1.09807100	-0.72904700
Pt	0.77193600	0.25447800	1.38675700
C	1.02413700	0.57736900	-1.74376700
H	-3.07310000	-0.47685600	0.32669400
H	1.97321200	1.13678900	-1.83100700
C	-3.36179200	-1.49883400	-0.48178700
H	-4.41166100	-1.18015600	-0.37530100
H	-3.26634100	-2.50275600	-0.04851200
H	-3.11314700	-1.48239400	-1.54894000
H	0.54632100	0.33242400	-2.71503200

³³-TS10

Pt	-1.46851100	-0.56109900	0.16203100
Pt	-0.16457400	1.59535500	-0.65322900

Pt	1.24304000	-1.16452500	-0.67218200
Pt	0.70742100	0.25912600	1.40793500
C	1.12377300	0.50232100	-1.71504000
H	-3.09068300	-0.35182000	0.22851400
H	2.10200900	1.01469000	-1.76056500
C	-3.38555200	-1.47703400	-0.45547600
H	-4.43091800	-1.13361900	-0.39645900
H	-3.30594400	-2.42443700	0.09387900
H	-3.12741100	-1.59243800	-1.51484800
H	0.66834300	0.28505300	-2.70270700

3-IM12



¹³-IM12

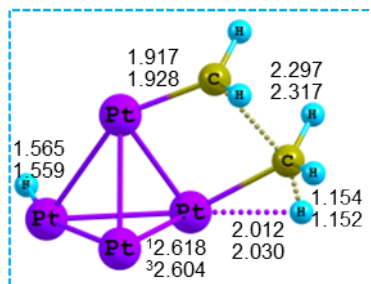
Pt	-0.55317000	-1.53350200	-0.69573800
Pt	-0.55230000	1.53384000	-0.69564200
Pt	1.51244600	-0.00046900	0.20103600
Pt	-0.76271100	0.00015800	1.44192000
C	3.80350100	-0.00053900	-0.43417300
H	2.84167400	-0.00078800	-1.08948800
H	3.69241000	0.00035400	0.67188600
C	-1.20815800	0.00038900	-1.76373900
H	-2.31421800	0.00069400	-1.79781300
H	4.33882400	0.90734500	-0.73089700
H	-0.72204800	0.00028300	-2.75966100
H	4.33862000	-0.90897600	-0.72955200

³³-IM12

Pt	0.66074800	1.52553900	-0.61967400
Pt	0.66479100	-1.52396000	-0.62007500
Pt	-1.55805200	-0.00148800	-0.01857700
Pt	0.55623200	0.00027900	1.48814100
C	-3.82813900	-0.00463400	-0.47477400
H	-3.06127600	-0.00257800	-1.31859900
H	-3.42756300	-0.00441400	0.59469000
C	1.53128600	0.00198700	-1.53523300
H	2.62082800	0.00357500	-1.34625000
H	-4.42296200	-0.91574700	-0.59429900

H	1.24832200	0.00173000	-2.60795100
H	-4.42634800	0.90442900	-0.59309100

3-TS11



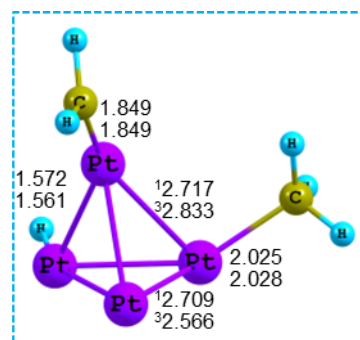
¹³3-TS11

Pt	0.76811200	-0.55023000	1.22490200
Pt	0.55380200	1.24312300	-0.59940100
Pt	-1.67025700	0.41643300	0.48007300
Pt	-0.22870200	-1.20232700	-1.11276500
C	2.67814900	1.09434300	-0.75481500
H	2.23227400	1.77926400	-1.56973200
H	3.22527000	0.35883500	-1.34865000
C	2.64474400	-0.56404100	0.83429100
H	3.10214200	-1.27638900	0.14204700
H	-2.13913900	1.53242900	1.47184400
H	3.34555200	-0.04787000	1.50769100
H	3.30616400	1.72595900	-0.11914300

³³3-TS11

Pt	0.72887200	-0.61443900	1.19035000
Pt	0.56496100	1.27337700	-0.51528100
Pt	-1.71504600	0.37962700	0.44939100
Pt	-0.15854300	-1.14386600	-1.16027700
C	2.70745300	1.18794800	-0.60322000
H	2.28410800	1.95562900	-1.35080400
H	3.27418100	0.50348200	-1.23780600
C	2.63671800	-0.55568200	0.92115200
H	3.16193600	-1.22061400	0.23020300
H	-2.15440700	1.43623800	1.50849200
H	3.27364800	-0.01672000	1.63553600
H	3.31646900	1.76184200	0.10055400

3-IM13



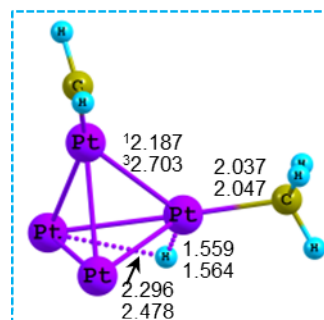
¹³3-IM13

Pt	1.10029300	0.99866300	0.49590200
Pt	-1.27576400	0.54705700	-0.74149200
Pt	-0.69422200	-0.91384100	1.17873500
Pt	0.92606900	-1.01533300	-0.97005200
C	-2.84269600	1.77787900	-0.38223400
H	-2.82524500	2.46825300	-1.25396400
H	-2.74001100	2.36304500	0.54065600
C	2.83376200	1.64166800	0.48900700
H	3.69628000	1.24861700	-0.06044800
H	-1.71963900	-0.44183300	2.27211900
H	3.03629500	2.53436000	1.11207800
H	-3.79130600	1.21971100	-0.37228800

³³3-IM13

Pt	1.33565100	-0.23790600	-0.80434300
Pt	-1.43157200	-0.62905700	-0.34000100
Pt	-0.34469900	1.68166100	-0.07017500
Pt	0.33419300	-0.49530200	1.51764200
C	-1.81389600	-2.18375000	-1.58511400
H	-2.26489100	-2.97375400	-0.95961400
H	-0.92245500	-2.56273700	-2.09684000
C	3.08237100	-0.83512700	-0.91353600
H	3.74176800	-1.11315400	-0.08247900
H	-0.87426500	2.49921100	-1.29007300
H	3.56378100	-0.84468300	-1.90956000
H	-2.55353400	-1.80446400	-2.31307200

3-TS12



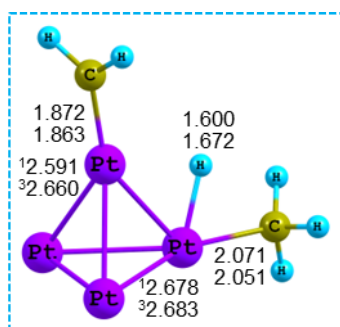
¹³3-TS12

Pt	-0.42165000	1.37940400	-0.51573000
Pt	1.64725900	-0.17840600	0.19856100
Pt	-0.59335900	-1.23031200	-0.99627900
Pt	-0.95916700	-0.35088500	1.29777500
C	3.56451200	0.50819600	0.23414700
H	4.21696000	-0.28809200	0.62990400
H	3.60636600	1.38793900	0.89964300
C	-1.13338100	3.05458200	-0.17178800
H	-1.52050400	3.44152700	0.77821300
H	1.70123400	-1.25467400	-0.92842800
H	-1.23705100	3.73813600	-1.03596500
H	3.90664000	0.79724600	-0.76994100

³³-TS12

Pt	-0.93999900	1.22335900	-0.35125400
Pt	1.56476900	0.21212400	-0.24649000
Pt	-0.55968400	-1.33478300	-0.90336100
Pt	-0.27936500	-0.53857900	1.48494300
C	3.27009300	1.30512300	0.04806700
H	4.01044700	0.72588900	0.61787400
H	3.02310300	2.23409700	0.58632600
C	-1.85549000	2.75620200	0.16051400
H	-2.06875000	3.05897700	1.19482900
H	1.91314400	-1.19131300	-0.84230300
H	-2.33003400	3.39869700	-0.60261300
H	3.67827800	1.56022600	-0.94495100

3-IM14



¹³-IM14

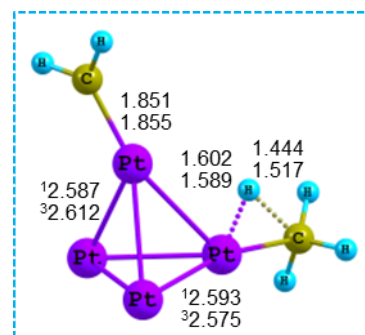
Pt	-1.33451700	0.79796300	-0.51020300
Pt	1.54445700	0.75507500	0.14007700
Pt	0.29531100	-1.33358000	-0.94471000
Pt	-0.50096300	-0.73219000	1.31109600
C	2.88846100	2.04395100	0.09956400
H	0.21776300	1.66593000	-0.30381600
H	3.90300500	1.82486900	0.47515900
C	-2.64940900	2.26289000	-0.02252100
H	-2.23863300	3.05125300	0.62114000

H	-3.58081000	1.86539600	0.40579200
H	-2.86353600	2.69863500	-1.02605600
H	2.79341800	3.04597400	-0.34279800

³³-IM14

Pt	-1.52936000	0.45934900	-0.29570900
Pt	1.17905400	1.07408300	-0.21699300
Pt	0.36602600	-1.31276100	-0.97764700
Pt	0.08235400	-0.68441500	1.45122600
C	2.58262200	2.20365700	0.25639000
H	-0.50290400	1.77768900	-0.22790000
H	2.99553800	2.30146500	1.27001900
C	-3.09972800	1.71943000	0.09351700
H	-2.86632100	2.51885600	0.80833300
H	-3.92931800	1.10549800	0.48256600
H	-3.39570200	2.17650300	-0.86796800
H	3.15153200	2.75354400	-0.51290300

3-TS13



¹³-TS13

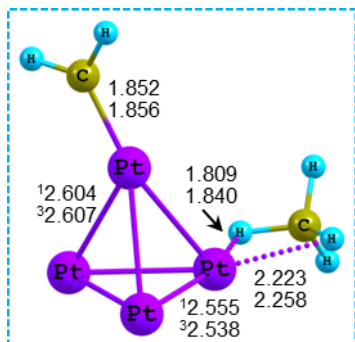
Pt	-1.60619700	0.25569300	0.09532600
Pt	0.91348300	1.22956700	-0.42101200
Pt	0.15809500	-1.26590100	-1.04370400
Pt	0.70567700	-0.67668500	1.31577800
C	2.31693000	2.39956300	-0.12417500
H	-2.16627400	1.19321100	1.26798100
H	3.01631900	2.39012800	0.72162000
C	-3.29640600	1.54487300	0.44158400
H	-3.36411100	2.42409300	1.10085000
H	-4.14392100	0.87897000	0.64700400
H	-3.30731500	1.91865100	-0.59437700
H	2.49962200	3.19975600	-0.86581800

³³-TS13

Pt	1.47293400	-0.57022400	-0.24162800
Pt	-1.32470600	-0.87596700	-0.42568000
Pt	-0.02988000	1.43127900	-0.84681000
Pt	-0.19871700	0.47166500	1.50746700
C	-2.86755600	-1.85071400	-0.09254600
H	1.56987300	-2.12468400	0.07409100

H	-3.36455200	-1.95942700	0.88148400
C	3.07741900	-1.96253000	0.10429000
H	3.01817500	-3.00390700	0.45481900
H	3.64580700	-1.38711000	0.84689300
H	3.56752700	-1.96323600	-0.88076500
H	-3.42727500	-2.30884200	-0.92824200

3-IM15



¹³3-IM15

Pt	-1.57506700	0.26263900	0.02265400
Pt	0.95548800	1.21498900	-0.41572100
Pt	0.16621700	-1.28966200	-1.02037400
Pt	0.61987500	-0.66426900	1.35579400

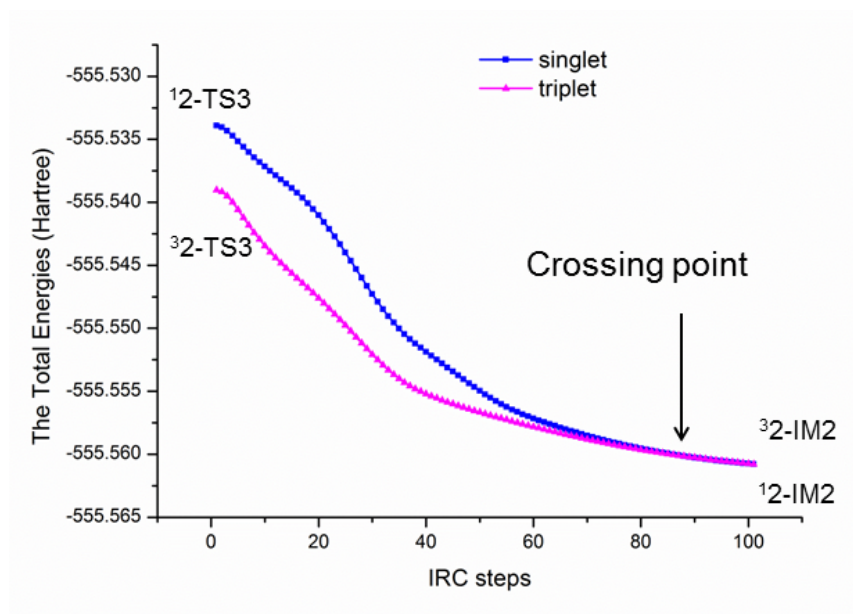
C	2.35633400	2.38808600	-0.11578400
H	-2.45426700	1.31892200	1.19847300
H	3.04206100	2.38350100	0.74172100
C	-3.28489900	1.77680400	0.50068600
H	-3.14219800	2.85443600	0.63254800
H	-4.23078800	1.42733200	0.92716100
H	-3.27301700	1.55981800	-0.58889100
H	2.54811600	3.19100200	-0.85190900

³³3-IM15

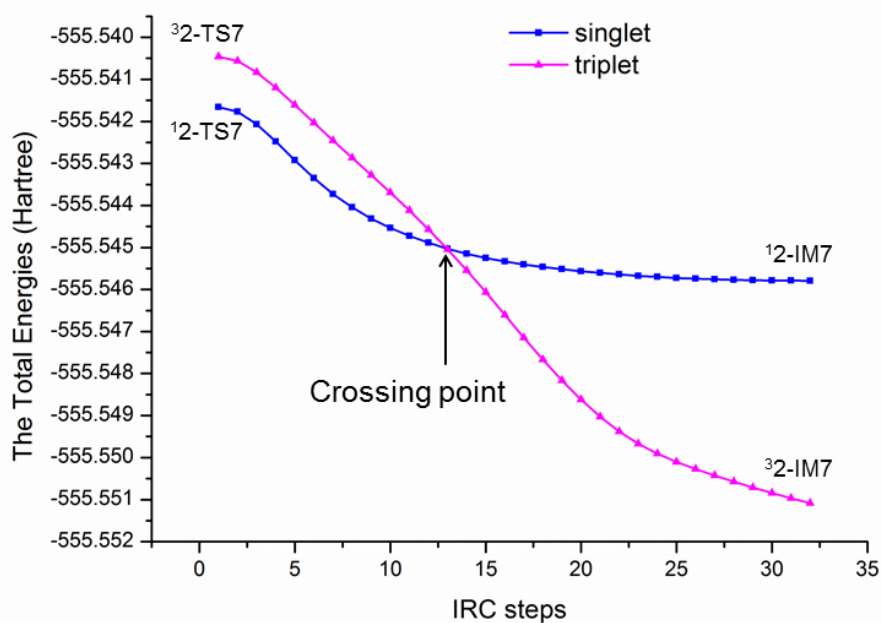
Pt	-1.47451500	0.49030400	-0.10367100
Pt	1.22180900	0.97046100	-0.43792000
Pt	0.00362600	-1.39912700	-0.93119100
Pt	0.33497100	-0.57552800	1.46465000
C	2.72998400	2.01417700	-0.15535200
H	-2.25213700	1.79973800	0.92806600
H	3.30012000	2.08886000	0.78086500
C	-2.95654400	2.32560900	0.16273700
H	-2.62097400	3.36768600	0.17384300
H	-3.95940900	2.20711400	0.58652600
H	-2.97278900	1.98349300	-0.89232000
H	3.16505900	2.59784100	-0.98698100

Table S4: IRC analysis of 2-TS3, 2-TS7, 3-TS6 and 3-TS11 for the minimum energy crossing points (MECPs).

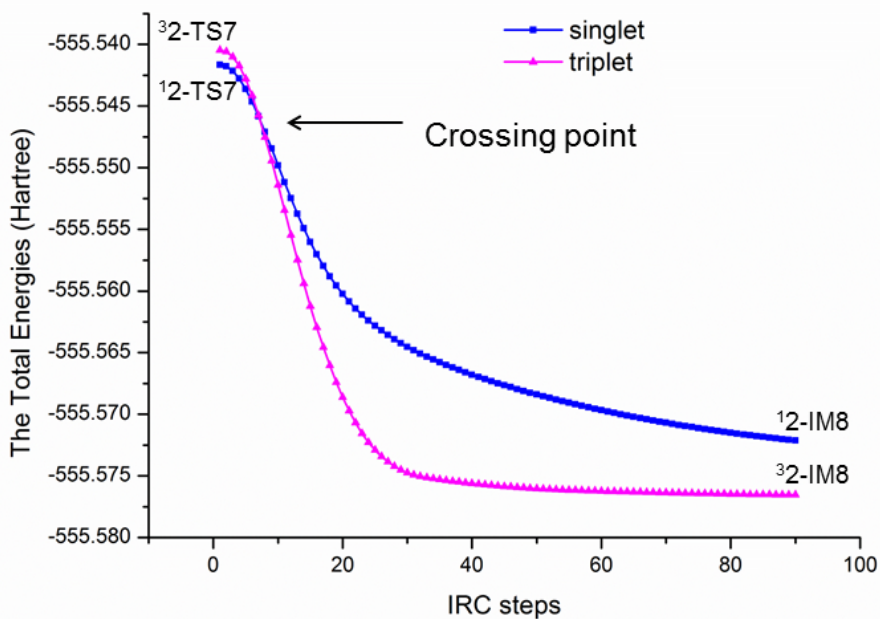
1. IRC analysis for $^12\text{-TS3} \rightarrow ^12\text{-IM2}$ and $^32\text{-TS3} \rightarrow ^32\text{-IM2}$.



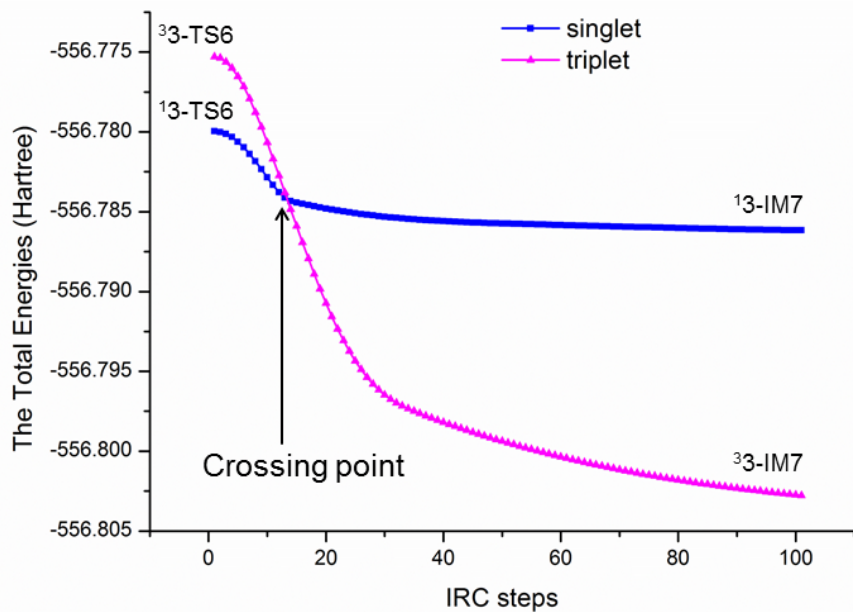
2. IRC analysis for $^12\text{-TS7} \rightarrow ^12\text{-IM7}$ and $^32\text{-TS7} \rightarrow ^32\text{-IM7}$.



3. IRC analysis for ${}^1_2\text{-TS7} \rightarrow {}^1_2\text{-IM8}$ and ${}^3_2\text{-TS7} \rightarrow {}^3_2\text{-IM8}$.



4. IRC analysis for ${}^1_3\text{-TS6} \rightarrow {}^1_3\text{-IM7}$ and ${}^3_3\text{-TS6} \rightarrow {}^3_2\text{-IM7}$.



5. IRC analysis for $^1\text{3-TS11} \rightarrow ^1\text{3-IM13}$ and $^3\text{3-TS11} \rightarrow ^3\text{3-IM13}$.

