

Supporting Information

Mechanisms of the PtCl₂-Catalyzed Intramolecular Cyclization of *o*-Isopropyl-Substituted Aryl Alkynes for the Synthesis of Indenes and Comparison of Three sp³ C-H Bond Activation Modes

Yi Wang,^{†,§} Wei Liao,^{†,§} Genping Huang,[‡] Yuanzhi Xia,[‡] and Zhi-Xiang Yu^{*,†}

[†]Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of Ministry of Education, College of Chemistry, Peking University, Beijing 100871, China

[‡]College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, Zhejiang Province 325035, China

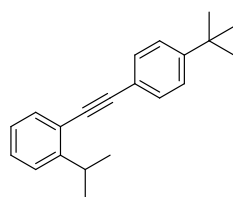
[§]These authors contributed equally

*E-mail: yuzx@pku.edu.cn

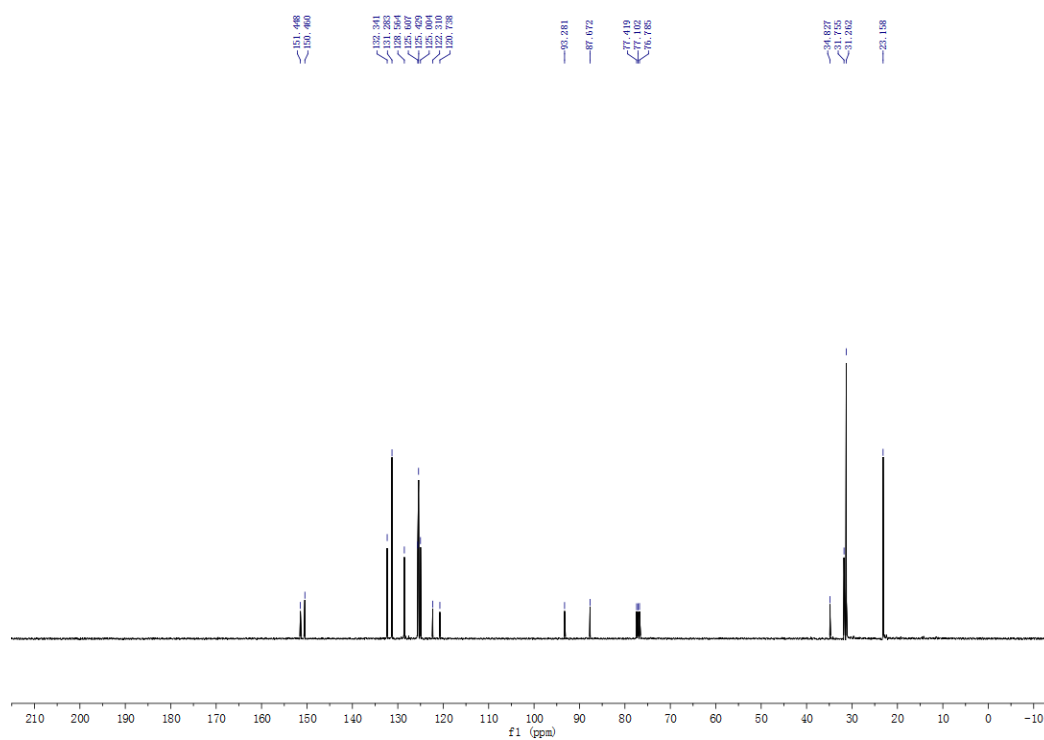
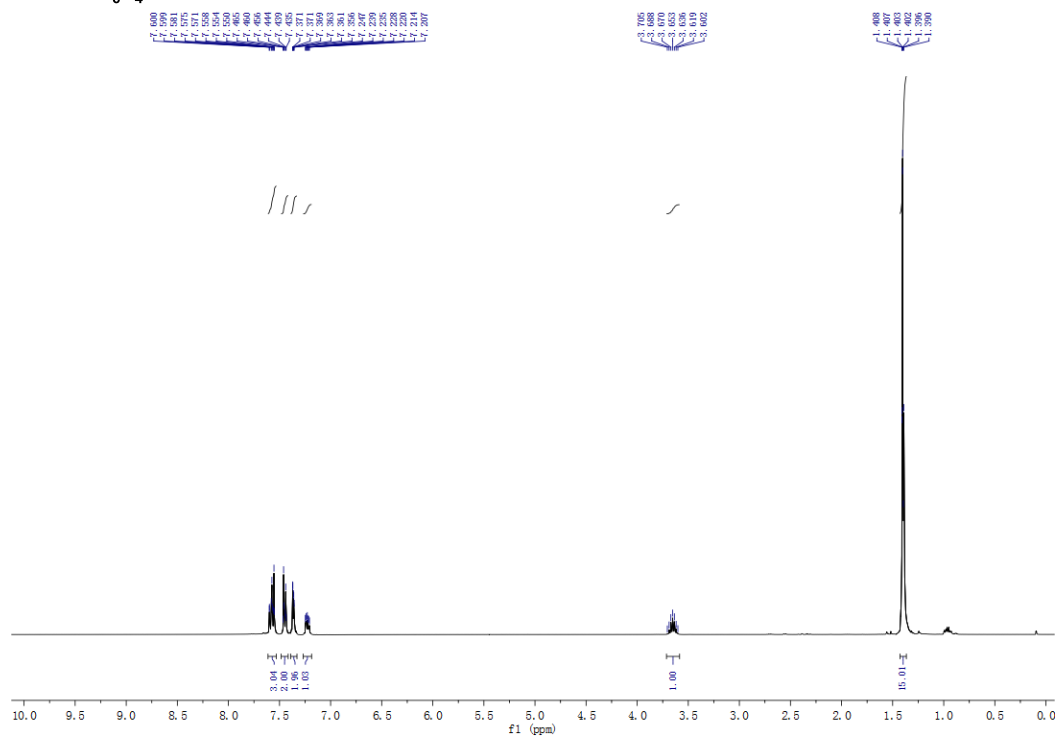
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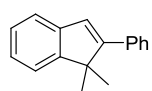
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1. ^1H and ^{13}C -NMR Spectra

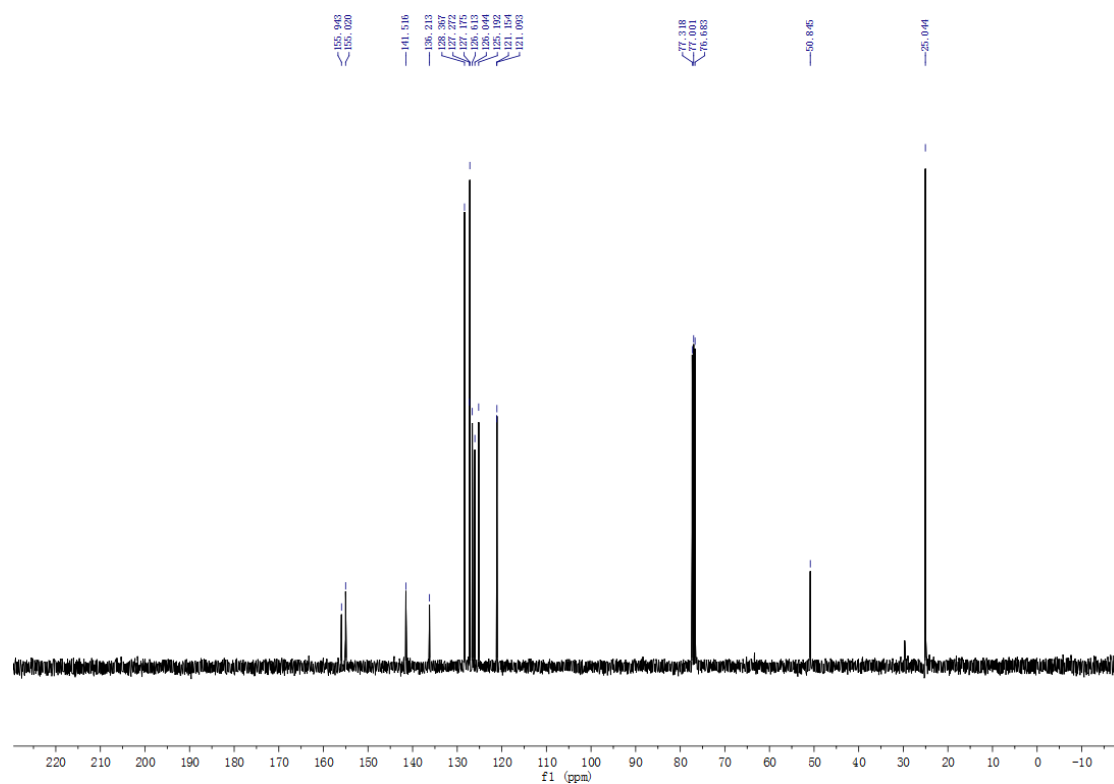
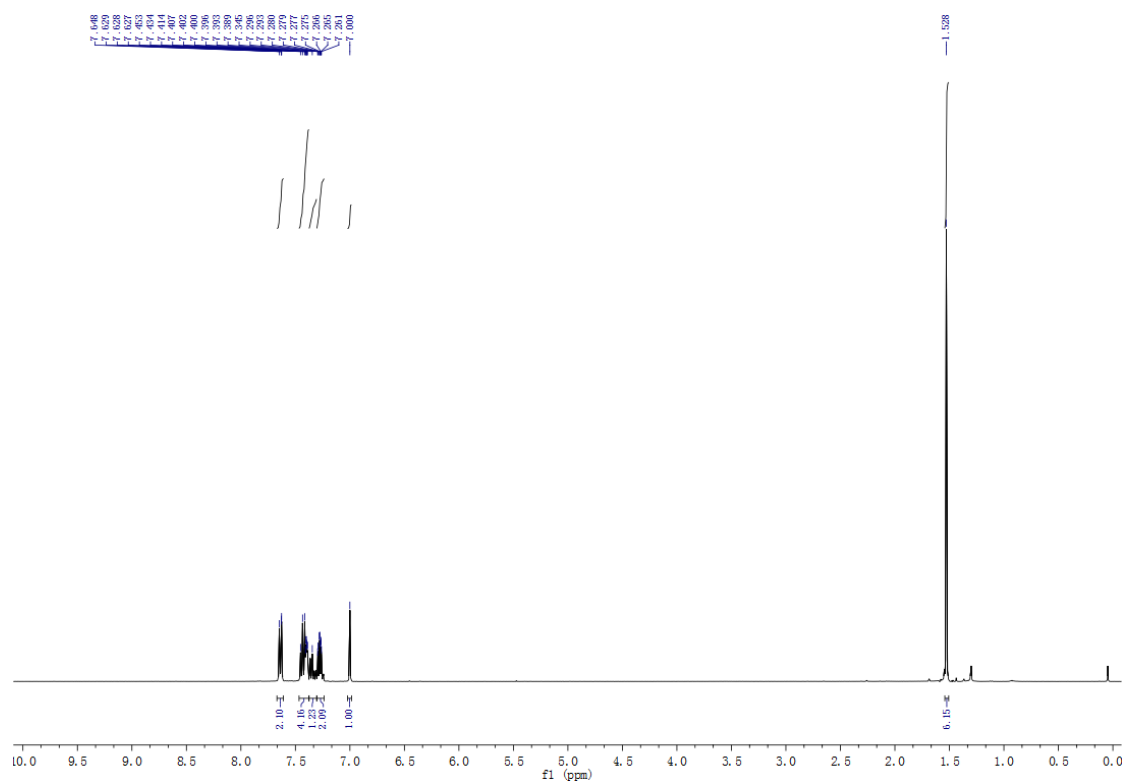


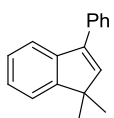
3- $t\text{BuC}_6\text{H}_4$



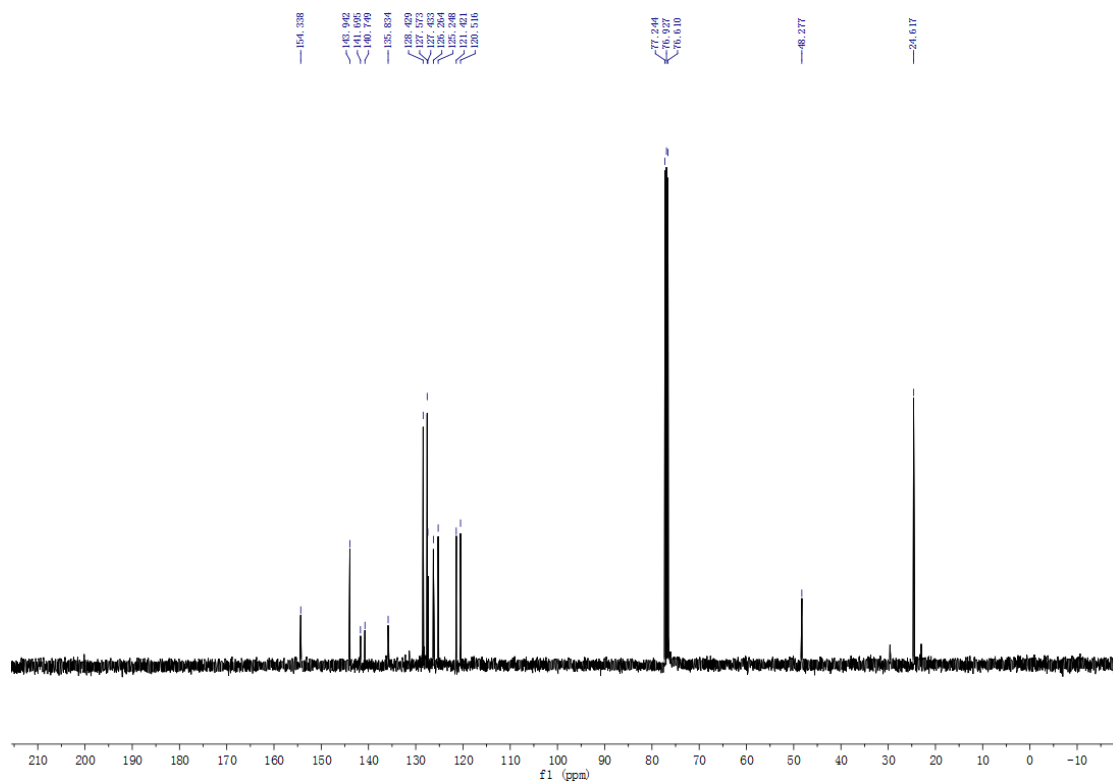
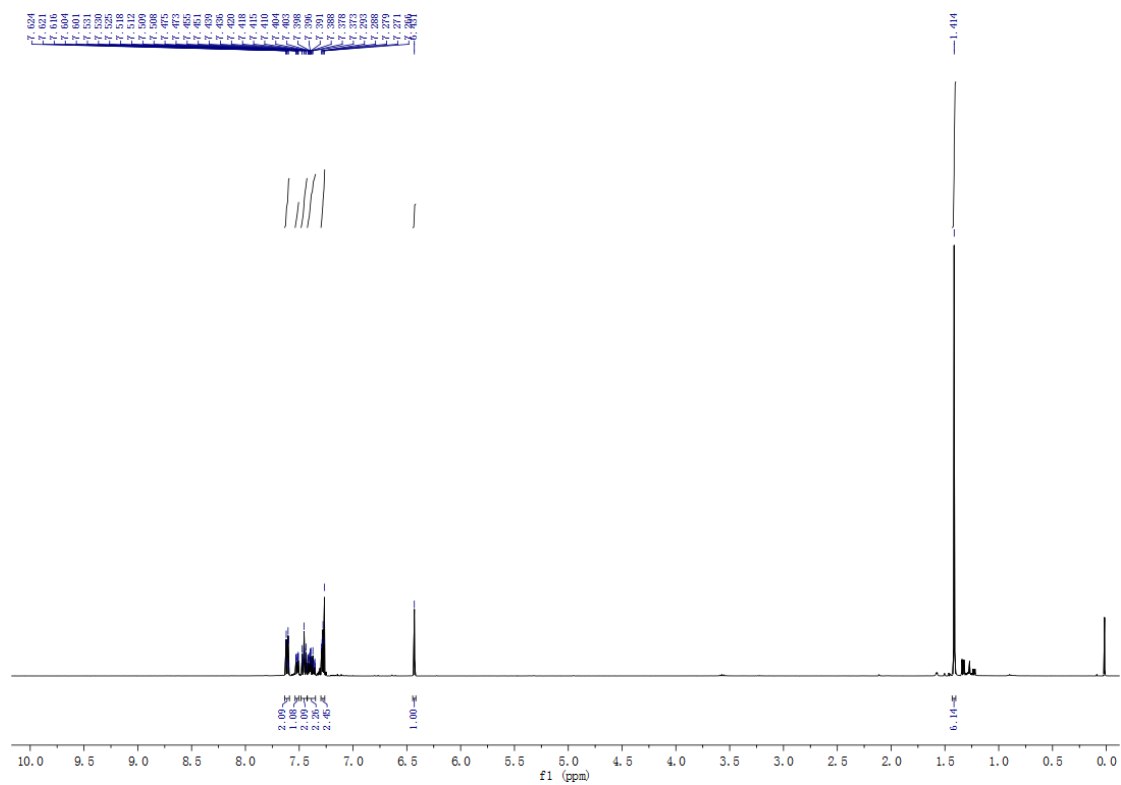


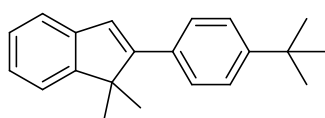
3P-C₆H₅



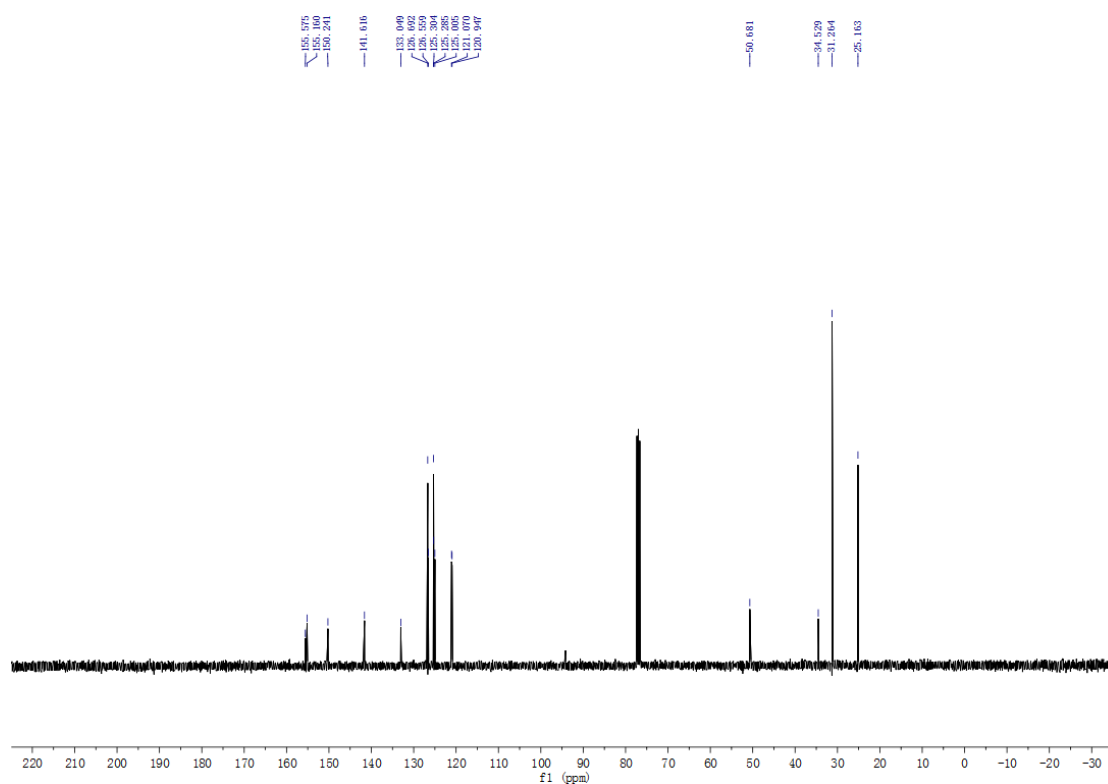
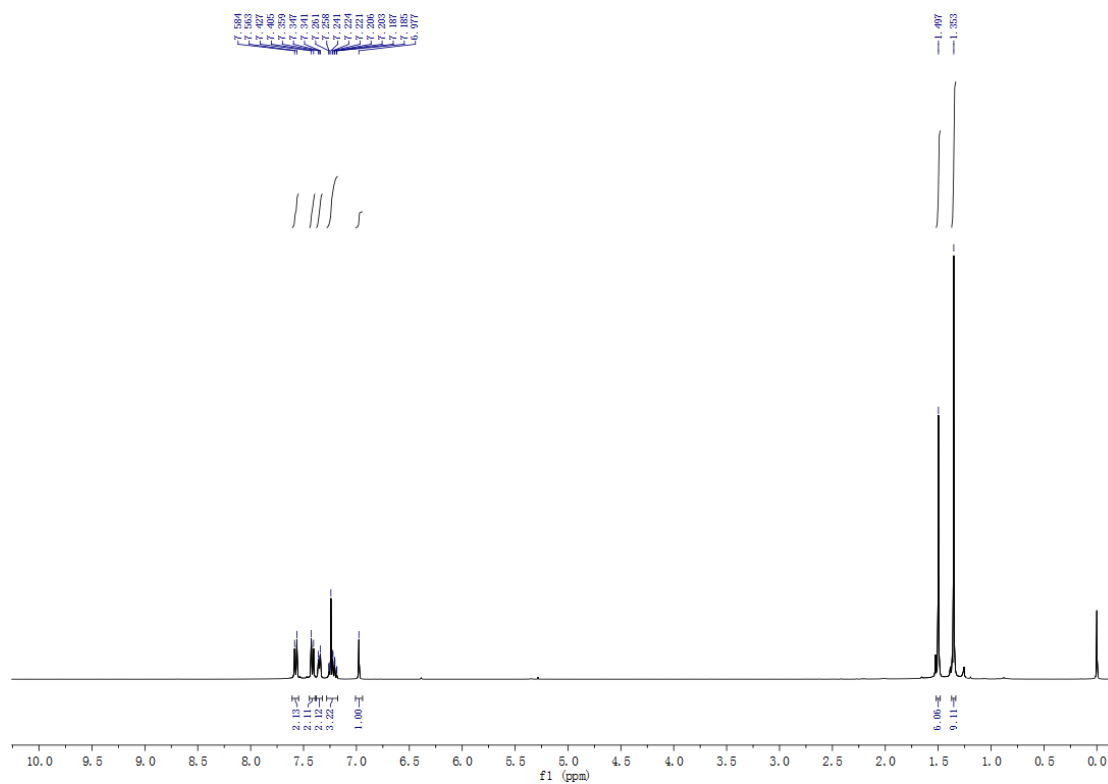


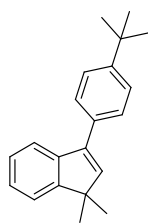
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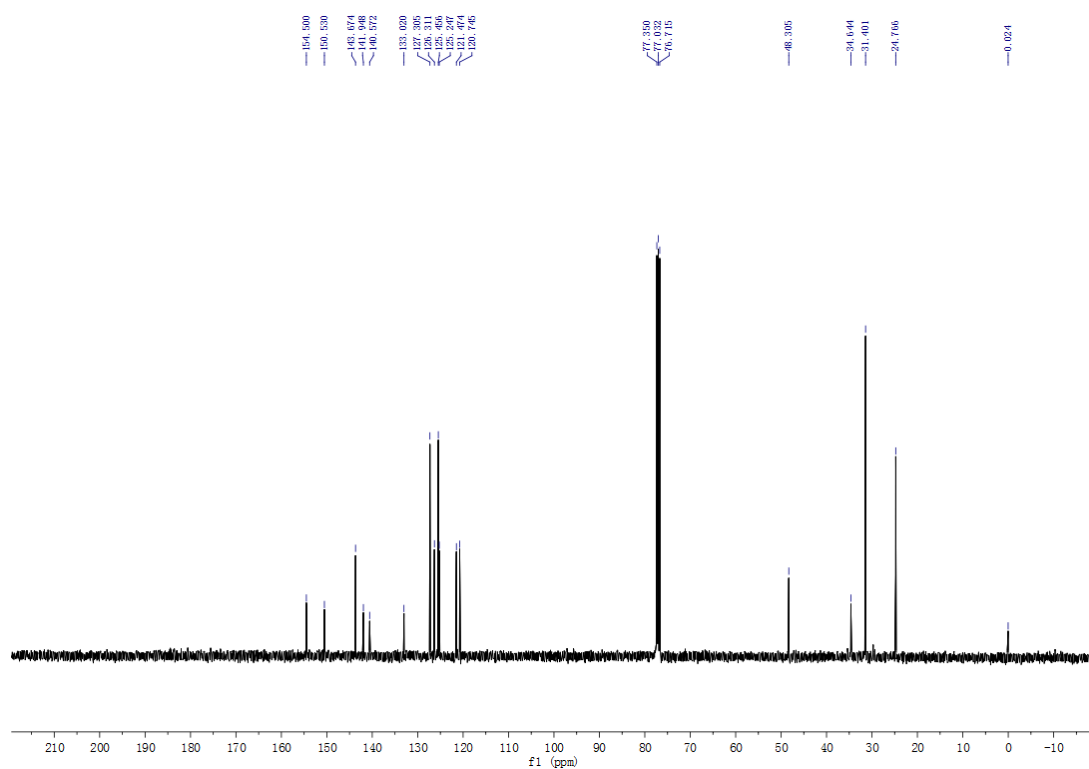
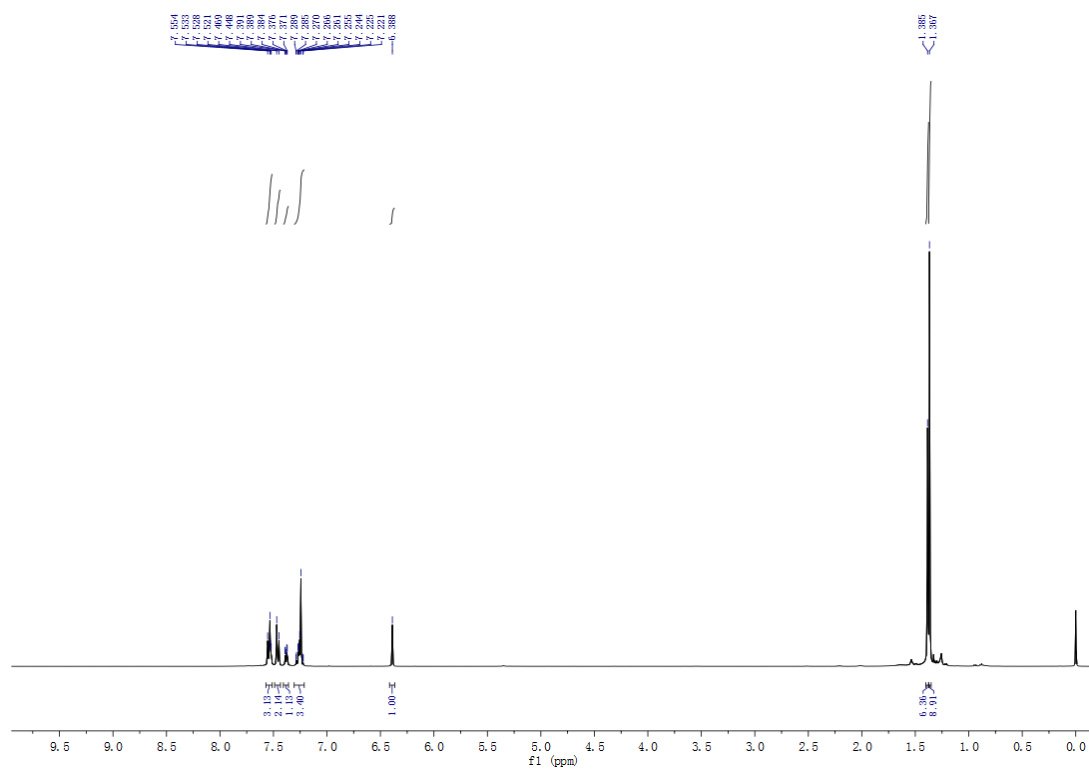


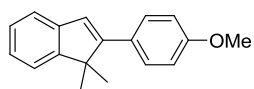
3P-^tBuC₆H₄



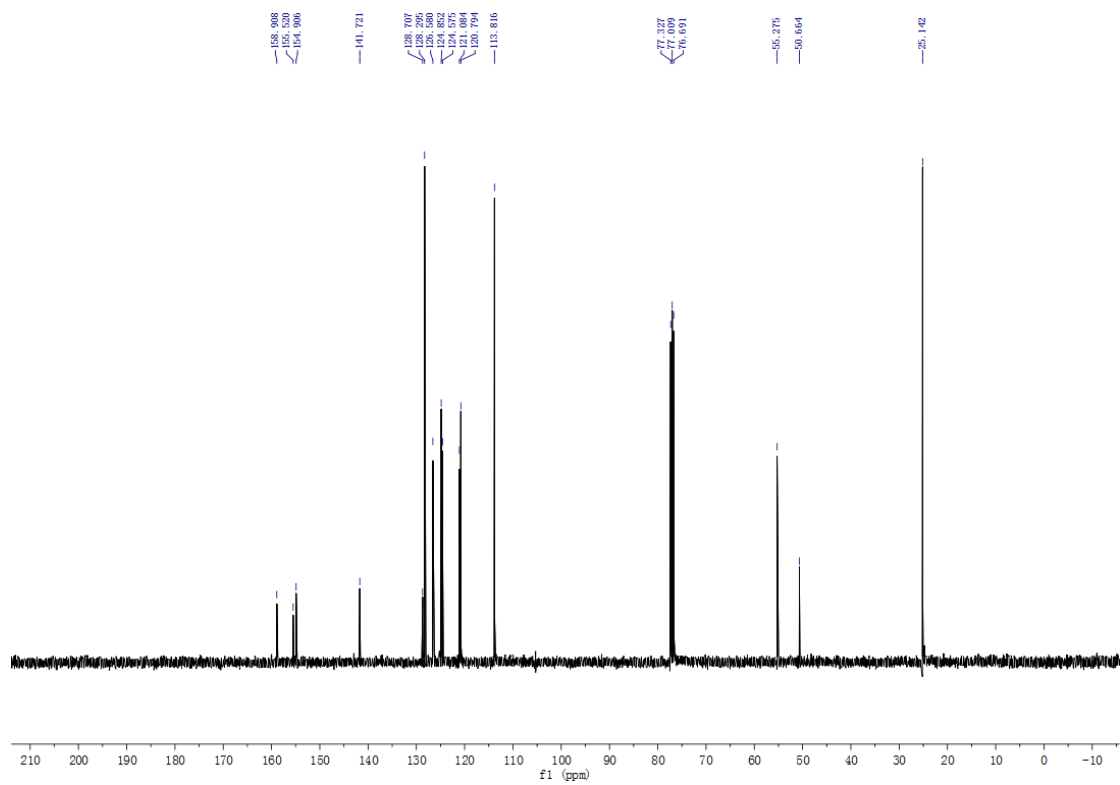
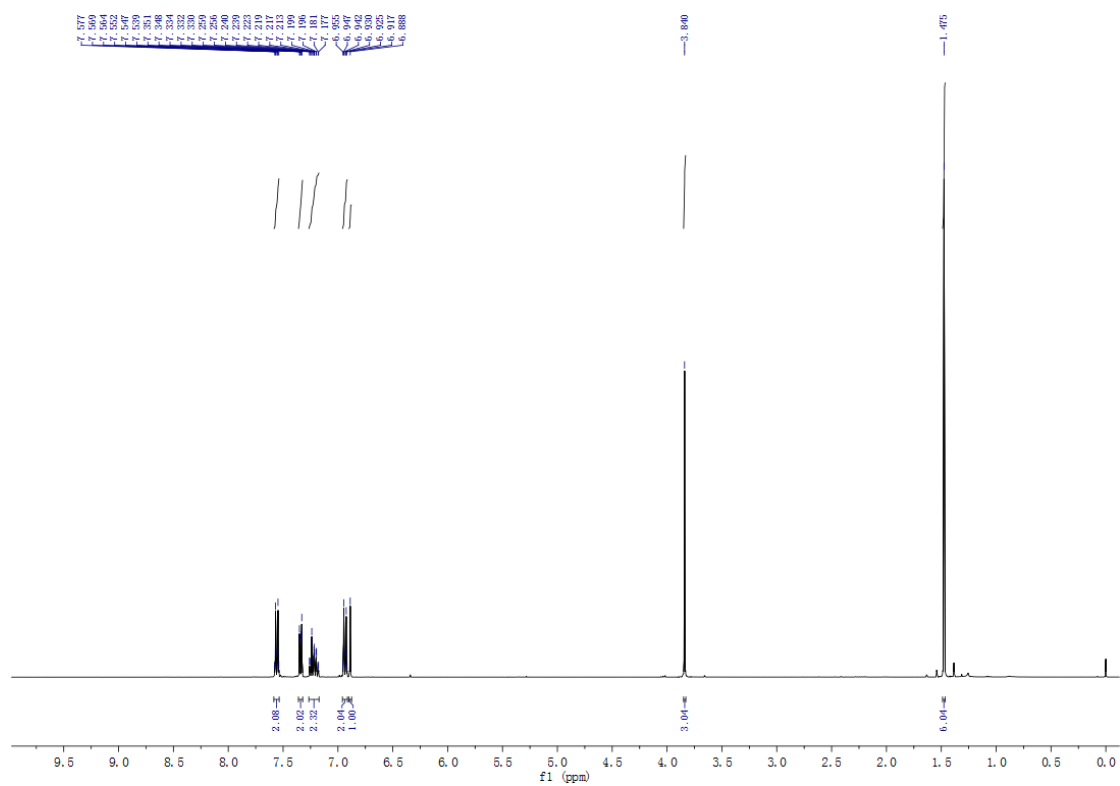


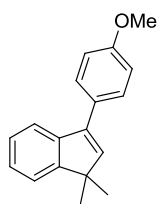
3P'-tBuC₆H₄



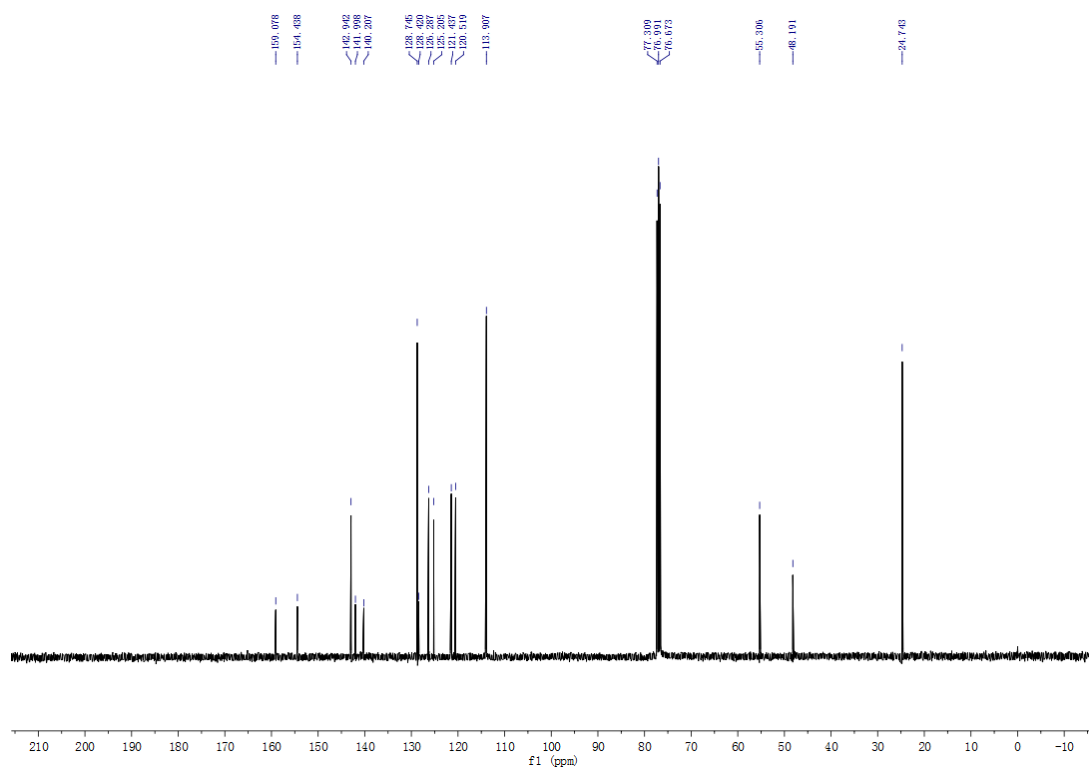
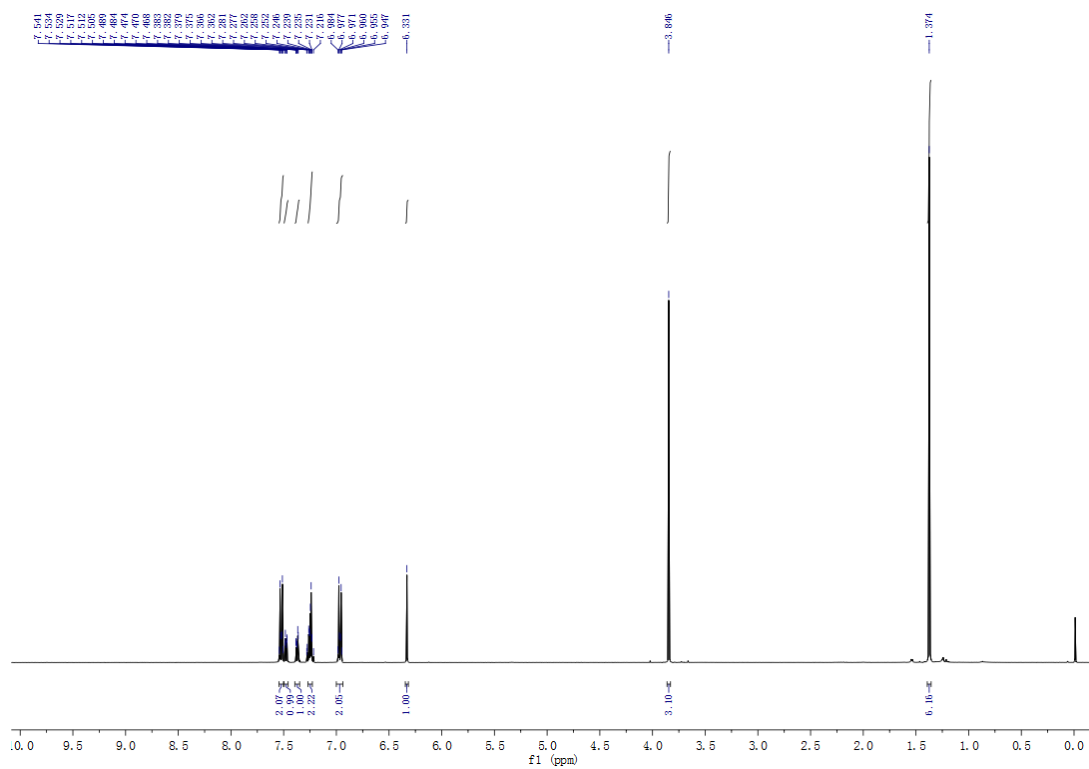


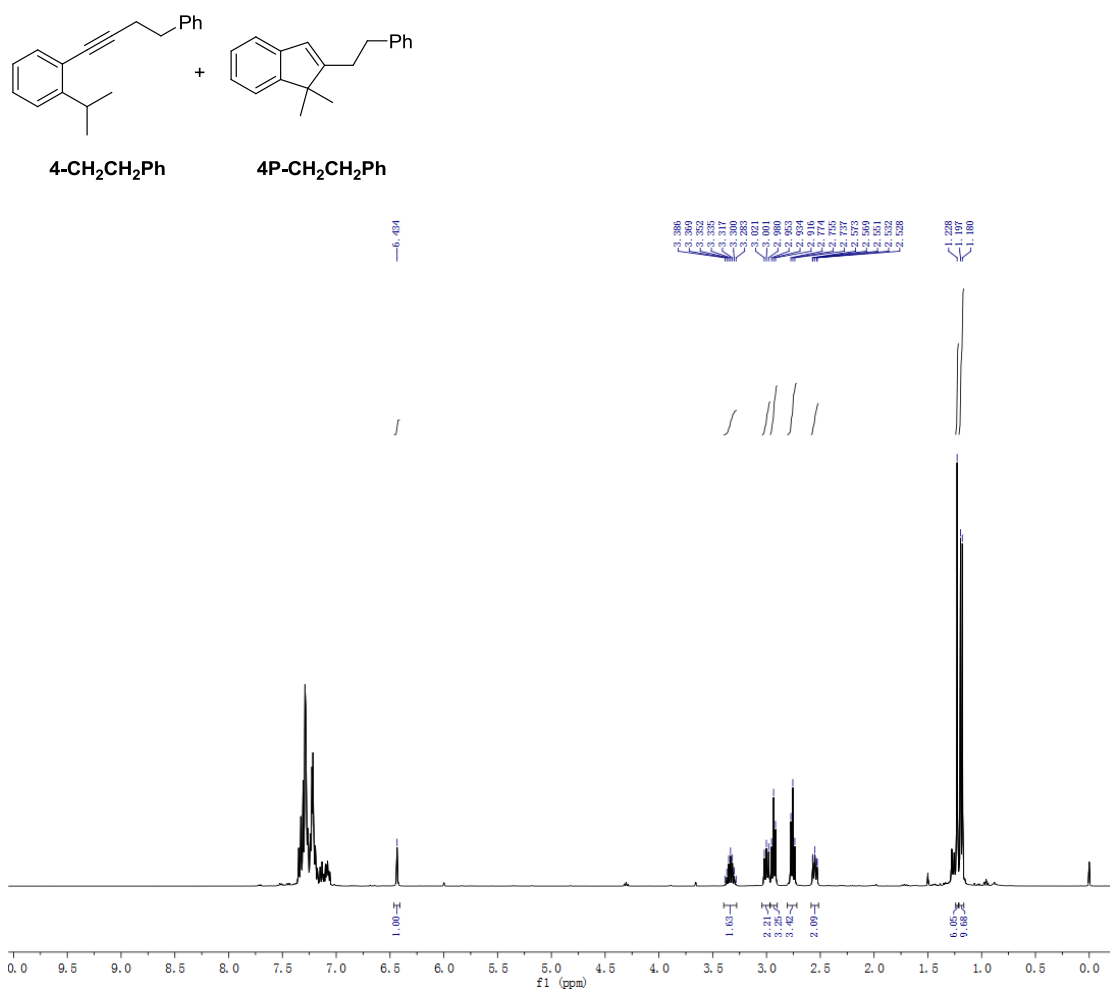
3P-MeOC₆H₄



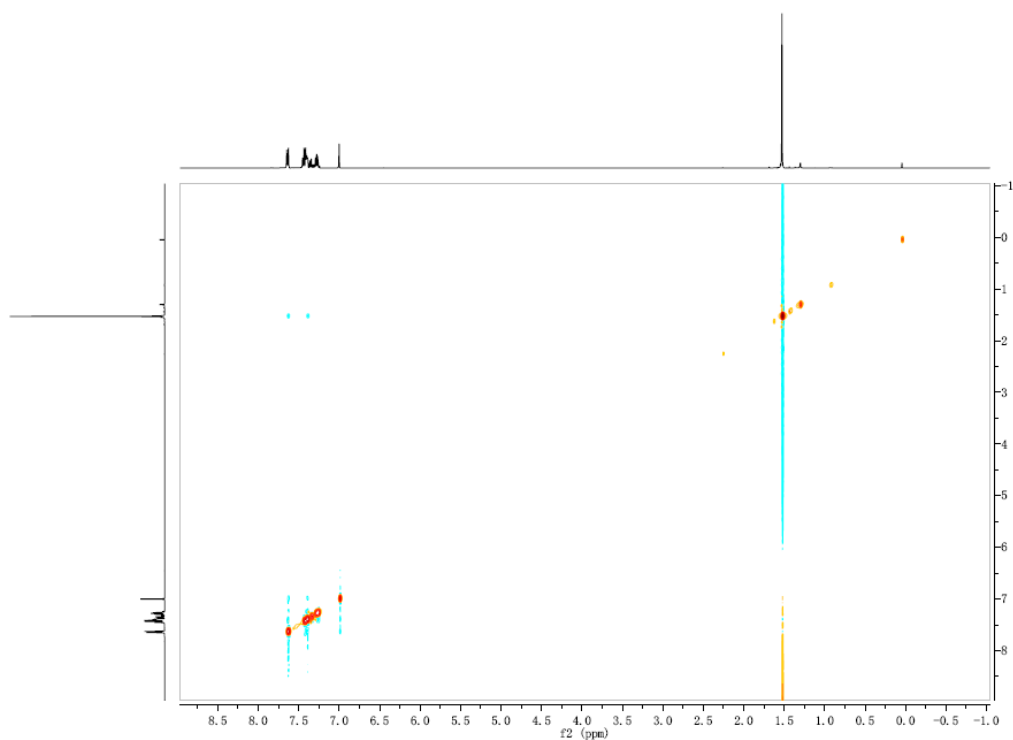
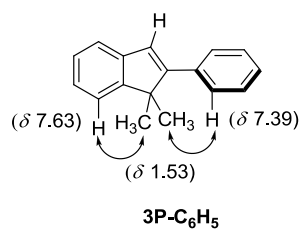


3P'-MeOC₆H₄

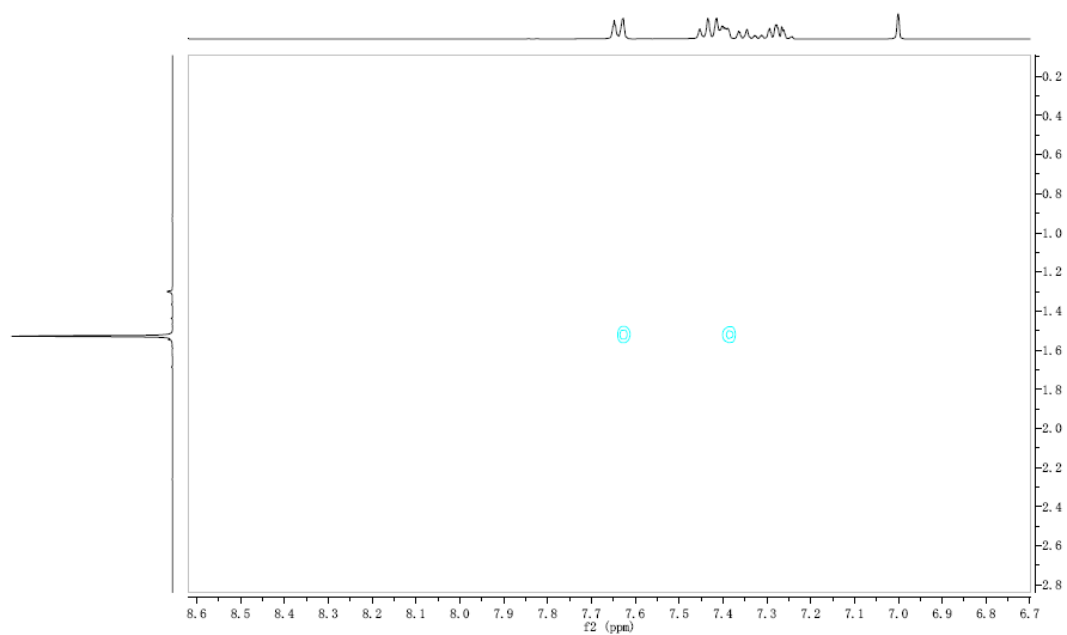


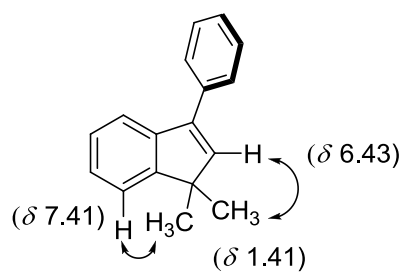


Structure was confirmed by the NOESY measurements:

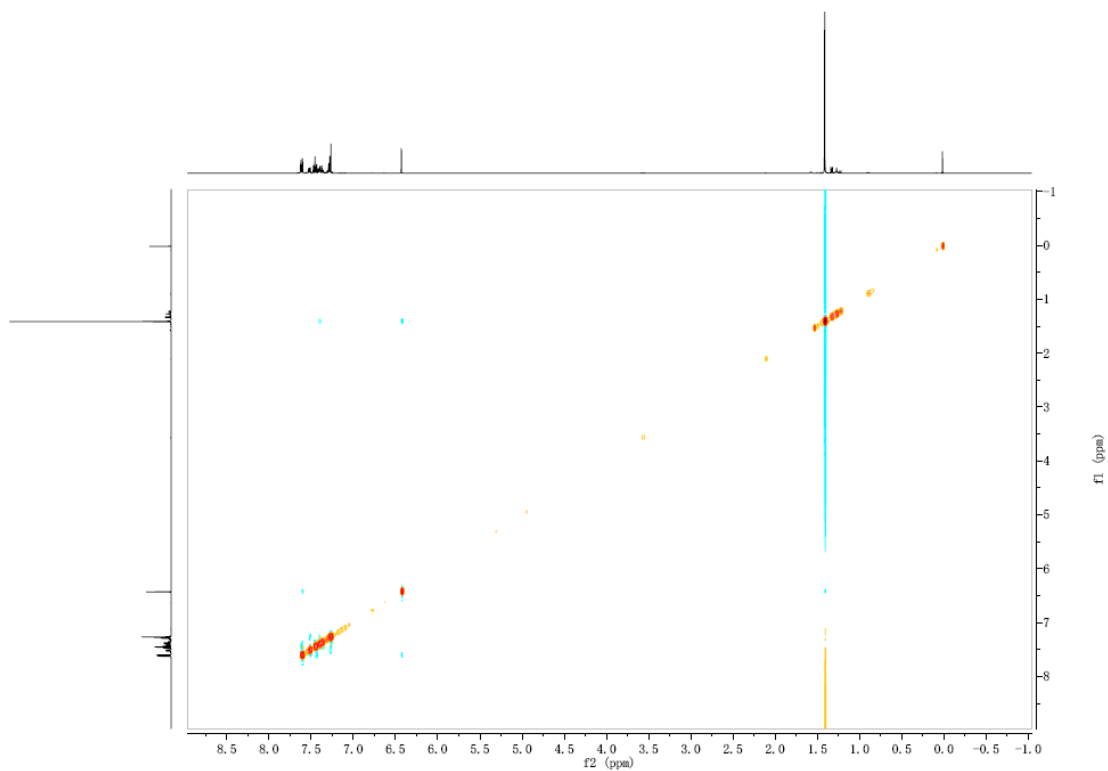


The magnified spectra:

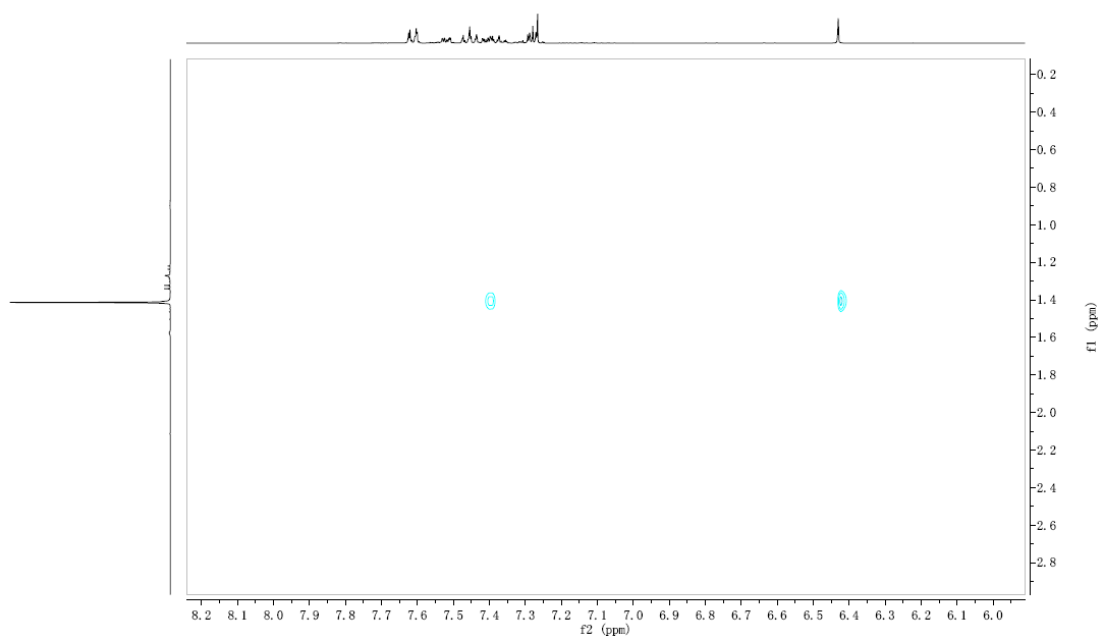


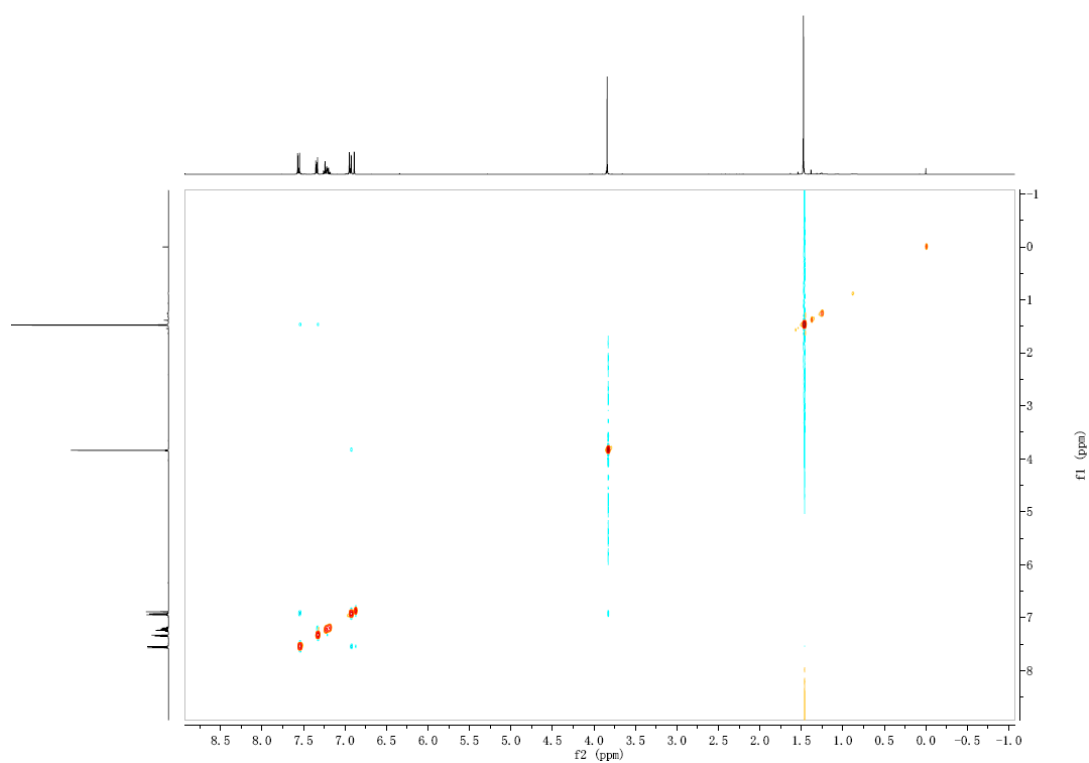
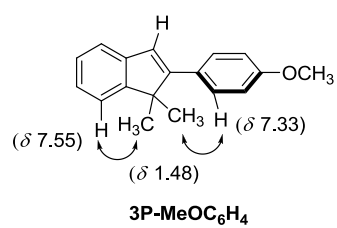


3P'-C₆H₅

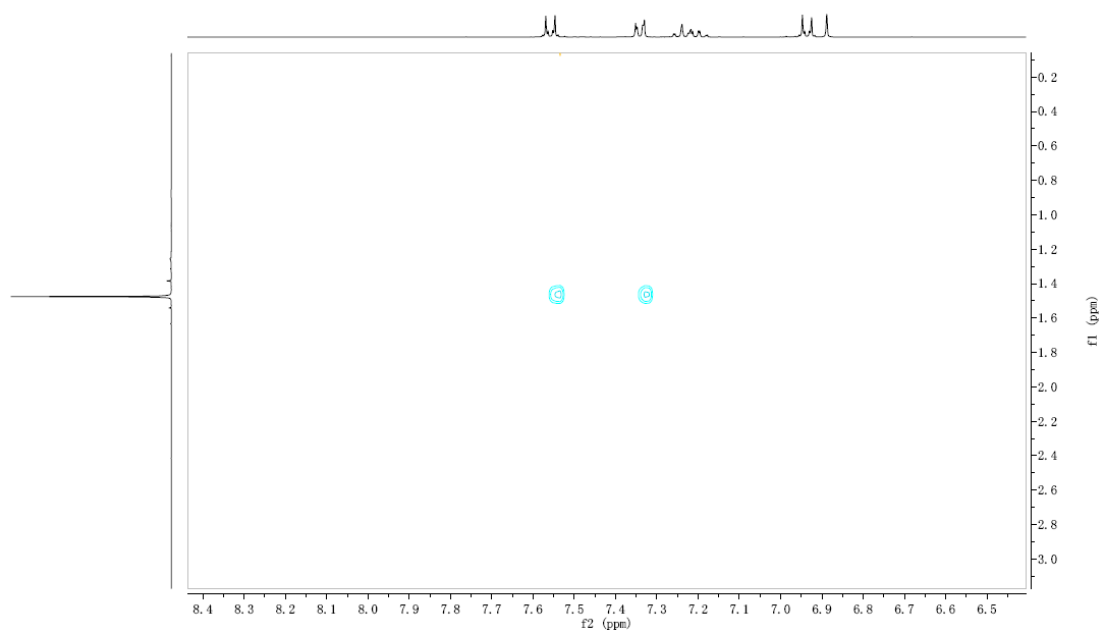


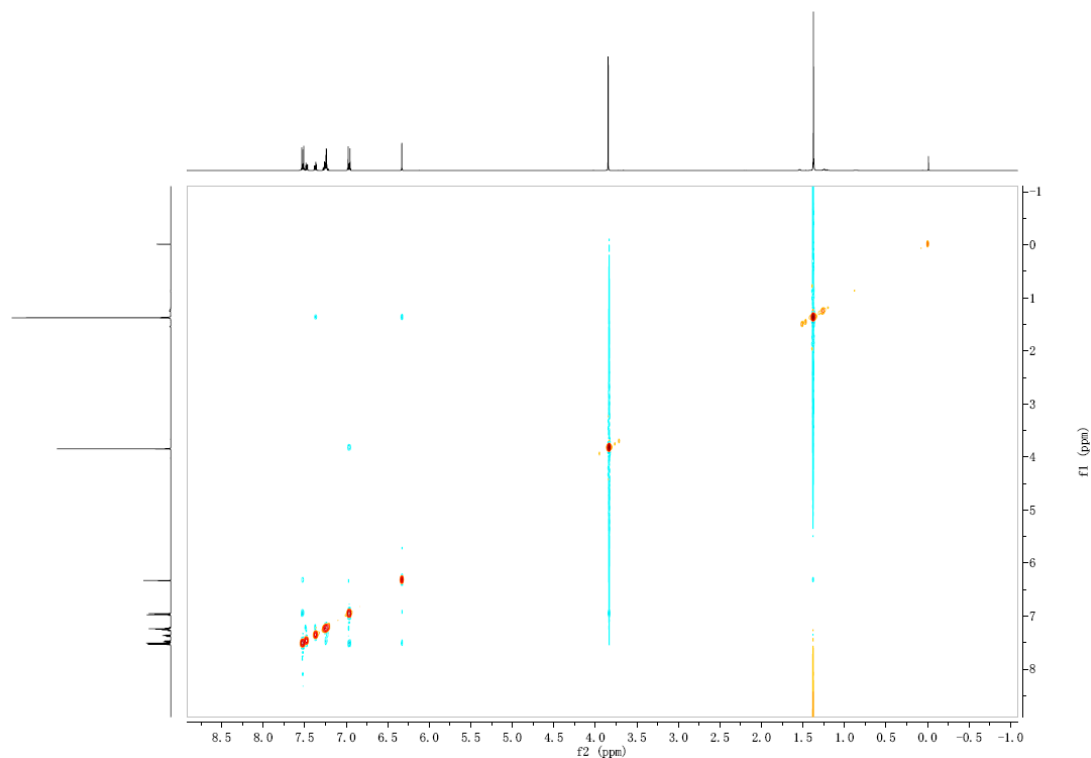
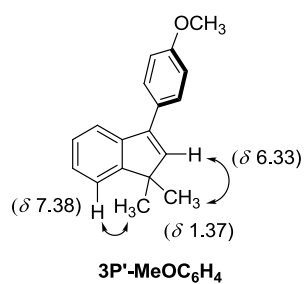
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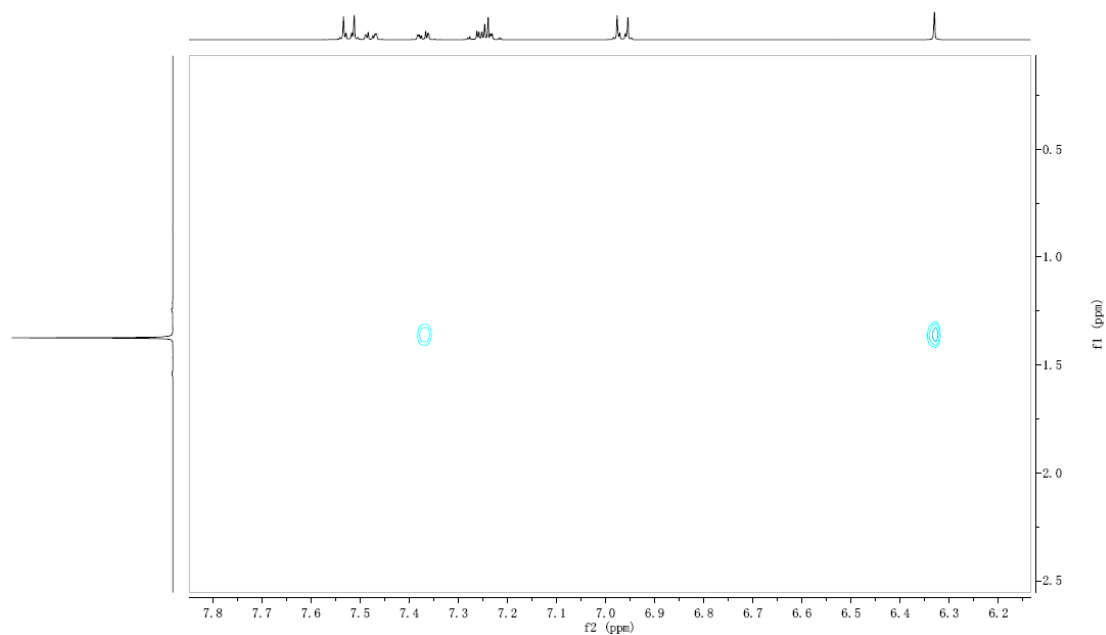


The magnified spectra:





The magnified spectra:

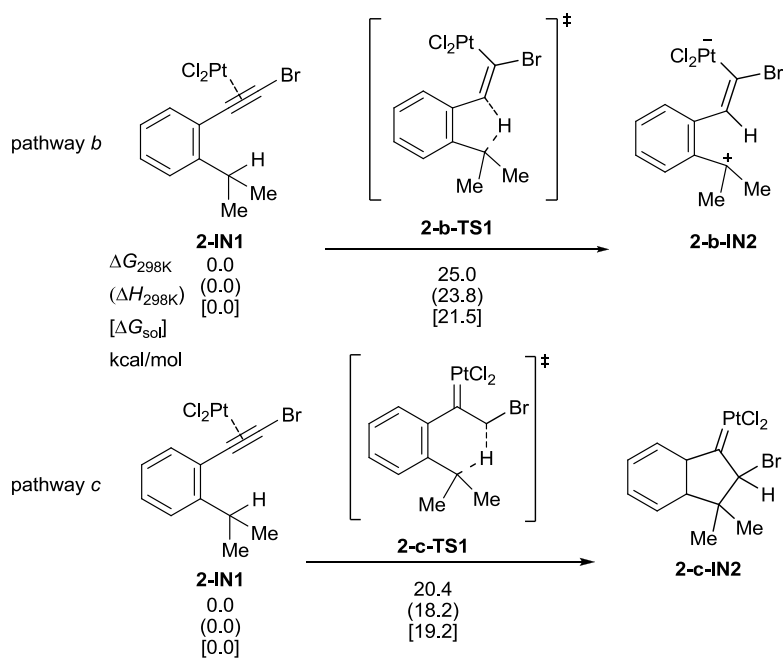


2. Full Citation of G09

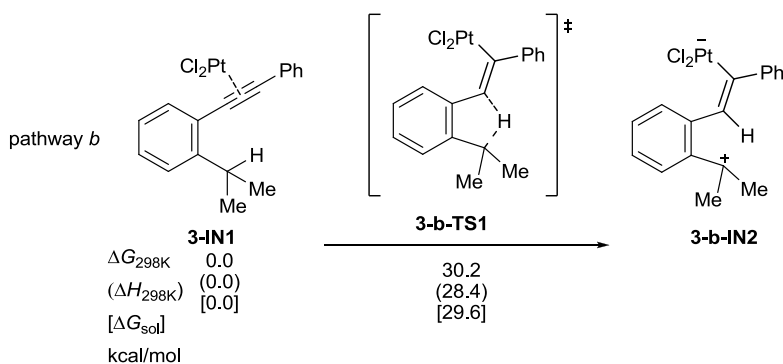
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3. Some Disfavored Pathways Calculated by M06//B3LYP Method

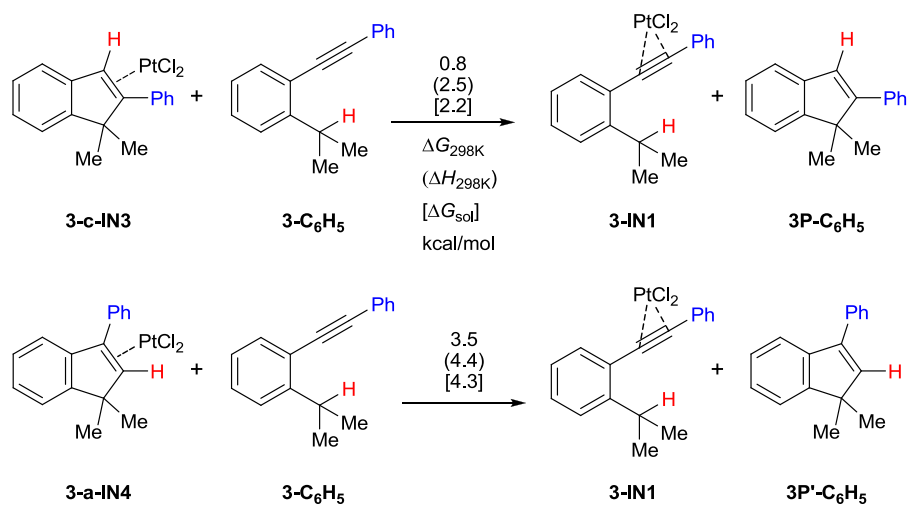
Scheme S1. Computed Activation Energies of **2** in Pathways *b* and *c*



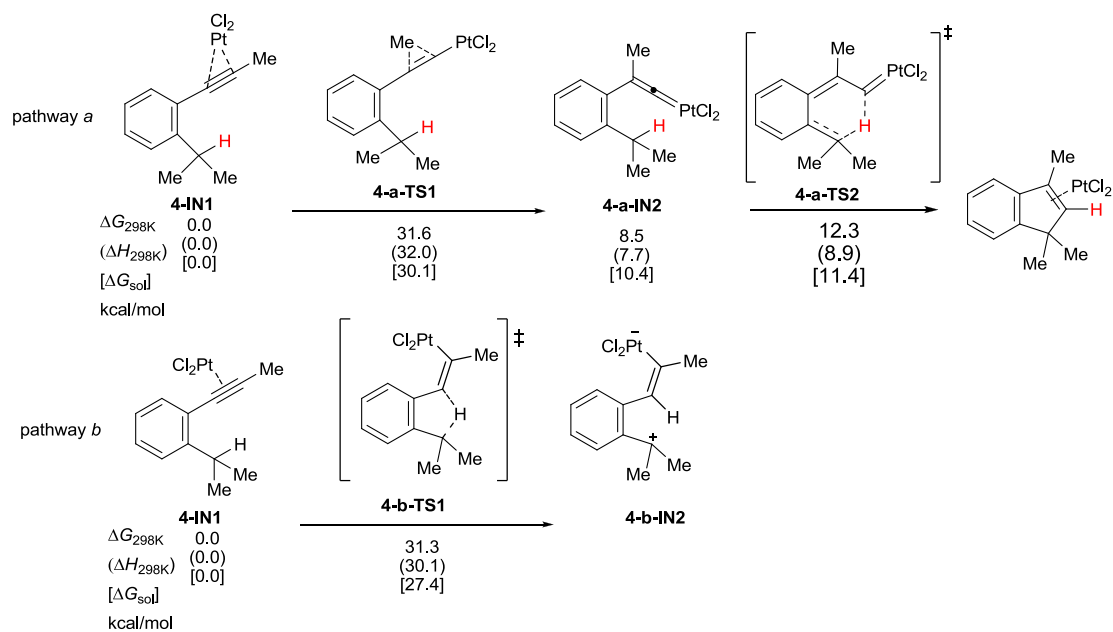
Scheme S2. Computed Activation Energies of **3-C₆H₅** in Pathway *b*



Scheme S3. Computed Energies of Catalyst Transfer Steps



Scheme S4. Computed Activation Energies of 4-CH₃ in Pathways *a* and *b*



4. Computed Energy Surfaces Using B3LYP Method

4.1 B3LYP Computed Energy Surface for the PtCl₂-catalyzed Cyclization of 1-Ethynyl-2-isopropylbenzene **1**.

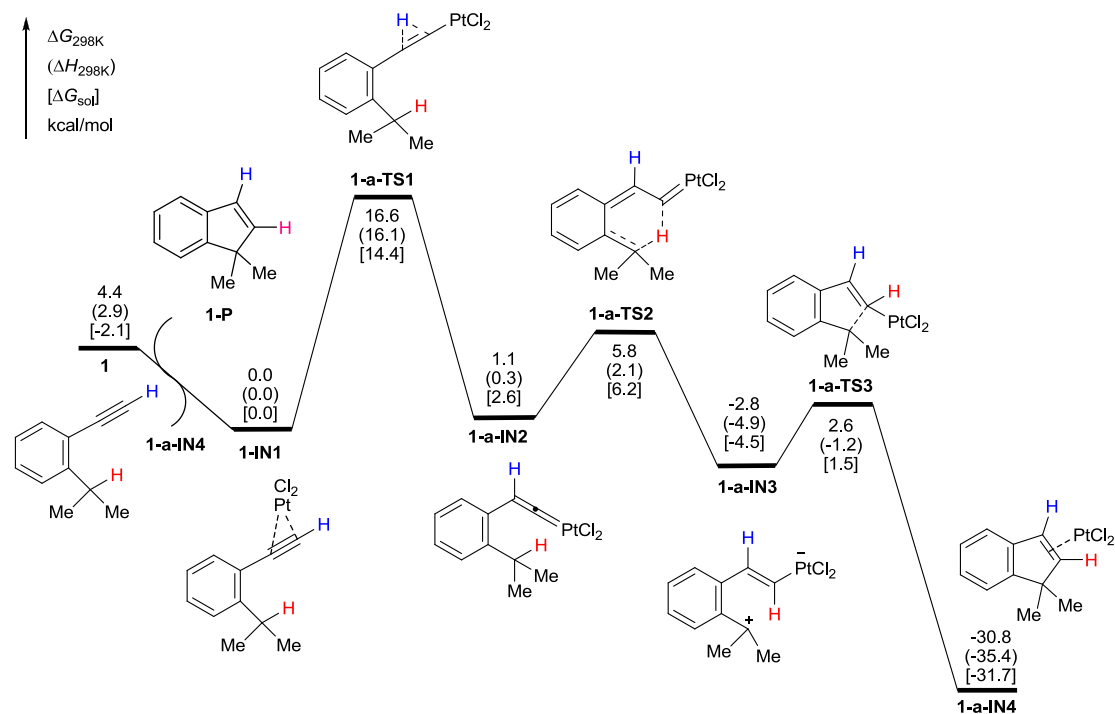


Figure S1. B3LYP computed energy surface for the PtCl₂-catalyzed cyclization of 1-ethynyl-2-isopropylbenzene **1** in pathway *a*.

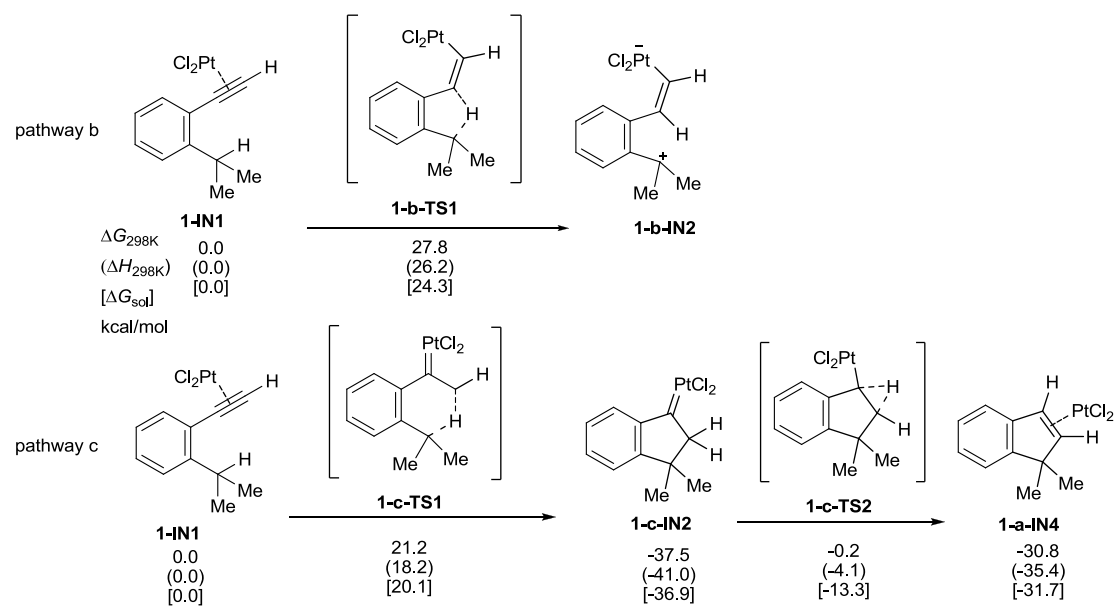


Figure S2. B3LYP computed alternative mechanisms of **1** via pathways *b* and *c*.

4.2 B3LYP Computed Energy Surface for the PtCl₂-catalyzed Cyclization of 1-(Bromoethynyl)-2-isopropylbenzene 2.

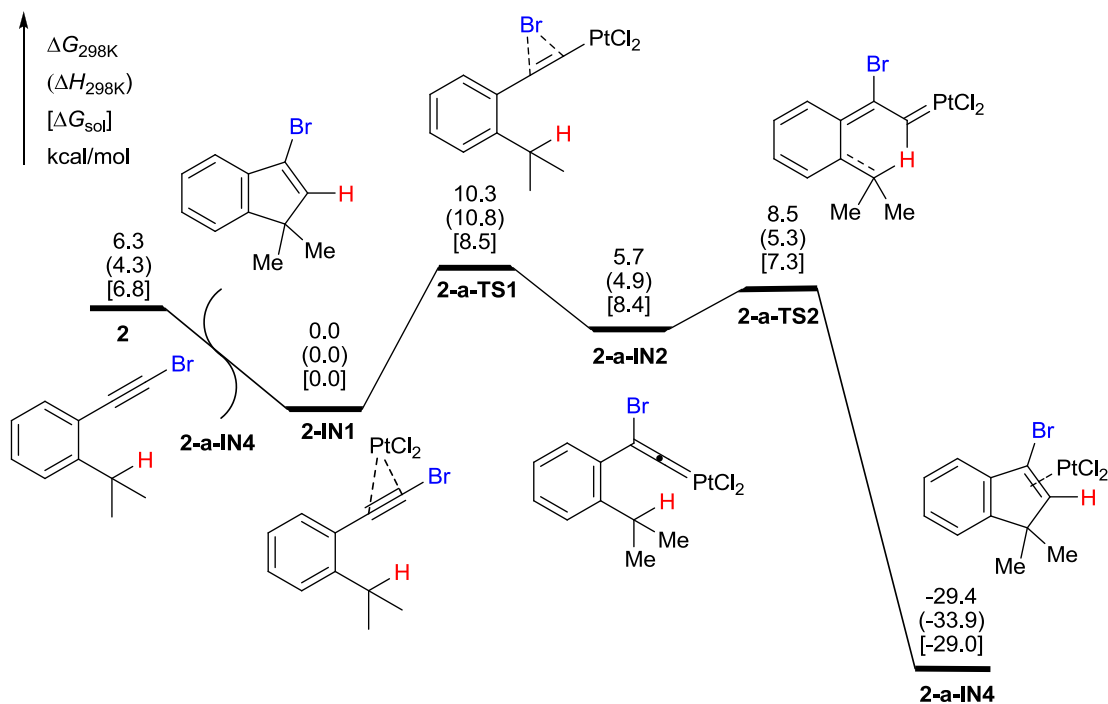


Figure S3. B3LYP computed energy surface for the PtCl₂-catalyzed cycloaddition of 1-(bromoethynyl)-2-isopropylbenzene 2 in pathway a.

4.3 B3LYP Computed Energy Surface for the PtCl₂-catalyzed Cyclization of 1-Isopropyl-2-(phenylethynyl)benzene 3.

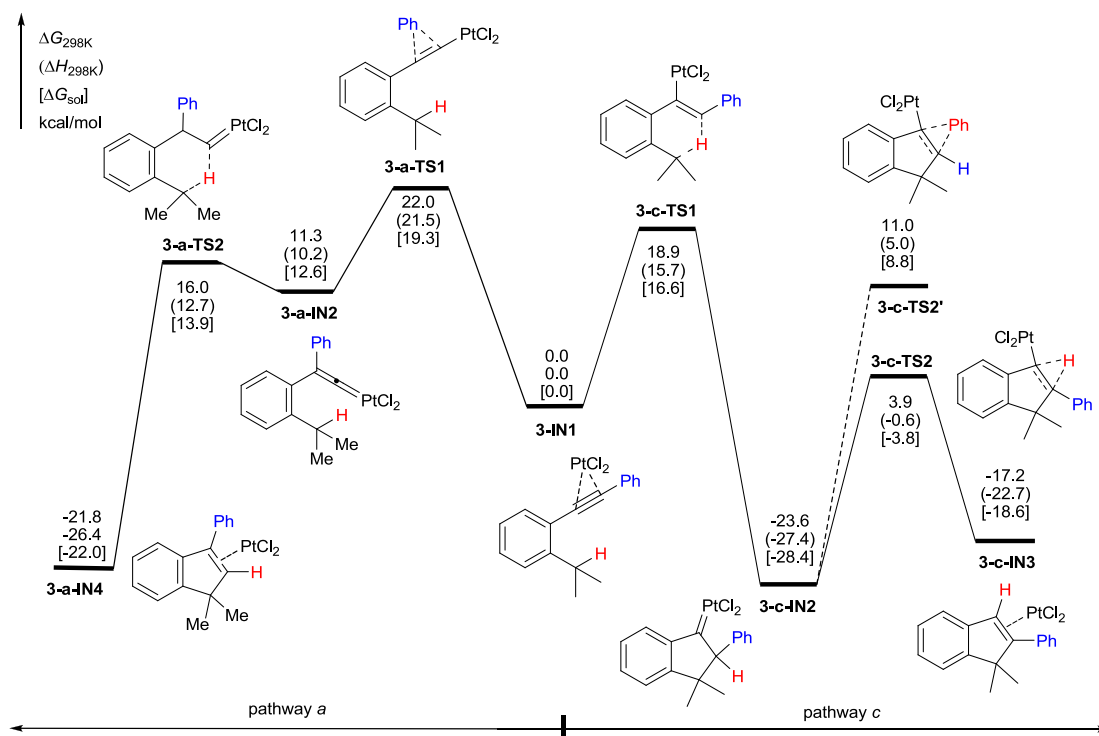


Figure S4. B3LYP computed energy surface for the PtCl₂-catalyzed cycloaddition of 1-isopropyl-2-(phenylethynyl)benzene 3-C₆H₅ in pathways a and c.

4.4 B3LYP Computed Energy Surface for the PtCl₂-catalyzed Cyclization of 1-Isopropyl-2-(prop-1-ynyl)benzene **4-Me**.

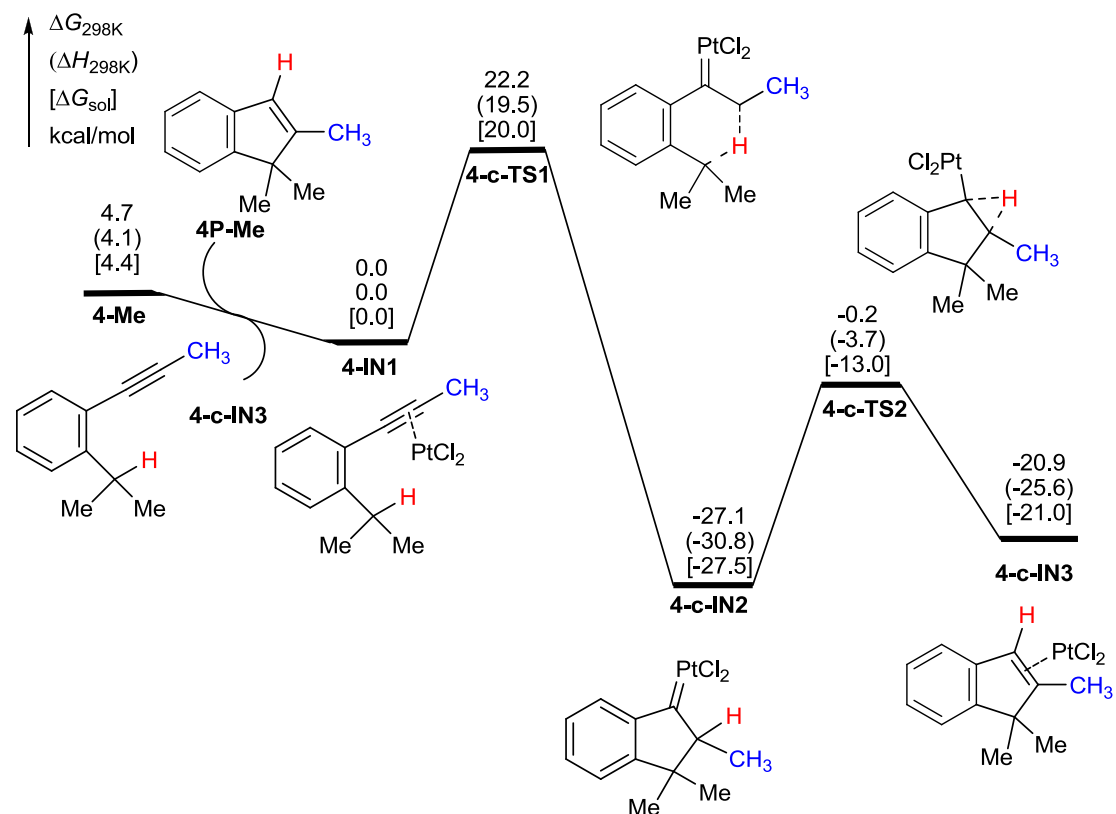
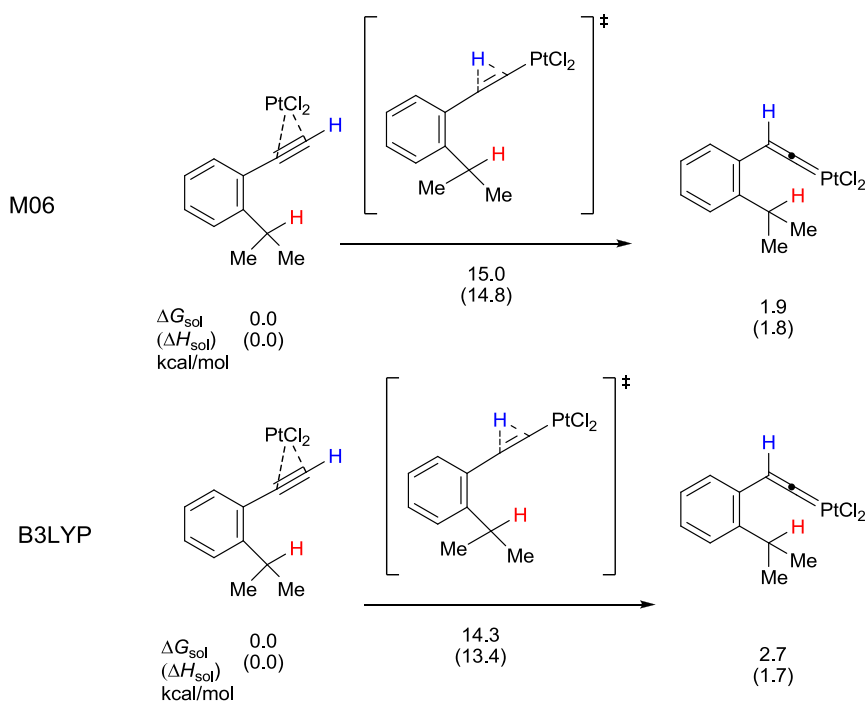


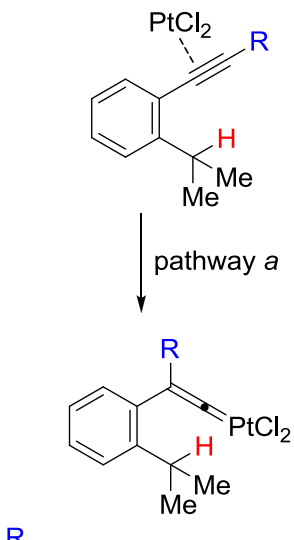
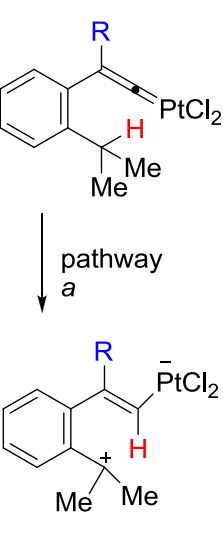
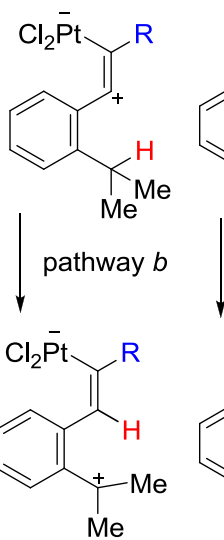
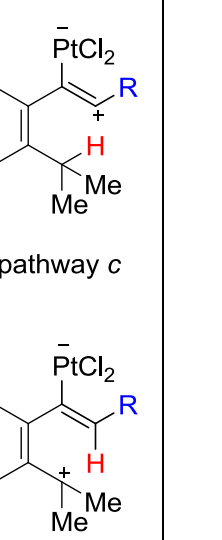
Figure S5. B3LYP computed energy surface for the PtCl₂-catalyzed cycloaddition of 1-isopropyl-2-(prop-1-ynyl)benzene **4-Me** in pathway c.

5. Energies of [1,2]-H Shift Step Optimized in Solvent Using B3LYP and M06 Method

Scheme S5. Energies of [1,2]-H Shift Step Optimized in Toluene Using B3LYP and M06 Methods.

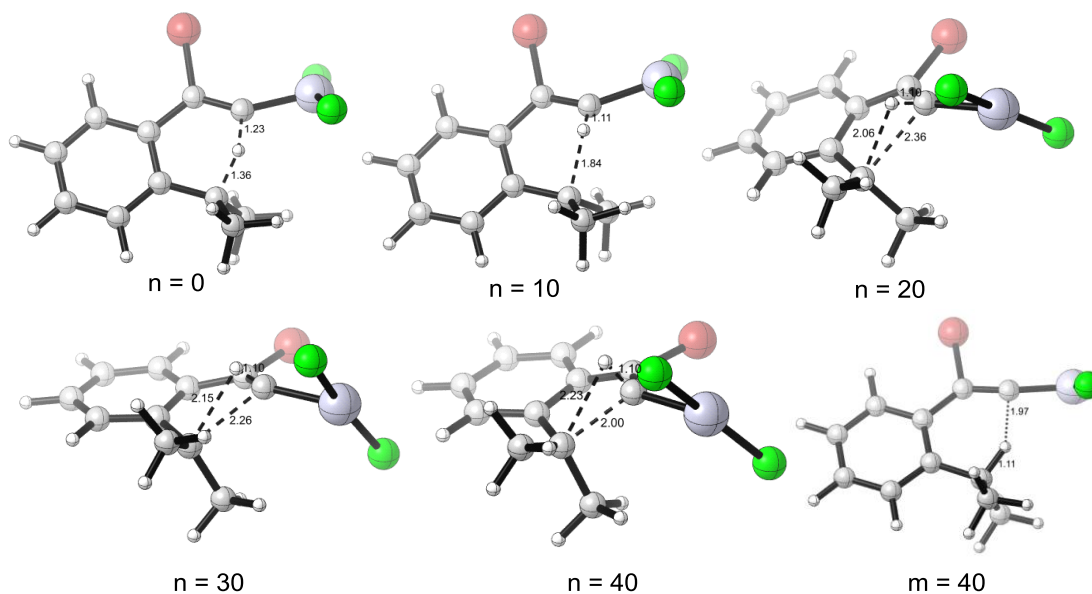
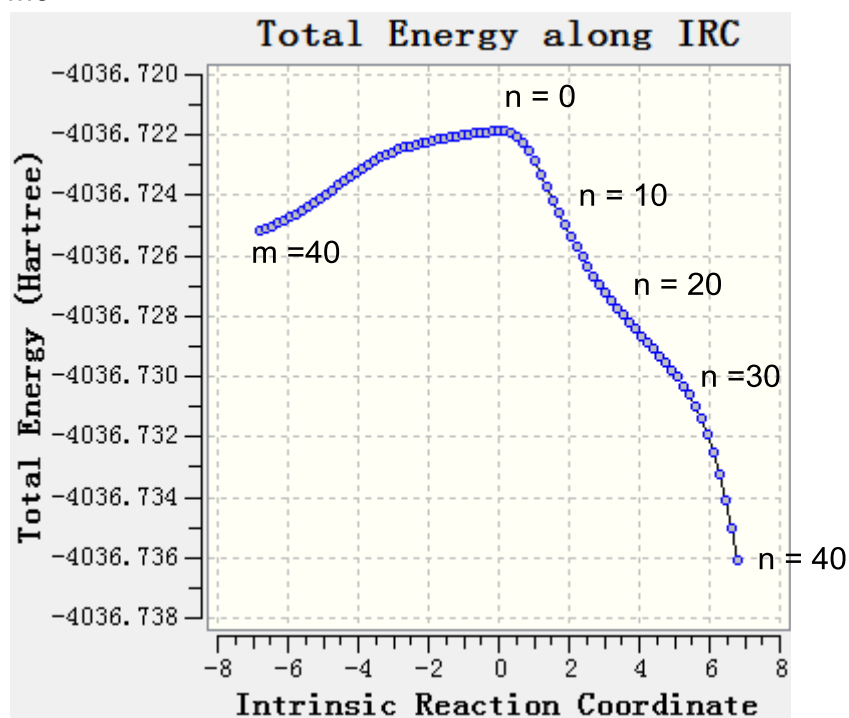
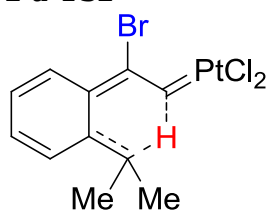


6. DFT Computed Activation Free Energies for [1,2]-R Migration and C-H Activations Using M06//B3LYP Method

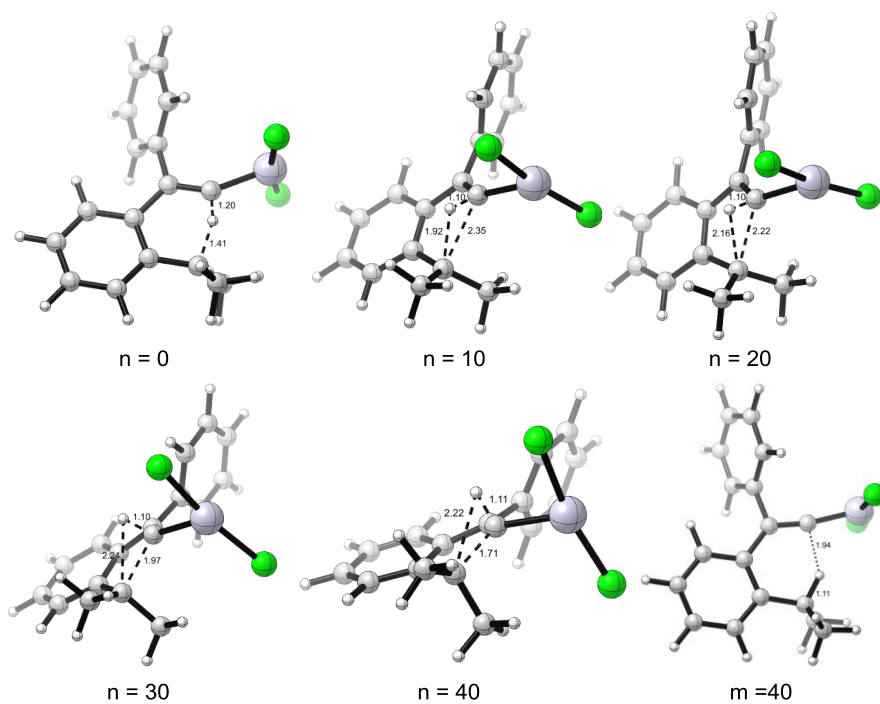
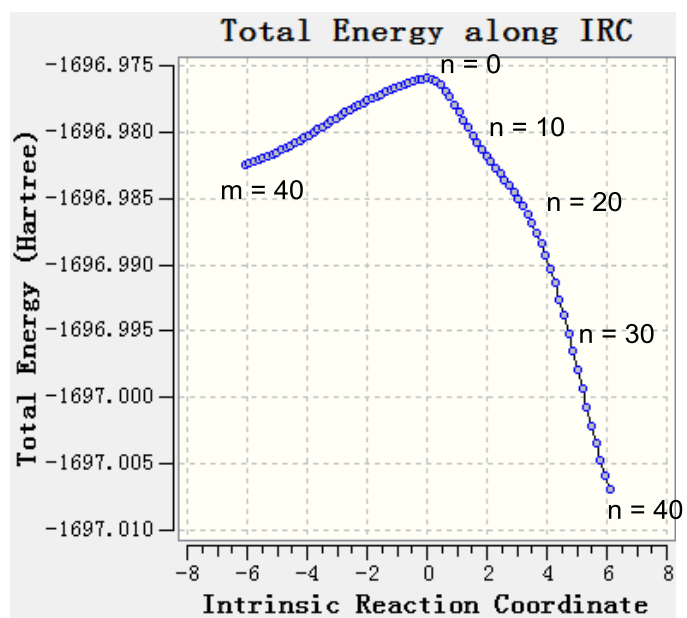
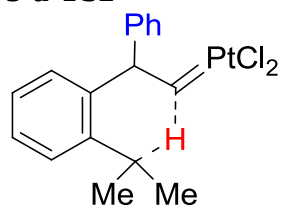
[1,2]-R migration		Three modes of C-H activations			
					
ΔG_{298K} (ΔH_{298K}) $[\Delta G_{sol}]$ kcal/mol	H	18.6 (18.1) [16.3]	5.2 (2.3) [4.1]	30.2 (28.6) [26.5]	20.7 (17.7) [19.7]
	Br	15.9 (16.5) [14.2]	3.8 (1.4) [-0.4]	25.0 (23.8) [21.5]	20.4 (18.2) [19.2]
	Ph	19.7 (18.6) [17.0]	5.8 (3.6) [2.2]	30.2 (28.4) [29.6]	17.7 (14.5) [15.5]
	Me	31.6 (32.0) [30.1]	3.8 (1.2) [1.0]	31.3 (30.1) [27.4]	21.5 (18.8) [19.4]

7. IRC Calculations of Some Transition States

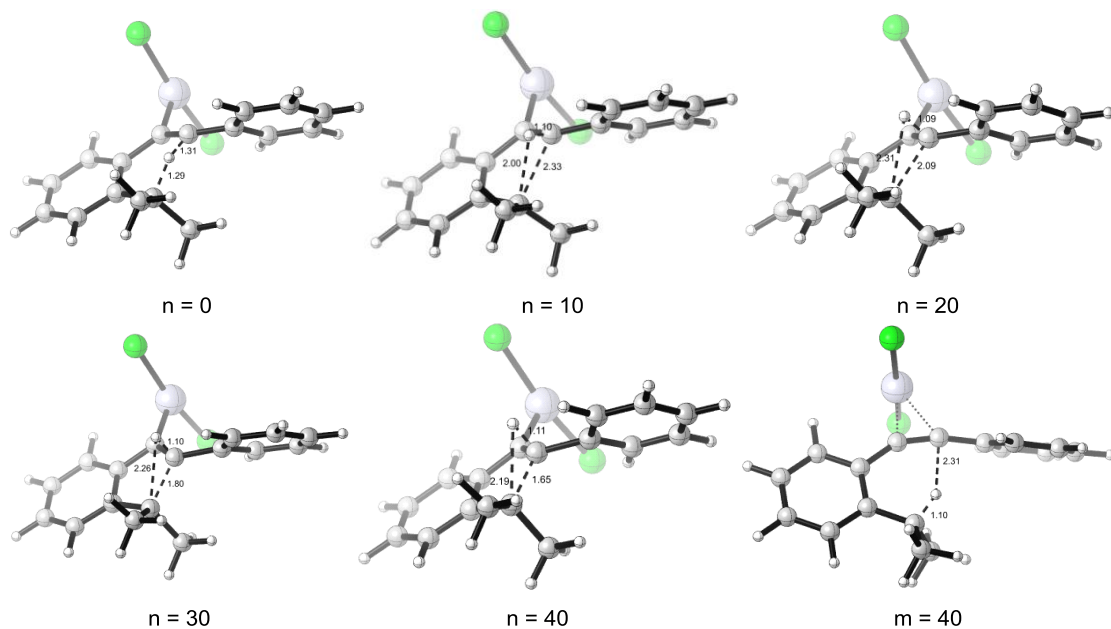
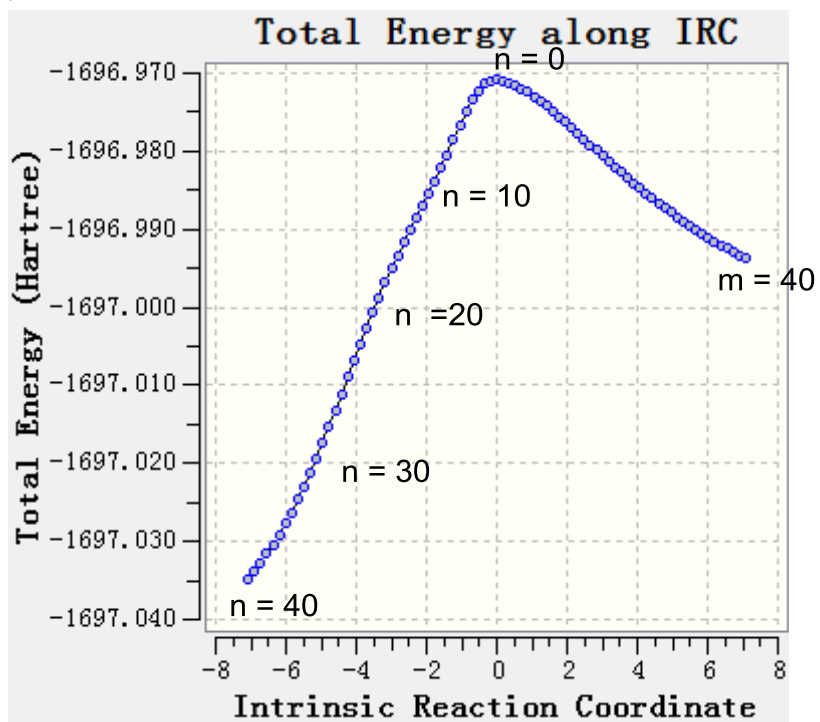
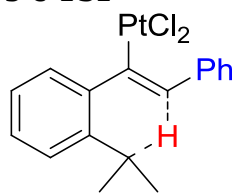
2-a-TS2



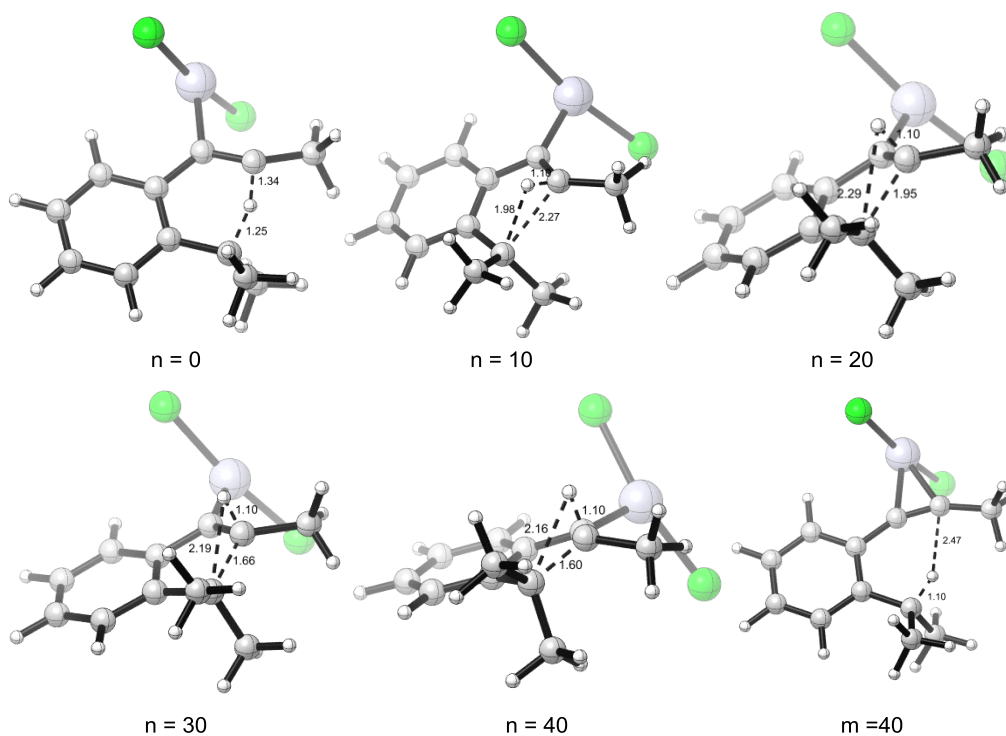
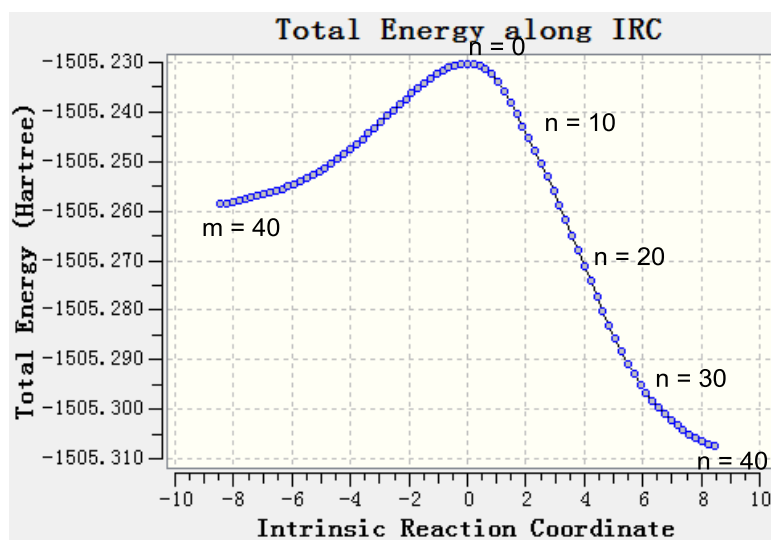
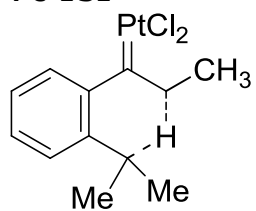
3-a-TS2



3-c-TS1



4-c-TS1



8. Computed Energies of All Stationary Points

Thermal correction to Gibbs Free Energy ($TCGFE_{B3LYP}$ in Hartree)

Sum of electronic and thermal Enthalpies (H_{B3LYP} , in Hartree)

Sum of electronic and thermal Free Energies (G_{B3LYP} , in Hartree)

Single point energies were calculated by M06//B3LYP method (E_{M06} , in Hartree)

Total free energy in solution calculated by M06//B3LYP method ($E_{M06,sol}$, in Hartree)

Total free energy in solution ($E_{B3LYP,sol}$, in Hartree)

name	$TCGFE_{B3LYP}$	H_{B3LYP}	G_{B3LYP}	E_{M06}	$E_{M06,sol}$	$E_{B3LYP,sol}$
1	0.157285	-426.122294	-426.171252	-425.979754	-425.985386	-426.333922
1-IN1	0.149537	-1465.722288	-1465.788481	-1465.491853	-1465.517801	-1465.963642
1-IN1'	0.151041	-1465.716726	-1465.781397	-1465.48782	-1465.508482	-1465.953039
1-a-TS1	0.146365	-1465.696585	-1465.761974	-1465.459096	-1465.488643	-1465.937476
1-a-IN2	0.150269	-1465.721840	-1465.786781	-1465.490235	-1465.513859	-1465.960303
1-a-TS2	0.151196	-1465.718928	-1465.779193	-1465.482855	-1465.508356	-1465.955457
1-a-IN3	0.152885	-1465.730098	-1465.792924	-1465.497343	-1465.526254	-1465.974117
1-a-TS3	0.153798	-1465.724192	-1465.784417	-1465.492868	-1465.520600	-1465.965455
1-a-IN4	0.158498	-1465.778782	-1465.837531	-1465.557385	-1465.584692	-1466.023044
1-P	0.163514	-426.183381	-426.227377	-426.034591	-426.039759	-426.387298
1-b-TS1	0.146535	-1465.680563	-1465.744144	-1465.440661	-1465.472550	-1465.921900
1-c-TS1	0.149836	-1465.693339	-1465.754765	-1465.459174	-1465.486778	-1465.931895
1-c-IN2	0.156502	-1465.787637	-1465.848313	-1465.561394	-1465.586422	-1466.029459
1-c-TS2	0.152577	-1465.728865	-1465.788784	-1465.500844	-1465.547946	-1465.987835
1B-a-IN2	0.184774	-465.409718	-465.460895	-465.276694	-465.282206	-465.660280
1B-a-TS2	0.182524	-465.363527	-465.411149	-465.222892	-465.227937	-465.607759
1B-a-IN3	0.185440	-465.394295	-465.444388	-465.258452	-465.264019	-465.644534
1C-a-IN2	0.182911	-427.345664	-427.393587	-427.234165	-427.239138	-427.589677
1C-a-TS2	0.179871	-427.281648	-427.326631	-427.165297	-427.169979	-427.519340
1C-a-IN3	0.181813	-427.313248	-427.361034	-427.201666	-427.206638	-427.556043
1D-a-IN3	0.197052	-465.783045	-465.834353	-465.658554	-465.705021	-466.087089
1D-a-TS3	0.198202	-465.771104	-465.819744	-465.646648	-465.694035	-466.074439
1D-a-IN4	0.201613	-465.799186	-465.847319	-465.682352	-465.731496	-466.106983
1E-a-IN3	0.170722	-426.488249	-426.536073	-426.366631	-426.413707	-426.762379
1E-a-TS3	0.172294	-426.477037	-426.521941	-426.354313	-426.401768	-426.750058
1E-a-IN4	0.174648	-426.516026	-426.561225	-426.399971	-426.449857	-426.793955
2	0.146654	-2996.927420	-2996.980215	-2996.623963	-2996.628729	-2997.131344
2-a-IN1	0.137367	-4036.527234	-4036.597716	-4036.135168	-4036.159904	-4036.759531
2-a-TS1	0.134954	-4036.509945	-4036.581359	-4036.107356	-4036.134888	-4036.743557
2-a-IN2	0.138134	-4036.519416	-4036.588655	-4036.129885	-4036.150199	-4036.746857
2-a-TS2	0.137752	-4036.518758	-4036.584112	-4036.123365	-4036.150357	-4036.748355
2-a-IN4	0.145047	-4036.581294	-4036.644498	-4036.200886	-4036.224986	-4036.813466
2-P	0.150447	-2996.988306	-2997.037011	-2996.686981	-2996.692134	-2997.192299
2-b-TS1	0.133434	-4036.490884	-4036.559451	-4036.091338	-4036.121704	-4036.722762
2-c-TS1	0.136652	-4036.494842	-4036.561798	-4036.101995	-4036.128545	-4036.724673
3-C₆H₅	0.231154	-657.099023	-657.161085	-656.858254	-656.865872	-657.399418
3-IN1	0.223902	-1696.698564	-1696.776817	-1696.372178	-1696.397582	-1697.025648

3-a-TS1	0.223792	-1696.664292	-1696.740804	-1696.340621	-1696.370452	-1696.993898
3-a-IN2	0.225120	-1696.682322	-1696.758843	-1696.358927	-1696.382233	-1697.006817
3-a-TS2	0.224608	-1696.678330	-1696.751334	-1696.349180	-1696.378202	-1697.004268
3-a-IN4	0.232628	-1696.740684	-1696.810973	-1696.428043	-1696.454241	-1697.069461
3-b-TS1	0.221205	-1696.651890	-1696.727202	-1696.321320	-1696.347781	-1696.974454
3-c-TS1	0.224119	-1696.673585	-1696.746770	-1696.344211	-1696.373142	-1696.999358
3-c-IN2	0.231213	-1696.742200	-1696.813901	-1696.426180	-1696.459661	-1697.078172
3-c-TS2	0.227473	-1696.699469	-1696.770643	-1696.380433	-1696.418242	-1697.035317
3-c-TS2'	0.232143	-1696.690544	-1696.759274	-1696.377320	-1696.406323	-1697.019816
3-c-IN3	0.233514	-1696.734794	-1696.804252	-1696.424089	-1696.451484	-1697.064850
3P-C₆H₅	0.237754	-657.140027	-657.19607	-656.905869	-656.913282	-657.440820
3P'-C₆H₅	0.237994	-657.142453	-657.197967	-656.906641	-656.913728	-657.442629
3-IN1-tBu	0.330859	-1853.833255	-1853.923229	-1853.498178	-1853.524049	-1854.279439
3-a-TS1-tBu	0.329490	-1853.800756	-1853.890218	-1853.467558	-1853.498384	-1854.250040
3-c-TS1-tBu	0.330939	-1853.809137	-1853.894127	-1853.470594	-1853.500291	-1854.254299
3-IN1-OMe	0.252359	-1811.187246	-1811.272444	-1810.837301	-1810.865138	-1811.552072
3-a-TS1-OMe	0.253658	-1811.157068	-1811.239421	-1810.807939	-1810.839890	-1811.524485
3-c-TS1-OMe	0.254067	-1811.164478	-1811.243121	-1810.810256	-1810.841295	-1811.527713
4-Me	0.182948	-465.417455	-465.471425	-465.270877	-465.276426	-465.659600
4-IN1	0.176658	-1505.020164	-1505.089346	-1504.787134	-1504.811505	-1505.290002
4-a-TS1	0.174166	-1504.971403	-1505.041313	-1504.734314	-1504.761049	-1505.241825
4-a-IN2	0.177905	-1505.006243	-1505.074111	-1504.774869	-1504.796138	-1505.272958
4-a-TS2	0.177832	-1505.005023	-1505.068852	-1504.768768	-1504.794547	-1505.271932
4-b-TS1	0.172791	-1504.973704	-1505.040877	-1504.733343	-1504.763996	-1505.243627
4-c-TS1	0.176405	-1504.989108	-1505.053985	-1504.752583	-1504.780323	-1505.257824
4-c-IN2	0.183745	-1505.069289	-1505.132526	-1504.843975	-1504.869000	-1505.340961
4-c-TS2	0.178309	-1505.025984	-1505.089663	-1504.798054	-1504.842886	-1505.312320
4-c-IN3	0.185154	-1505.061017	-1505.122689	-1504.840257	-1504.864637	-1505.332006
4P-Me	0.189803	-465.464851	-465.512299	-465.322784	-465.328082	-465.707056

9. Coordinates of All Stationary Points

1

C	2.68573800	-0.63135800	0.09732800
C	1.86449700	-1.75984800	0.10856000
C	0.47915500	-1.61646400	0.02087100
C	-0.12786500	-0.35914600	-0.07954700
C	0.71334000	0.78280500	-0.08310100
C	2.11104600	0.63162500	0.00266200
C	-1.64285100	-0.20597500	-0.13739200
C	0.17404800	2.10668500	-0.16816300
C	-0.25508000	3.23708600	-0.23425700
C	-2.23130400	-0.12708100	1.28716400
C	-2.34246400	-1.30056700	-0.96015800
H	3.76541000	-0.73394300	0.16117700
H	2.30013200	-2.75275900	0.18325600
H	-0.14200700	-2.50719300	0.02849100
H	2.73359400	1.52112400	-0.00767900
H	-1.84894400	0.75357400	-0.62576300
H	-0.63376100	4.23182900	-0.29384300
H	-3.31550700	0.03376200	1.24791500
H	-1.78504000	0.69731500	1.85301600
H	-2.04611300	-1.05675000	1.83917400
H	-3.40723300	-1.06334200	-1.06650200
H	-1.91188100	-1.38640900	-1.96395900
H	-2.27820400	-2.28378000	-0.47908100

1-IN1

Pt	-1.64028400	-0.10316000	-0.08177900
Cl	-2.22069800	2.17227400	-0.10892300
Cl	-1.30429600	-2.40603000	-0.37325700
H	3.49783400	-3.10134200	1.39450600
C	3.62331900	-2.02304400	1.24731100
C	2.60392300	-1.51352300	0.20762900
H	3.48942000	-1.52980500	2.21651900
H	4.65502700	-1.84758400	0.91993300
C	2.70025000	-0.00663100	0.04087500
C	2.76488400	-2.24191100	-1.14126300
H	1.60172800	-1.74829400	0.57931500
C	3.84967800	0.58739000	-0.48949000
C	1.63768500	0.86699800	0.42133800
H	2.63875700	-3.31991200	-0.99501600
H	2.00876200	-1.91208600	-1.86036700
H	3.75638100	-2.07608000	-1.57937500
C	3.95163900	1.96930600	-0.65297100
H	4.68310300	-0.04209700	-0.78627900
C	1.74316900	2.27289500	0.24182500
C	0.45397800	0.37356300	0.99477700
C	2.89669200	2.81898100	-0.29156500
H	4.86144200	2.38997500	-1.07298100
H	0.89444300	2.89337100	0.51030800
C	-0.59686900	0.00330200	1.60344900
H	2.98015000	3.89173200	-0.43388700
H	-0.97009000	-0.22153300	2.59170100

1-IN1'

C	2.35763200	2.90278400	0.16099200
C	3.69471200	2.50300400	0.10681100

C	4.02714900	1.15216200	-0.01357600
C	3.05040700	0.15379300	-0.08104500
C	1.68940300	0.57112300	-0.01455400
C	1.36180900	1.93842500	0.09996400
C	3.43256500	-1.31766200	-0.18137300
C	0.61691300	-0.38117500	-0.05614400
C	0.09399600	-1.56812500	-0.11210900
C	3.49784000	-1.95424600	1.22483700
C	4.74086100	-1.56706600	-0.95073400
H	2.09639300	3.95255800	0.24950900
H	4.48671200	3.24542800	0.15464200
H	5.07454200	0.87382600	-0.06022400
H	0.31493400	2.22280800	0.14003900
H	2.63722400	-1.82550400	-0.73931800
H	0.18279700	-2.64124700	-0.15581300
H	3.72011300	-3.02499100	1.14976500
H	2.55375200	-1.83838900	1.76788100
H	4.28705100	-1.48607800	1.82448200
H	4.87701400	-2.64302300	-1.10434600
H	4.73071500	-1.08285100	-1.93310400
H	5.61832800	-1.20728500	-0.40139400
Pt	-1.41168200	-0.29732000	-0.03196100
Cl	-2.97636200	0.35578500	1.58359000
Cl	-3.01470200	0.47054600	-1.55403400

1-a-TS1

Pt	-2.08254400	-0.00897700	-0.01969400
Cl	-2.25283500	-1.60035600	1.71119800
Cl	-2.29701900	1.61076900	-1.67435400
H	2.99210500	3.58927800	0.68112700
C	3.33588600	2.70559200	0.13256500
C	2.95040500	1.42477300	0.90040800
H	2.88012600	2.72610800	-0.86289100
H	4.42233300	2.78790400	0.01018200
C	3.34960600	0.18013800	0.12235300
C	3.54461000	1.42433800	2.32273300
H	1.85968800	1.42158500	1.00052400
C	4.69901400	-0.11684800	-0.10719800
C	2.39269900	-0.71802900	-0.41788900
H	3.18253300	2.29628100	2.87823600
H	3.25702500	0.52517700	2.87838300
H	4.63950700	1.47396900	2.30457800
C	5.09040900	-1.24618300	-0.82459800
H	5.46100800	0.55001900	0.28493500
C	2.79052400	-1.86001700	-1.14868300
C	0.99057200	-0.48546800	-0.25877700
C	4.13684000	-2.12526900	-1.34923100
H	6.14815200	-1.44208000	-0.97784900
H	2.02786400	-2.51975600	-1.55022900
C	-0.24309000	-0.31833800	-0.13084000
H	4.44353700	-3.00262200	-1.90984000
H	0.24722600	-1.07081500	0.72756800

1-a-IN2

Pt	1.79398000	-0.02663500	-0.03827100
Cl	1.57194200	2.27249500	-0.27913800
Cl	2.87732500	-2.06793000	0.21759800
H	-1.19859900	2.68166100	1.70208800
C	-1.91976000	1.86316400	1.60738500
C	-2.05325500	1.43622100	0.13139900

H	-1.57935600	1.03363700	2.23643600
H	-2.88598600	2.20602500	1.99665000
C	-2.95345700	0.22207600	-0.00313600
C	-2.47425600	2.61952800	-0.75665500
H	-1.04645000	1.14931300	-0.21452900
C	-4.34688200	0.36046000	-0.00464300
C	-2.42518000	-1.08801300	-0.08524200
H	-1.71287300	3.40441700	-0.70967500
H	-2.58814200	2.31523000	-1.80239200
H	-3.42245800	3.05766100	-0.42335500
C	-5.19885600	-0.74109700	-0.08627700
H	-4.77647500	1.35539300	0.06153700
C	-3.28769400	-2.19663100	-0.16719100
C	-0.98466400	-1.37216600	-0.08428700
C	-4.66750000	-2.02863000	-0.16995900
H	-6.27496500	-0.59186600	-0.08501300
H	-2.86476900	-3.19569200	-0.23278700
C	0.11036000	-0.65666200	-0.07477700
H	-5.32017700	-2.89392000	-0.23724300
H	-0.69090700	-2.43142600	-0.10014100

1-a-TS2

Pt	1.73243500	-0.10065500	-0.05818100
Cl	1.83016700	2.24438200	-0.28905500
Cl	2.18860700	-2.37207600	0.23461500
H	-0.29421200	2.05185800	1.70795800
C	-1.27540200	1.56928300	1.69165600
C	-1.76570700	1.37479000	0.26943900
H	-1.23427400	0.63014900	2.24638800
H	-1.99416300	2.23454900	2.19106300
C	-2.83289000	0.36926100	0.05552700
C	-1.81826100	2.63800700	-0.56636700
H	-0.68595300	0.76037300	-0.37390400
C	-4.18228400	0.72883900	-0.05973400
C	-2.46325000	-0.99562900	-0.04108700
H	-0.87243500	3.18041100	-0.50878800
H	-2.05908000	2.42766600	-1.61122800
H	-2.60789800	3.28477300	-0.15560900
C	-5.16202700	-0.25643000	-0.17338300
H	-4.47272600	1.77419900	-0.01002500
C	-3.46014500	-1.97632500	-0.16309200
C	-1.04448000	-1.29451500	-0.10706400
C	-4.80034600	-1.60802600	-0.21729200
H	-6.20856800	0.02972200	-0.21933800
H	-3.17315400	-3.02164500	-0.23210500
C	-0.12587700	-0.32152900	-0.21047000
H	-5.56679000	-2.37185900	-0.31039900
H	-0.69580100	-2.32464300	-0.12924400

1-a-IN3

Pt	1.81000400	-0.05282400	-0.08681900
Cl	1.74824300	2.30108800	-0.35621700
Cl	2.29756500	-2.32119000	0.22381600
H	-0.44392400	2.06024600	1.30499900
C	-1.41414600	1.64303400	1.60722200
C	-2.35089300	1.52270300	0.43969700
H	-1.23631500	0.70094300	2.12440200
H	-1.85697900	2.36730900	2.30710300
C	-2.93637100	0.32362900	-0.00564500
C	-2.79094000	2.85509500	-0.09844400

H	-0.47775800	0.57828300	-0.97794500
C	-4.27968400	0.34862100	-0.52484300
C	-2.31857000	-0.97919200	0.19013800
H	-1.90127500	3.48301800	-0.22981600
H	-3.31536200	2.79793600	-1.05301000
H	-3.42816100	3.37605400	0.63071300
C	-5.02858300	-0.79839100	-0.58803500
H	-4.74525300	1.29980900	-0.75489900
C	-3.15126900	-2.12874600	0.20240700
C	-0.90556000	-1.11984900	0.24195700
C	-4.46923700	-2.04146500	-0.18608300
H	-6.06291500	-0.75474200	-0.91476200
H	-2.70458900	-3.09233200	0.42970900
C	-0.05842700	-0.18933800	-0.32407400
H	-5.07996300	-2.93908800	-0.22686700
H	-0.48447500	-2.03205800	0.65727300

1-a-TS3

C	-4.82096200	-1.00735500	-0.85632900
C	-5.01734900	0.29044800	-0.32958000
C	-3.96463000	1.02081200	0.20315100
C	-2.68915100	0.42670700	0.26650900
C	-2.46995600	-0.82236700	-0.38609100
C	-3.55952700	-1.57101000	-0.88823100
C	-1.53459700	0.98014500	0.95600000
C	-0.99684000	0.27655900	2.18624600
C	-1.31158700	2.46818600	0.94718600
C	-1.08986200	-1.09545100	-0.57990600
C	-0.20522800	-0.00981300	-0.48493100
H	-5.66933000	-1.55126300	-1.26086700
H	-6.01933600	0.70971400	-0.31438500
H	-4.14209500	1.99592300	0.64626700
H	-3.38884000	-2.54384400	-1.33989200
H	-0.48121500	0.91350600	-0.99848800
H	-1.12891300	-0.80517000	2.15331900
H	0.06411100	0.49296800	2.33394000
H	-1.54850800	0.67650600	3.05131400
H	-1.83326700	2.96827500	0.12686200
H	-1.63490500	2.90762800	1.90128300
H	-0.23789400	2.67484500	0.84682300
Pt	1.67719500	-0.11178500	-0.13203400
Cl	2.00359700	2.09199200	-0.90075400
Cl	1.63621300	-2.28948100	0.76488200
H	-0.71967400	-2.10372900	-0.74185100

1-a-IN4

C	-3.53536100	-1.56485300	-1.27338500
C	-4.11092100	-0.85789700	-0.20876100
C	-3.42532900	0.18653400	0.42481200
C	-2.14898200	0.51374900	-0.01449700
C	-1.56557300	-0.21247000	-1.07563500
C	-2.25276900	-1.24817200	-1.71627600
C	-1.22500300	1.63552300	0.45460800
Pt	1.25093200	-0.31377100	0.13099100
C	0.04062500	1.35495700	-0.36254700
C	-0.22787200	0.31423400	-1.32991800
C	-1.76588400	3.00135300	-0.06026500
C	-1.03040900	1.71043200	1.97864400
Cl	2.93985500	0.65742900	-1.18946300
Cl	0.14630700	-1.69262000	1.66625500

H	-4.08995100	-2.36881700	-1.74796400
H	-5.10913500	-1.12260700	0.12906300
H	-3.89250600	0.72569300	1.24443000
H	-1.78963600	-1.80408500	-2.52666400
H	0.72636100	2.17047800	-0.57394200
H	0.27856100	0.22997200	-2.28663900
H	-1.08489100	3.81387600	0.21692100
H	-2.74259200	3.20446500	0.39139000
H	-1.88949000	3.00529700	-1.14854800
H	-0.69958000	0.75272100	2.38514300
H	-0.28662200	2.47470700	2.23065000
H	-1.97310100	1.99035400	2.46273300

1-P

C	2.25668100	-1.30547900	0.00003600
C	0.86167600	-1.44776300	0.00001500
C	0.06848100	-0.30834800	-0.00004200
C	0.66022700	0.97288400	-0.00007800
C	2.04817500	1.11548300	0.00000000
C	-1.45077200	-0.16877200	-0.00007600
C	-1.60759500	1.34489300	-0.00013500
C	-0.41631400	1.96949300	-0.00013500
C	-2.08375500	-0.79225700	-1.26527600
C	-2.08354200	-0.79174600	1.26556500
H	3.92507900	0.05652500	0.00001800
H	2.88824400	-2.19000100	0.00003500
H	0.41721500	-2.44075600	-0.00001500
H	2.50690200	2.10137500	-0.00002600
H	-2.58207100	1.82414500	-0.00017100
H	-0.25386700	3.04297900	-0.00017200
H	-3.16536600	-0.61222500	-1.28481700
H	-1.92371500	-1.87661800	-1.28474400
H	-1.64805500	-0.36609000	-2.17454700
H	-1.64762000	-0.36520200	2.17454400
H	-3.16513700	-0.61164700	1.28523100
H	-1.92354500	-1.87610600	1.28541500

1B-a-IN2

H	2.28589000	2.14890200	1.18090100
C	1.34793400	1.58404800	1.24723900
C	0.78299000	1.29880100	-0.16026700
H	1.54982700	0.65689100	1.79250900
H	0.63611900	2.17468300	1.83685200
C	-0.46223300	0.42402600	-0.07431700
C	0.56913000	2.61263400	-0.93295400
H	1.54254600	0.73273800	-0.70781100
C	-1.72291900	1.01989800	0.06989000
C	-0.39606900	-0.99432600	-0.11466200
H	1.53242000	3.11360300	-1.08448500
H	0.12178100	2.43204700	-1.91663900
H	-0.07546200	3.31528600	-0.39203900
C	-2.89741600	0.27433900	0.16508600
H	-1.79129800	2.10288800	0.10436800
C	-1.59469000	-1.73151000	-0.03540300
C	0.83109100	-1.80940700	-0.24718500
C	-2.83345600	-1.11681700	0.10641400
H	-3.85316200	0.77950700	0.27685700
H	-1.54015100	-2.81673900	-0.08184700
C	2.10842400	-1.50955700	-0.13491500
H	-3.73648800	-1.71792900	0.16878600

H	0.62757800	-2.86379600	-0.44907700
C	3.39689200	-1.31913100	-0.02094200
H	4.01566200	-1.04147000	-0.87347100
H	3.90667700	-1.41459600	0.93719100

1B-a-TS2

H	2.70351500	1.02057400	1.17391700
C	1.62224900	1.07204400	1.35871000
C	0.82998300	1.13232400	0.05878300
H	1.34657300	0.20636300	1.96518400
H	1.42277800	1.98045000	1.94453300
C	-0.46292000	0.47701300	0.01832600
C	1.00700000	2.44123400	-0.68999100
H	1.57393500	0.07213500	-0.64214400
C	-1.67179900	1.18670000	-0.19071200
C	-0.52663600	-0.95777400	0.10147200
H	2.07183500	2.64861400	-0.84806700
H	0.51199900	2.42811500	-1.66560000
H	0.60478000	3.28910300	-0.11456600
C	-2.89703200	0.55093900	-0.12456600
H	-1.63427000	2.26476500	-0.31853200
C	-1.80332900	-1.58249700	0.17553500
C	0.64644800	-1.73006000	-0.13748400
C	-2.96309200	-0.84528000	0.08434000
H	-3.81304800	1.12936200	-0.21020000
H	-1.84776500	-2.66451300	0.27597900
C	1.87137400	-1.15807000	-0.42648200
H	-3.92965500	-1.33831800	0.14520100
H	0.51002000	-2.79428200	-0.32682300
C	3.18091000	-1.44286800	-0.35453300
H	3.91675800	-0.90203800	-0.94360500
H	3.56361700	-2.20255500	0.32433000

1B-a-IN3

H	2.30400800	1.76253700	0.57907500
C	1.35512800	1.61137300	1.11320100
C	0.16394600	1.59091400	0.19017100
H	1.45428000	0.68925300	1.68977600
H	1.25347100	2.45584900	1.80929600
C	-0.56099300	0.46221100	-0.11447100
C	-0.26289500	2.97454200	-0.24736700
H	2.02316200	0.14092900	-1.15357000
C	-1.91829100	0.56356000	-0.64850100
C	-0.12518700	-0.91585200	0.23137000
H	0.62258600	3.59413300	-0.43589800
H	-0.86998500	2.98367500	-1.15538900
H	-0.83502900	3.48285600	0.54329500
C	-2.82909900	-0.42321900	-0.44711100
H	-2.23372200	1.48649300	-1.12272200
C	-1.17097100	-1.85776400	0.59397300
C	1.16110300	-1.38507300	0.11151500
C	-2.46662700	-1.62969700	0.25810900
H	-3.85262500	-0.29724500	-0.79027200
H	-0.87218100	-2.80150900	1.04513100
C	2.25933200	-0.75282800	-0.57885700
H	-3.23063300	-2.37205200	0.47301700
H	1.35264300	-2.39356800	0.48082900
C	3.52277200	-1.22035000	-0.59063900
H	4.30309000	-0.73835000	-1.17159200
H	3.81163300	-2.09990100	-0.01933400

1C-a-IN2

H	3.37581400	-0.52236200	-1.09976100
C	2.28472500	-0.57630400	-1.19880100
C	1.60028900	-0.32235800	0.15924500
H	1.97395900	0.15768600	-1.95103800
H	2.03206900	-1.57038600	-1.58715600
C	0.07816700	-0.33489400	0.03143800
C	2.10232500	-1.32529100	1.21720400
H	1.89942100	0.67139700	0.50268500
C	-0.56747700	-1.56239900	-0.18846600
C	-0.72455900	0.82659700	0.16181000
H	3.18627800	-1.22317400	1.34896700
H	1.62418600	-1.14974900	2.18706900
H	1.90415000	-2.36418100	0.92928400
C	-1.95355200	-1.67375900	-0.26264500
H	0.03547600	-2.46017100	-0.29748700
C	-2.12712500	0.68995400	0.12620700
C	-0.21949400	2.20681400	0.34922900
C	-2.74394900	-0.53620600	-0.09244500
H	-2.41227500	-2.64337900	-0.43799500
H	-2.73773800	1.58091600	0.25488400
H	-3.82789700	-0.60387200	-0.12905800
H	-0.82835900	2.81649100	1.01866600
C	0.81683300	2.80267900	-0.25381000
H	1.05302500	3.84380700	-0.05127700
H	1.44479800	2.29798000	-0.98157400

1C-a-TS2

H	-3.19220500	0.05256500	1.07294600
C	-2.15858300	-0.26077200	1.27512000
C	-1.39245400	-0.58765800	-0.00160600
H	-1.66715000	0.51632000	1.86698800
H	-2.21152500	-1.16074300	1.90444500
C	0.03549900	-0.39321000	0.01653900
C	-1.95694700	-1.79629700	-0.72990800
H	-1.71761100	0.70994900	-0.72371200
C	0.93979100	-1.47858600	-0.15956700
C	0.60578500	0.93947900	0.09101500
H	-3.02380200	-1.64932800	-0.93682900
H	-1.45068900	-1.97440700	-1.68354300
H	-1.87926700	-2.71505200	-0.12753800
C	2.30359300	-1.31715900	-0.04848600
H	0.53287800	-2.47756300	-0.28700300
C	2.02776200	1.06566800	0.21057300
C	-0.16745800	2.05264300	-0.30337500
C	2.85397800	-0.02833900	0.16419800
H	2.95804900	-2.18344800	-0.09937800
H	2.44659000	2.06425500	0.31177500
H	3.92968400	0.09226000	0.26214300
H	0.38844600	2.88628200	-0.73060000
C	-1.57522500	2.00012400	-0.50617100
H	-1.96805100	2.70993700	-1.24000900
H	-2.23979600	1.95361400	0.36032800

1C-a-IN3

H	-3.08969200	0.33231900	0.39440000
C	-2.26222900	-0.07517800	0.99377500
C	-1.28904000	-0.87325400	0.16661800
H	-1.78370800	0.75952100	1.51157800

H	-2.72378200	-0.73300900	1.74360000
C	-0.01132600	-0.46353200	-0.11703800
C	-1.80854200	-2.24897900	-0.18882900
H	-1.73048300	1.32812200	-1.43311400
C	1.00949600	-1.41581200	-0.55669200
C	0.49449900	0.91405600	0.14356200
H	-2.87203300	-2.18938000	-0.45281200
H	-1.28816000	-2.71469800	-1.02870000
H	-1.73941600	-2.93442000	0.66913100
C	2.32615400	-1.19641900	-0.31443800
H	0.70030100	-2.36153600	-0.98863600
C	1.88851400	1.01873200	0.57449900
C	-0.18090700	2.06535100	-0.12951500
C	2.76808000	0.01571300	0.34116100
H	3.06160100	-1.95028400	-0.58346200
H	2.22182200	1.96651900	0.99190800
H	3.81693900	0.12775000	0.60298000
H	0.32444000	2.99406800	0.13944800
C	-1.46770000	2.23258200	-0.87512000
H	-1.38427400	3.06904000	-1.58078500
H	-2.31555100	2.46641800	-0.21343600

1D-a-IN3

H	2.01658700	2.17777400	0.69521600
C	1.10264300	1.79784600	1.16888700
C	0.01132900	1.61986900	0.15917400
H	1.34185400	0.90279800	1.73810800
H	0.78038800	2.59324300	1.85700800
C	-0.66040000	0.40556900	-0.08578900
C	-0.44965300	2.91161500	-0.44886900
C	-2.04043900	0.48631500	-0.49029800
C	-0.13074100	-0.90314100	0.26200900
H	0.40913900	3.57642900	-0.58962300
H	-0.96566900	2.79311100	-1.40234900
H	-1.12110100	3.43398700	0.24935000
C	-2.88618800	-0.58997000	-0.35471200
H	-2.44948900	1.43795400	-0.80585500
C	-1.03726900	-1.95793900	0.44831400
C	1.28785500	-1.21123600	0.28639300
C	-2.38672000	-1.80857100	0.14967000
H	-3.93625400	-0.49518700	-0.61022300
H	-0.65804500	-2.92856200	0.75346300
H	-3.05728800	-2.65457500	0.27037300
H	1.58617800	-2.05025200	0.91403900
C	2.21032400	-0.65292000	-0.53131700
C	3.65394900	-1.02474000	-0.56919900
H	4.28145600	-0.14243300	-0.37877800
H	3.90506700	-1.79454400	0.16529800
H	3.93229600	-1.38380900	-1.56884900
H	1.88674000	0.09789400	-1.25276300

1D-a-TS3

H	2.57126500	0.92892000	1.48269600
C	1.47927500	0.94387400	1.54765900
C	0.83115300	1.01095400	0.18177200
H	1.13212100	0.10063000	2.14575200
H	1.20680700	1.87161200	2.07372200
C	-0.51489100	0.48044900	-0.00583200
C	1.27522900	2.17116400	-0.66519000
H	1.41572100	-0.35847200	-1.48391200

C	-1.65302800	1.25927600	-0.27734400
C	-0.64785000	-0.93462200	0.12949300
H	2.36769800	2.22409200	-0.71648100
H	0.86258400	2.14416700	-1.67647700
H	0.94860100	3.10671900	-0.18630200
C	-2.90069900	0.64709600	-0.23659000
H	-1.57549900	2.33171800	-0.42381600
C	-1.92214800	-1.53414300	0.20600400
C	0.61034800	-1.59440200	0.03882600
C	-3.03758700	-0.73580300	0.01771600
H	-3.79295400	1.25073300	-0.37273000
H	-2.01741500	-2.60681400	0.34462700
C	1.65816100	-0.92598500	-0.58794300
H	-4.02918000	-1.17665700	0.03958600
H	0.77349400	-2.56418800	0.50892400
C	3.10152300	-1.30144000	-0.43311800
H	3.45036200	-1.84583700	-1.32019100
H	3.72974600	-0.40485400	-0.35838800
H	3.27972600	-1.92027300	0.45026700

1D-a-IN4

H	-2.60632600	-1.30619800	1.32626500
C	-1.52128600	-1.16991100	1.31707000
C	-1.05602400	-0.66686900	-0.07650000
H	-1.24997400	-0.47611400	2.11866200
H	-1.05989900	-2.13734000	1.53682900
C	0.43865800	-0.43823600	-0.03696900
C	-1.46106200	-1.69251300	-1.15732900
H	-1.84703500	0.80187600	-1.48152700
C	1.47692500	-1.35544400	0.06069300
C	0.74976400	0.96494300	-0.09234300
H	-2.55158500	-1.78206900	-1.19891000
H	-1.10307700	-1.40015700	-2.15031100
H	-1.05826800	-2.68409100	-0.92808300
C	2.78787100	-0.87011000	0.12808400
H	1.29089800	-2.42408100	0.09512100
C	2.09274900	1.44461500	-0.01714600
C	-0.42747600	1.66492900	-0.27427700
C	3.10027600	0.51417700	0.09306200
H	3.60532300	-1.58118600	0.21424500
H	2.30150800	2.50944300	-0.05496600
C	-1.60597600	0.77621800	-0.40035500
H	4.13780500	0.82591600	0.14963500
H	-0.49376300	2.74902600	-0.35325200
C	-2.87136200	1.27734900	0.32717700
H	-3.15558600	2.26711800	-0.04325600
H	-3.70681000	0.59883500	0.13497800
H	-2.72155200	1.34412400	1.40756100

1E-a-IN3

C	-2.76203600	-0.10602100	0.20779800
C	-2.24155300	-1.36447100	-0.14573100
C	-0.88149700	-1.51558000	-0.30885000
C	0.02186500	-0.42026900	-0.08221200
C	-0.54684000	0.89764600	0.13073600
C	-1.92645100	1.00206600	0.33805300
C	0.21648700	2.13492800	-0.01791400
C	1.18647800	2.32305900	-0.93003500
C	1.38116900	-0.74114400	0.12952100
C	2.30216100	0.03510700	1.01533000

C	1.97687500	-2.01678000	-0.38349200
H	-3.83265300	0.01356300	0.34706600
H	-2.90363700	-2.21516800	-0.26757300
H	-0.48444600	-2.50305600	-0.50897500
H	-2.35796400	1.97986500	0.52976800
H	-0.12803100	2.98305400	0.57164900
H	1.67193700	3.28793600	-1.03908700
H	1.48991500	1.54349900	-1.62384300
H	1.84342200	0.88502900	1.51400500
H	2.68903300	-0.66571400	1.77049700
H	3.18385800	0.37618500	0.45861200
H	3.03707400	-1.85984400	-0.60944300
H	1.47976900	-2.41415200	-1.26890100
H	1.95177600	-2.78245000	0.40699500

1E-a-TS3

H	-3.09001900	0.19605300	1.28418600
C	-2.04698500	-0.09958600	1.42357400
C	-1.38318800	-0.48615000	0.12230000
H	-1.50821300	0.67501200	1.96925100
H	-2.05520100	-1.00988900	2.04414200
C	0.06570100	-0.38181300	-0.01475800
C	-2.11337300	-1.52513700	-0.67798600
H	-1.49125500	0.88370600	-1.67652400
C	0.92114400	-1.49022600	-0.14498600
C	0.62142100	0.93272100	0.03392000
H	-3.16677000	-1.25559800	-0.80280800
H	-1.66047000	-1.71027000	-1.65453700
H	-2.10737300	-2.46974600	-0.11215000
C	2.29398200	-1.28516800	-0.05713900
H	0.52429400	-2.49746100	-0.21866000
C	2.01104800	1.12024500	0.15387000
C	-0.36636600	1.94327400	-0.18540500
C	2.83633300	0.00713400	0.10442700
H	2.96148400	-2.14104000	-0.08559700
H	2.42598200	2.12158300	0.21731400
C	-1.52176400	1.58478400	-0.84838400
H	3.91325100	0.12913200	0.16331300
H	-0.24489000	2.94453800	0.22599600
H	-2.40853800	2.21351900	-0.81051000

1E-a-IN4

H	-3.14947700	-0.67286400	1.27292500
C	-2.06561900	-0.82561500	1.26833300
C	-1.45080400	-0.18315200	0.00008900
H	-1.65147800	-0.39162300	2.18450100
H	-1.87921600	-1.90373400	1.28599600
C	0.05644100	-0.32561400	0.00001300
C	-2.06620200	-0.82575400	-1.26780400
H	-2.19794000	1.73876600	-0.87113800
C	0.83953900	-1.47202100	-0.00026100
C	0.70187200	0.96153300	0.00013800
H	-3.14999700	-0.67250000	-1.27210800
H	-1.65215200	-0.39215800	-2.18421000
H	-1.88033900	-1.90397100	-1.28540500
C	2.23156600	-1.32559500	-0.00023900
H	0.39781500	-2.46336700	-0.00050800
C	2.12482700	1.09329900	0.00016200
C	-0.27235400	1.94046300	-0.00014700
C	2.87484000	-0.05956900	0.00003100

H	2.85134100	-2.21847800	-0.00046500
H	2.58796000	2.07529600	0.00041200
C	-1.63465400	1.36697000	-0.00024000
H	3.95872300	-0.01505200	0.00013600
H	-0.07349500	3.01049500	-0.00055400
H	-2.19845200	1.73951400	0.86997300

1-b-TS1

Pt	-1.78141900	0.01575500	0.05405600
Cl	-1.41144400	1.79370100	1.54644500
Cl	-2.53338100	-1.49933800	-1.57343300
H	3.11000900	-2.29328600	2.49058300
C	3.39930800	-1.34103200	2.03476900
C	3.22722200	-1.35670300	0.53509700
H	2.84920800	-0.52047500	2.49982000
H	4.47051200	-1.19021500	2.23955200
C	3.15147100	-0.03856500	-0.16606200
C	3.82940300	-2.52250600	-0.20246100
H	1.79766700	-1.59056800	0.39662800
C	4.19516400	0.73615400	-0.66665100
C	1.81666400	0.38790800	-0.25177200
H	3.68266900	-3.46881000	0.32603700
H	3.44721700	-2.59929900	-1.22352700
H	4.91445900	-2.34423400	-0.27015200
C	3.87921500	1.98817600	-1.20265200
H	5.22763600	0.40188100	-0.61372400
C	1.50103300	1.65009400	-0.76653000
C	0.96647100	-0.69059300	0.22387400
C	2.55103700	2.43584700	-1.24269700
H	4.67408700	2.62479500	-1.57981600
H	0.47349100	1.99208600	-0.79844600
C	-0.26461500	-1.03248100	0.59019200
H	2.33045800	3.41288700	-1.66260200
H	-0.47894100	-1.95563600	1.12745900

1-c-TS1

C	2.38519900	2.59000200	-1.16168700
C	3.66421500	2.08169100	-0.91988800
C	3.82803100	0.82249100	-0.33942300
C	2.71557200	0.04039500	-0.01685500
C	1.41954700	0.57089000	-0.24919400
C	1.26280300	1.84038900	-0.82322900
C	2.85087100	-1.34098500	0.56339000
C	3.91081700	-1.49750600	1.65412900
C	2.90183800	-2.45387600	-0.48905000
C	0.30962900	-0.26002800	0.18824900
C	0.41853000	-1.35231900	0.91832700
H	2.26336200	3.57463500	-1.60252000
H	4.54086800	2.66595400	-1.18505500
H	4.82951300	0.44206400	-0.16113700
H	0.26312600	2.23133100	-0.97242600
H	1.82443000	-1.48248400	1.18284900
H	3.82162100	-0.72112600	2.41880800
H	3.83297600	-2.47885500	2.13254600
H	4.91227800	-1.43019000	1.21020600
H	2.10536500	-2.35284000	-1.23058200
H	3.86431800	-2.39979400	-1.01279800
H	2.82948900	-3.44257800	-0.02307400
Pt	-1.61566600	0.00278800	0.03385700
Cl	-1.99403200	-1.97848800	-1.17014000

Cl	-1.71915100	2.05486300	1.15221100
H	0.05641700	-2.36883800	0.95847400

1-c-IN2

C	-2.43553400	2.60680200	-1.08999600
C	-3.67941000	1.98236800	-0.88324400
C	-3.77443400	0.68771300	-0.36468700
C	-2.60421200	0.00335500	-0.04890400
C	-1.35010300	0.62988400	-0.26371500
C	-1.25954700	1.93972900	-0.78402500
C	-2.45380100	-1.39429800	0.53071300
C	-3.05452800	-2.45525000	-0.41672500
C	-3.11935600	-1.48854000	1.92048500
C	-0.30895900	-0.26710900	0.12774400
C	-0.90292500	-1.54779500	0.63248700
H	-2.40127100	3.61601800	-1.48818800
H	-4.58950300	2.52274800	-1.13048500
H	-4.74894700	0.23272400	-0.21165000
H	-0.28788200	2.40125800	-0.91864000
H	-0.50626500	-2.37554300	0.02780100
H	-2.59318300	-2.41057600	-1.40911500
H	-2.89518700	-3.46051300	-0.01082500
H	-4.13385800	-2.30846400	-0.53608500
H	-2.70564300	-0.74638300	2.61194200
H	-4.20000600	-1.32137800	1.85034500
H	-2.96131400	-2.48413000	2.35031100
Pt	1.53029700	0.02209200	0.01687300
Cl	1.66371400	2.04981400	1.17247200
Cl	2.03473100	-1.92207700	-1.18824300
H	-0.55684500	-1.74166100	1.65576300

1-c-TS2

C	-2.47716000	2.72498000	-0.92791100
C	-3.71380700	2.07641800	-0.83054700
C	-3.80232700	0.76372500	-0.35356000
C	-2.63075100	0.11180900	0.01853300
C	-1.39224500	0.76888700	-0.08236500
C	-1.29798900	2.07714400	-0.55108600
C	-2.44848600	-1.30357900	0.55531900
C	-2.75454600	-2.37457900	-0.54292700
C	-3.25832800	-1.60540700	1.83460600
C	-0.31958300	-0.15756200	0.39620100
C	-0.96633300	-1.36669900	0.75859100
H	-2.43339600	3.74501100	-1.29808500
H	-4.61869200	2.59896000	-1.12808000
H	-4.76935900	0.27245900	-0.28076600
H	-0.33283700	2.56939900	-0.60715800
H	-0.43610200	-2.21984300	1.16834900
H	-2.14760000	-2.21568800	-1.43806400
H	-2.56993900	-3.38507800	-0.16494100
H	-3.81151200	-2.29002700	-0.81620500
H	-3.05399500	-0.86706900	2.61641700
H	-4.32928900	-1.57337300	1.60985400
H	-3.02251200	-2.60229500	2.22210400
Pt	1.58077800	-0.03651000	-0.03162200
Cl	2.01423600	2.05216000	0.93885800
Cl	1.44931500	-2.12967600	-1.09517200
H	-0.28654000	-0.15772300	1.59129600

C	2.60981100	-2.51835600	0.00004800
C	3.57558900	-1.50903500	0.00000600
C	3.18314800	-0.17143100	-0.00004100
C	1.83362300	0.20395400	-0.00006700
C	0.85974100	-0.82537300	-0.00005200
C	1.26271400	-2.17713100	0.00002700
C	1.44090100	1.67552100	-0.00004500
C	-0.54130700	-0.53659600	-0.00005000
C	-1.73656400	-0.33386800	-0.00005600
C	1.93246500	2.39502600	-1.27100700
C	1.93210000	2.39486400	1.27118900
H	2.90508700	-3.56384200	0.00011800
H	4.63230200	-1.76282800	0.00002100
H	3.94619500	0.60280700	-0.00003800
H	0.49939300	-2.94918200	0.00007400
H	0.34663900	1.72168600	-0.00019200
H	1.58963000	3.43651700	-1.27667300
H	1.55299000	1.90643900	-2.17501000
H	3.02747000	2.40515500	-1.32973400
H	1.58920600	3.43633100	1.27692400
H	1.55240900	1.90608400	2.17499300
H	3.02708600	2.40502600	1.33017900
Br	-3.50805000	-0.03227500	-0.00001100

2-IN1

Pt	-1.29571200	0.28373500	-0.81229200
Cl	-1.78266000	2.49677300	-0.19714400
Cl	-0.99069900	-1.81782500	-1.80854100
H	3.25371200	-3.52957000	0.27501400
C	3.45345500	-2.49426600	0.57213600
C	2.70163000	-1.52607800	-0.36427000
H	3.13610300	-2.37288500	1.61371700
H	4.53778800	-2.33658900	0.52951100
C	2.89247100	-0.08338900	0.07163400
C	3.11703500	-1.72978900	-1.83456500
H	1.63425400	-1.75953800	-0.29872700
C	4.15121400	0.52395900	0.02412500
C	1.80840400	0.71050600	0.55252000
H	2.91696300	-2.76393100	-2.13424900
H	2.54848600	-1.07300000	-2.50035400
H	4.18548400	-1.53614400	-1.98673400
C	4.33989900	1.85003600	0.41474300
H	5.00353300	-0.04835500	-0.32948700
C	2.00424300	2.06565200	0.93335400
C	0.51111400	0.18163600	0.67676400
C	3.26599300	2.62892500	0.86816800
H	5.33418500	2.28525200	0.35896900
H	1.14327800	2.64237900	1.25506800
C	-0.64936800	-0.26087700	0.96924000
H	3.41996300	3.66342900	1.15825400
Br	-1.55650400	-1.08692600	2.34889600

2-a-TS1

Pt	-2.03056400	0.19336700	-0.38593300
Cl	-1.61931800	2.48991600	-0.16634700
Cl	-2.89689500	-1.93978200	-0.78165400
H	3.44910300	3.07359700	1.56007200
C	3.74727700	2.07339900	1.22770300
C	2.87113000	1.63702500	0.03612900
H	3.63936400	1.38852400	2.07554800

H	4.80889800	2.11393800	0.95682500
C	3.19839300	0.21821000	-0.39940800
C	2.99064900	2.62529100	-1.14167800
H	1.82855800	1.65638100	0.36899500
C	4.47245500	-0.11158000	-0.87425100
C	2.23560600	-0.83120500	-0.35457600
H	2.69541200	3.62789800	-0.81477100
H	2.33760700	2.33628800	-1.97155200
H	4.01853000	2.68301000	-1.51926400
C	4.79027300	-1.40772800	-1.27999800
H	5.23313100	0.66123500	-0.92956800
C	2.56461500	-2.14801100	-0.76374600
C	0.91247100	-0.58314900	0.07962400
C	3.83713500	-2.43348600	-1.22850800
H	5.79227000	-1.62201900	-1.64195500
H	1.80157400	-2.91791600	-0.71122000
C	-0.33682100	-0.31463800	0.12184000
H	4.09121400	-3.43870900	-1.54926500
Br	0.22185300	-0.75262500	2.22446100

2-a-IN2

Pt	1.85499400	0.33571400	-0.04898800
Cl	1.72713000	2.62839600	-0.38452800
Cl	2.98533000	-1.64866800	0.28368100
H	-0.73147200	3.05311700	1.78594100
C	-1.54281900	2.32640800	1.67466400
C	-1.78028700	2.01406500	0.18282500
H	-1.27428800	1.42659300	2.23843700
H	-2.44983200	2.74699500	2.12513300
C	-2.80718100	0.90958500	0.01709400
C	-2.10632300	3.29247600	-0.60770400
H	-0.82758700	1.64939300	-0.23206500
C	-4.17277100	1.21529100	0.00155200
C	-2.43188400	-0.45577500	-0.07972700
H	-1.25482200	3.97799400	-0.56137500
H	-2.31171100	3.07229700	-1.66050600
H	-2.97491600	3.81608700	-0.19141100
C	-5.15219500	0.22978000	-0.10978500
H	-4.47772500	2.25389000	0.07891400
C	-3.42581800	-1.44402200	-0.19341300
C	-1.01416200	-0.86410300	-0.06040200
C	-4.77481600	-1.10758100	-0.21045500
H	-6.20218100	0.50843800	-0.11901200
H	-3.13926300	-2.48522100	-0.27275900
C	0.14296900	-0.23751100	-0.06559700
H	-5.52218400	-1.88987800	-0.30302300
Br	-0.54981800	-2.74978300	-0.01848900

2-a-TS2

Pt	-1.83702800	-0.18075600	-0.01321800
Cl	-2.02324100	-1.84335600	-1.67717000
Cl	-2.11343600	1.35007400	1.72084200
H	-0.21206900	-2.16293100	2.00929800
C	0.83543700	-1.85085500	1.96392000
C	1.36564900	-1.90284900	0.54334500
H	0.93118400	-0.85937000	2.41002800
H	1.42903700	-2.55930500	2.55832800
C	2.59309300	-1.12035800	0.25341600
C	1.19124300	-3.23897900	-0.15239800
H	0.46102100	-1.22241800	-0.21140300

C	3.86304000	-1.70784500	0.25321700
C	2.45471100	0.26008200	-0.03176500
H	0.13903100	-3.53962400	-0.15765200
H	1.56089300	-3.21657300	-1.17970500
H	1.75314000	-3.99839500	0.41023800
C	4.99711700	-0.92036600	0.05915200
H	3.96802600	-2.77153600	0.44624000
C	3.60268700	1.03905500	-0.22891200
C	1.08470500	0.75603700	-0.17949700
C	4.86367700	0.45181500	-0.17233300
H	5.98208100	-1.37593600	0.09628600
H	3.49772800	2.09733000	-0.43962800
C	0.02823900	-0.07410800	-0.16352700
H	5.74670300	1.06513300	-0.32529800
Br	0.77363800	2.59653200	-0.51988200

2-a-IN4

C	-3.67499200	0.96301500	-1.42689700
C	-4.25620500	-0.03213800	-0.62828100
C	-3.53389000	-0.65191900	0.39784900
C	-2.21516200	-0.27062300	0.61616600
C	-1.63516600	0.72002100	-0.20060500
C	-2.35364300	1.34937200	-1.21935700
C	-1.24260000	-0.75304300	1.68956800
Pt	1.12024100	-0.68394100	-0.36297600
C	0.04649000	-0.01083800	1.30378200
C	-0.24882600	0.91870700	0.22868800
C	-1.66804000	-0.20061400	3.07759000
C	-1.10766000	-2.28475100	1.76026500
Cl	3.07518300	0.03762200	0.71903500
Cl	-0.25449300	-1.86288400	-1.85268900
H	-4.25755900	1.42914700	-2.21569400
H	-5.28713400	-0.32485400	-0.80702200
H	-4.00422700	-1.41622900	1.01031300
H	-1.88483300	2.10973300	-1.83580500
H	0.76599400	0.23453000	2.07964400
H	-0.94783300	-0.50003800	3.84716400
H	-2.64867400	-0.60413200	3.35097800
H	-1.74141000	0.89217300	3.07463200
H	-2.04881000	-2.72695700	2.10646000
H	-0.86455000	-2.70499200	0.78176800
H	-0.32224000	-2.56731300	2.46968900
Br	0.54996900	2.63064700	0.00370000

2-P

C	1.33958800	2.81434000	-0.00000300
C	2.57852400	2.16561000	0.00000500
C	2.65371600	0.76556400	0.00000900
C	1.47640200	0.02844000	0.00000500
C	0.23217400	0.68990100	-0.00000400
C	0.14936300	2.08000100	-0.00000900
C	1.26349100	-1.48305400	0.00001500
C	-0.25651500	-1.57634500	-0.00001700
C	-0.80141600	-0.34976200	-0.00000300
C	1.85471200	-2.14378300	-1.26686900
C	1.85466200	-2.14376400	1.26693400
H	1.30088400	3.90028000	-0.00000500
H	3.49313100	2.75245900	0.00001100
H	3.62323500	0.27275700	0.00001800
H	-0.81684000	2.57588200	-0.00001600

H	-0.79304200	-2.51776300	-0.00002900
H	1.62705400	-3.21612600	-1.28428300
H	2.94485500	-2.03081400	-1.28721300
H	1.44636200	-1.69012500	-2.17539900
H	1.44626900	-1.69009700	2.17544100
H	1.62701100	-3.21610800	1.28435300
H	2.94480400	-2.03078800	1.28732700
Br	-2.65462700	0.05164400	-0.00001700

2-b-TS1

Pt	-1.63846200	-0.57813100	0.03690800
Cl	-1.39076100	-1.40799000	-2.14590000
Cl	-2.22092000	-0.15807100	2.26748900
H	2.97438100	2.88294400	-1.33081900
C	3.34652400	1.85470500	-1.29128900
C	3.15241500	1.24298400	0.07872600
H	2.86996300	1.25835400	-2.07244200
H	4.42749600	1.87951400	-1.49358700
C	3.22824700	-0.25620000	0.17519800
C	3.66106100	2.04865500	1.25041000
H	1.80848200	1.29978600	0.24883700
C	4.34672100	-1.07627800	0.26665100
C	1.93289200	-0.79156700	0.12383700
H	3.40307100	3.10786700	1.16270100
H	3.29725400	1.65394600	2.20236400
H	4.75888000	1.96887500	1.25416900
C	4.14306900	-2.46124300	0.26448600
H	5.35157300	-0.66579400	0.31394200
C	1.72471500	-2.17432900	0.10095100
C	1.00124800	0.31890200	0.11378400
C	2.85081100	-2.99580300	0.17758800
H	4.99865300	-3.12768100	0.31984400
H	0.72336500	-2.58289300	0.03350000
C	-0.25148900	0.72272100	-0.07831000
H	2.71839900	-4.07370300	0.17423800
Br	-0.65571900	2.55773600	-0.36716500

2-c-TS1

C	2.22658700	-3.30831500	0.52980000
C	3.53847700	-2.83863600	0.42150300
C	3.78453700	-1.48693400	0.17832500
C	2.72666600	-0.58004800	0.06841300
C	1.39571200	-1.06345900	0.15948200
C	1.15889100	-2.42801000	0.39301500
C	2.95279800	0.88763900	-0.14646100
C	4.02716400	1.25359700	-1.16960400
C	3.04591700	1.70064600	1.14760700
C	0.30874900	-0.11322500	-0.05046700
C	0.47410300	1.12703400	-0.49725200
H	2.03647600	-4.36205000	0.70912600
H	4.37372600	-3.52493600	0.52843000
H	4.80850800	-1.13401400	0.09853000
H	0.13584300	-2.78120900	0.45024400
H	1.94168600	1.22212800	-0.68311600
H	3.90075700	0.69961200	-2.10380600
H	4.00579000	2.32640500	-1.38678000
H	5.02125900	1.02337400	-0.76495000
H	2.25503800	1.43427300	1.85374900
H	4.01202200	1.49794100	1.62637400
H	2.99114500	2.77565600	0.94363700

Pt	-1.59532200	-0.49929300	0.03852300
Cl	-1.89494900	0.43286000	2.17336100
Cl	-1.75484200	-1.55388200	-2.04537100
Br	-0.08109500	2.85495200	-0.36166400

3-C₆H₅

C	-3.28910100	-2.46074300	0.02571000
C	-4.21138600	-1.41338100	-0.00657500
C	-3.76461000	-0.09195500	-0.05772500
C	-2.40246800	0.22700600	-0.07785300
C	-1.46897400	-0.84293400	-0.03811100
C	-1.92850900	-2.17533500	0.01051300
C	-1.92006800	1.67217500	-0.09580300
C	-0.06167700	-0.60667200	-0.04306600
C	1.14404600	-0.43913100	-0.04223800
C	-1.76433200	2.20610800	1.34397300
C	-2.80455900	2.60939700	-0.93451200
H	-3.62736900	-3.49259800	0.06185100
H	-5.27785400	-1.62226700	0.00567100
H	-4.49773000	0.70871100	-0.08527800
H	-1.19733400	-2.97769600	0.03443200
H	-0.92209400	1.66951600	-0.55009000
H	-1.36945600	3.22944100	1.33586700
H	-1.07882800	1.58042000	1.92493000
H	-2.73154400	2.21994900	1.86104800
H	-2.33298700	3.59569800	-1.01349100
H	-2.95326100	2.22210900	-1.94856200
H	-3.79167500	2.76028100	-0.48158600
C	2.55599200	-0.24608700	-0.04131600
C	3.10543500	1.05062900	-0.11112900
C	3.42996800	-1.35042800	0.02958200
C	4.48584200	1.23251800	-0.11003800
H	2.43778200	1.90505200	-0.16595100
C	4.80909600	-1.15895000	0.03051200
H	3.01275000	-2.35128500	0.08352100
C	5.34273700	0.13078300	-0.03936400
H	4.89497500	2.23780000	-0.16462800
H	5.47055000	-2.01942600	0.08568000
H	6.41948000	0.27630500	-0.03878400

3-IN1

Pt	-0.60019700	-1.40797000	0.35260900
Cl	-0.84763000	-2.45012700	-1.73573600
Cl	-0.45310100	-0.74874100	2.60404700
H	2.05001100	3.65215300	2.11537800
C	2.39700600	3.20474500	1.17710100
C	2.37574900	1.66582000	1.28312300
H	1.74586100	3.55978300	0.37047300
H	3.40935500	3.57791600	0.98021500
C	2.78915900	1.02714800	-0.03397400
C	3.23856000	1.17488900	2.46069300
H	1.34614600	1.36035100	1.49370200
C	4.11448800	1.09351400	-0.48020900
C	1.85492200	0.36522700	-0.87689700
H	2.86498800	1.60458100	3.39652200
H	3.19795800	0.08492300	2.55266200
H	4.28848400	1.47310600	2.35413600
C	4.51268700	0.52017600	-1.68735600
H	4.85332300	1.60189800	0.13217100
C	2.26440000	-0.22771400	-2.09473000

C	0.47324100	0.28706600	-0.53210900
C	3.58814900	-0.14826000	-2.49834100
H	5.55274600	0.58885800	-1.99508800
H	1.52633800	-0.75839700	-2.68747900
C	-0.76845300	0.50890600	-0.35321100
H	3.90231700	-0.60536200	-3.43164900
C	-1.93585000	1.34950200	-0.48348000
C	-2.12493900	2.07897400	-1.67244900
C	-2.86894600	1.45778300	0.56261300
C	-3.22684500	2.92019700	-1.79975600
H	-1.41104700	1.97529400	-2.48350400
C	-3.96898700	2.29965700	0.42103700
H	-2.71453600	0.88597000	1.47214100
C	-4.14998700	3.03108400	-0.75614300
H	-3.36979800	3.48303400	-2.71770900
H	-4.68789700	2.38317400	1.23081900
H	-5.01257200	3.68287600	-0.86305200

3-a-TS1

C	-4.40616000	1.44471600	-1.39561900
C	-5.14672100	0.32146600	-1.01577500
C	-4.52018400	-0.76185400	-0.40135200
C	-3.14526500	-0.77022800	-0.13249600
C	-2.40278300	0.37391700	-0.53812000
C	-3.03845800	1.46558500	-1.16408300
C	-2.46706200	-1.97554700	0.50363000
C	-2.03224900	-2.98522800	-0.58164000
C	-3.32571000	-2.66465500	1.57781000
C	-0.98569100	0.40180800	-0.33723800
C	0.25221700	0.22536800	-0.13116900
C	-0.01962000	1.70885500	0.42918900
C	-0.26501700	1.89633500	1.80812000
C	-0.17158200	3.17015800	2.35279200
C	0.16880400	4.25511800	1.53363200
C	0.41955000	4.07506800	0.16735600
C	0.32078700	2.80699000	-0.39272900
H	-4.89159000	2.29151800	-1.87122400
H	-6.21757500	0.28983000	-1.19728600
H	-5.11732400	-1.62165300	-0.11542700
H	-2.44472700	2.32814500	-1.45045200
H	-1.55221800	-1.62666700	0.99556700
H	-1.36741100	-2.52262600	-1.31865900
H	-1.49081200	-3.81873100	-0.12173200
H	-2.90273000	-3.38825200	-1.11380800
H	-3.68747000	-1.95176400	2.32733200
H	-4.19450700	-3.17817100	1.14904700
H	-2.72454100	-3.42089500	2.09318400
H	-0.50785700	1.03558900	2.42279000
H	-0.35507500	3.32367800	3.41177200
H	0.24384100	5.24926300	1.96559000
H	0.69430600	4.92284200	-0.45267300
H	0.53926500	2.63182000	-1.44126700
Pt	1.91599400	-0.67016400	-0.16912200
Cl	1.46657200	-1.91657400	1.77378900
Cl	2.71694400	0.37549200	-2.11408700

3-a-IN2

Pt	-1.78628100	-0.72939000	-0.03136600
Cl	-1.47379800	-2.99547100	-0.46181300
Cl	-3.00432800	1.19194800	0.41375300

H	1.03002400	-3.31135700	1.71320700
C	1.76815400	-2.50704800	1.62826600
C	1.99876700	-2.14775300	0.14573000
H	1.40071600	-1.64687000	2.19839200
H	2.70369700	-2.84313900	2.09155700
C	2.92171300	-0.94997800	0.01740200
C	2.45583100	-3.37809500	-0.65657500
H	1.02407800	-1.86781900	-0.27831600
C	4.31066100	-1.12683700	0.02236300
C	2.42294800	0.37483900	-0.06504600
H	1.66861200	-4.13810200	-0.63844000
H	2.65916000	-3.12218000	-1.70191800
H	3.36083800	-3.83009200	-0.23336700
C	5.19570500	-0.05198600	-0.05424200
H	4.71018400	-2.13384400	0.08838800
C	3.32233600	1.45414200	-0.14460700
C	0.97710300	0.69526000	-0.06703600
C	4.69784800	1.24692900	-0.14067000
H	6.26725900	-0.23178400	-0.04798700
H	2.93620600	2.46475900	-0.21337700
C	-0.11363600	-0.03378100	-0.06055300
H	5.37208100	2.09599500	-0.20583900
C	0.48515800	2.13424500	-0.07251100
C	0.20829900	2.77577800	-1.28833600
C	0.33072100	2.82515800	1.13826000
C	-0.17668400	4.11590000	-1.29225700
H	0.30209300	2.22468700	-2.21906500
C	-0.05371500	4.16487400	1.12630400
H	0.51583400	2.31199600	2.07685100
C	-0.30526800	4.81071500	-0.08708300
H	-0.38585300	4.61334200	-2.23481100
H	-0.16919000	4.70008800	2.06427400
H	-0.61334600	5.85249100	-0.09244800

3-a-TS2

C	4.85854100	0.24232000	-0.40269700
C	5.01178000	-1.14659200	-0.33315100
C	3.89753600	-1.95932400	-0.13763400
C	2.63184100	-1.38479100	0.03862200
C	2.46534600	0.01806900	-0.07489100
C	3.59801200	0.82068800	-0.28873600
C	1.43238100	-2.20357800	0.31437600
C	0.94530700	-2.27164400	1.74640600
C	1.24164700	-3.48044800	-0.48157100
C	1.08702000	0.53276500	-0.09546200
C	0.07097100	-0.35323800	-0.17215100
C	0.79548900	1.99493100	-0.12161600
C	-0.01565900	2.53959900	-1.12892900
C	-0.30183900	3.90498000	-1.13868300
C	0.21411900	4.73959800	-0.14579500
C	1.01925200	4.20318400	0.86172900
C	1.31061000	2.83965500	0.87499800
H	5.72538000	0.87548800	-0.56867200
H	5.99660300	-1.59432400	-0.42756000
H	4.01753600	-3.03701400	-0.07553200
H	3.47968500	1.89368200	-0.38838400
H	0.47570000	-1.46270700	-0.40825100
H	1.08335100	-1.33146700	2.28121300
H	-0.11029900	-2.55168900	1.80352500
H	1.53511300	-3.05288400	2.24722900

H	1.51469000	-3.35689300	-1.53205300
H	1.88109800	-4.26020200	-0.04382900
H	0.20758800	-3.83169900	-0.41329600
H	-0.41899400	1.89063900	-1.90017900
H	-0.93106000	4.31416800	-1.92406900
H	-0.01232300	5.80223300	-0.15394500
H	1.41542200	4.84453800	1.64422700
H	1.92089200	2.42412000	1.67188300
Pt	-1.79972600	-0.45643000	0.01736400
Cl	-2.16410800	-0.96965400	-2.25142800
Cl	-1.89329700	0.01780200	2.30697900

3-a-IN4

C	-2.49067800	3.09109900	-1.19997700
C	-3.59162300	2.57270000	-0.50551000
C	-3.43413000	1.53396700	0.41829300
C	-2.16597500	1.00698500	0.62903500
C	-1.06206800	1.50750100	-0.09351000
C	-1.21680400	2.56649600	-0.99671700
C	-1.73829300	-0.05972700	1.62794000
C	-2.57231600	-1.35187900	1.55472400
C	-1.80294000	0.51520800	3.06973500
C	0.15730700	0.79887300	0.33112800
C	-0.25296800	-0.22478500	1.28441100
C	1.51337500	1.37607000	0.19549500
C	2.30811400	1.57683100	1.33544700
C	3.56031700	2.17804500	1.22440700
C	4.04227000	2.57036700	-0.02575700
C	3.26441900	2.36134000	-1.16802600
C	2.00629500	1.77472600	-1.05987000
H	-2.63210100	3.90750200	-1.90197900
H	-4.57935000	2.99130600	-0.67822900
H	-4.29401200	1.15388700	0.96312800
H	-0.36507700	2.97477000	-1.52912300
H	0.41920600	-0.55650000	2.07191300
H	-2.60751600	-1.74376800	0.53568200
H	-2.14703200	-2.11953500	2.21057800
H	-3.59766600	-1.15514000	1.88870800
H	-1.19829300	1.42334100	3.17114000
H	-2.83687100	0.77007100	3.32568300
H	-1.44425500	-0.22504500	3.79404900
H	1.94176600	1.27050300	2.31027500
H	4.16256100	2.33259500	2.11503500
H	5.02325000	3.02912500	-0.11165400
H	3.64203200	2.64774900	-2.14538900
H	1.41871500	1.57827400	-1.95149500
Pt	0.23827300	-1.34135600	-0.41175400
Cl	2.12671500	-2.11992200	0.75200600
Cl	-1.45827300	-1.19868300	-2.02724200

3-b-TS1

C	4.17961800	2.22117300	-0.77796200
C	5.07290300	1.15151800	-0.62840800
C	4.61284000	-0.12390700	-0.27884200
C	3.24828600	-0.30127000	-0.08668200
C	2.36178000	0.77980100	-0.20187700
C	2.80914500	2.05333800	-0.57865200
C	2.46031100	-1.55139400	0.21514100
C	2.74781700	-2.25913200	1.52429800
C	2.16241000	-2.46378400	-0.96258600

C	1.02599800	0.33701800	0.11753500
C	-0.28485300	0.52882400	0.11341200
C	-0.84501500	1.89261000	0.27685200
C	-0.34929300	2.72603200	1.29739100
C	-0.84567900	4.01969600	1.44795900
C	-1.83515300	4.49484900	0.58444200
C	-2.33226300	3.66807200	-0.42765000
C	-1.84991100	2.37076800	-0.58360100
H	4.55900700	3.20092400	-1.05349100
H	6.13341700	1.31041600	-0.79985300
H	5.30843000	-0.95317500	-0.18494200
H	2.11812400	2.88267100	-0.68313400
H	1.35636600	-0.98154400	0.41146100
H	2.86330100	-1.55132300	2.34896700
H	1.94705900	-2.96257000	1.76938000
H	3.68517800	-2.82480500	1.41998400
H	1.88460200	-1.89943000	-1.85624500
H	3.06490000	-3.04876900	-1.18772300
H	1.35527400	-3.16128800	-0.71800900
H	0.40272500	2.34389100	1.98087800
H	-0.46592200	4.65148900	2.24610300
H	-2.22549100	5.50154000	0.70589300
H	-3.10829600	4.03146400	-1.09542600
H	-2.23785100	1.72093500	-1.36064600
Pt	-1.40635700	-1.04881400	-0.06424600
Cl	-1.99485000	-0.77574700	-2.32177500
Cl	-1.00389400	-1.79591000	2.13138500

3-c-TS1

C	4.21039300	0.49323000	-0.21406800
C	4.34918600	1.88409400	-0.16155700
C	3.22130100	2.69821200	-0.07338500
C	1.94183600	2.13026000	-0.07322900
C	1.80142900	0.71947400	-0.08565200
C	2.94760400	-0.08759100	-0.16836300
C	0.70376600	2.95598500	-0.04690400
C	0.05822300	3.22889800	-1.40000700
C	0.69265900	4.15754000	0.88958200
C	0.44987400	0.18045500	0.07782800
C	-0.58643000	0.98177800	0.36617700
C	-2.01008600	1.13969200	0.21337500
C	-2.68848100	0.58131600	-0.89501600
C	-4.06477000	0.74400300	-1.01604200
C	-4.77676100	1.47576900	-0.06003400
C	-4.11356100	2.04306600	1.03383000
C	-2.74100300	1.87355400	1.17369500
H	5.09094800	-0.13918900	-0.27549900
H	5.33656400	2.33575900	-0.19548600
H	3.33647300	3.77798700	-0.04517700
H	2.82887600	-1.16496700	-0.17910800
H	-0.07084000	2.15908500	0.60225600
H	0.09934400	2.35800300	-2.05771900
H	-0.98498200	3.54401700	-1.28848200
H	0.60604200	4.04946200	-1.88200000
H	1.08294400	3.90673000	1.87947300
H	1.31936700	4.95326900	0.46471200
H	-0.31880800	4.56411400	0.99166100
H	-2.12826900	0.00262400	-1.62289500
H	-4.58405900	0.29981700	-1.86010100
H	-5.85115300	1.60057700	-0.16391200

H	-4.67030700	2.60304300	1.77939400
H	-2.22041800	2.28860200	2.03228800
Pt	0.05389700	-1.72138500	0.04527100
Cl	-0.24828300	-1.82445400	-2.29498000
Cl	0.28082500	-2.06197500	2.34957400

3-c-IN2

C	4.24919500	0.40041000	-0.40373800
C	4.32976300	1.79681700	-0.24884100
C	3.19543100	2.57498900	-0.00172200
C	1.95649800	1.94596500	0.09203900
C	1.87904800	0.53836900	-0.04148600
C	3.02587500	-0.24303400	-0.30131100
C	0.58980100	2.57458700	0.29122100
C	0.19950900	3.35560900	-0.98384000
C	0.55184600	3.52144200	1.50596900
C	0.52915600	0.11924700	0.16455000
C	-0.33018100	1.30204400	0.53506400
C	-1.74140600	1.35173500	-0.02217200
C	-2.04088200	0.93061200	-1.32642800
C	-3.34145100	1.03202400	-1.82137600
C	-4.36015400	1.55844100	-1.02463700
C	-4.07272700	1.97588000	0.27572900
C	-2.77318800	1.86842500	0.77299800
H	5.15065000	-0.17086500	-0.60198700
H	5.29872100	2.28256400	-0.32977500
H	3.28690500	3.65227000	0.10330200
H	2.93192600	-1.31688100	-0.41879400
H	-0.42711900	1.17789700	1.62859100
H	0.20463700	2.71552500	-1.87110800
H	-0.80085000	3.78578600	-0.88023100
H	0.91101500	4.17196300	-1.15097100
H	0.87047400	3.01372600	2.42307500
H	1.20777900	4.38550000	1.35033500
H	-0.46453100	3.90122900	1.65789900
H	-1.26431800	0.50336800	-1.95448300
H	-3.55716400	0.69227000	-2.83053100
H	-5.37266500	1.63383600	-1.41150400
H	-4.86050900	2.37406400	0.90935300
H	-2.56224400	2.17470900	1.79485100
Pt	-0.07865900	-1.64269200	0.14757600
Cl	0.47536400	-2.19092700	-2.06073600
Cl	-0.79854600	-1.71897600	2.37243700

3-c-TS2

C	4.34152600	-0.09535200	0.06690300
C	4.59066200	1.27907900	-0.02983000
C	3.53742800	2.19913200	-0.06418800
C	2.23192300	1.71887800	-0.00711100
C	1.99019000	0.34424300	0.09560100
C	3.03328500	-0.57825100	0.13688000
C	0.92450500	2.49690700	-0.05510700
C	0.73041100	3.13156100	-1.46462900
C	0.86513200	3.59503000	1.02827200
C	0.52029600	0.11701400	0.18196800
C	-0.13435200	1.38625100	0.05008600
C	-1.57991300	1.58588600	-0.05293100
C	-2.30629600	0.80500300	-0.97761300
C	-3.67553600	1.00648600	-1.14054700
C	-4.34413100	1.95556500	-0.36644100

C	-3.63784300	2.72093600	0.56713400
C	-2.26519800	2.55188800	0.71349900
H	5.17384400	-0.79261800	0.08950200
H	5.61530200	1.63677900	-0.08106900
H	3.74548700	3.26330900	-0.14255600
H	2.82218500	-1.63972000	0.21231500
H	0.17666200	0.44588500	1.29067200
H	0.77272100	2.37415400	-2.25317100
H	-0.22888800	3.65412000	-1.52681800
H	1.53697600	3.85095500	-1.64028000
H	0.88445900	3.16890500	2.03682300
H	1.74069000	4.24372400	0.92376200
H	-0.02238800	4.22350600	0.92215200
H	-1.78933000	0.06791100	-1.58182200
H	-4.21916500	0.40959800	-1.86658000
H	-5.41479100	2.09765400	-0.48433900
H	-4.15891900	3.44652100	1.18466300
H	-1.73739500	3.12922200	1.46276300
Pt	-0.27499000	-1.66800200	0.08228000
Cl	0.04043300	-1.99251600	-2.21826400
Cl	-0.76871500	-1.58379600	2.39147100

3-c-TS'

C	2.18198400	-1.46099200	2.86845700
C	3.36779100	-1.75728000	2.18618600
C	3.49406400	-1.47819300	0.82154500
C	2.41527200	-0.90327100	0.15333600
C	1.22896000	-0.60485100	0.84236400
C	1.09993000	-0.87750600	2.20364700
C	2.30062000	-0.52721500	-1.32021300
C	3.39475400	0.43617200	-1.83266300
C	2.28342900	-1.80137900	-2.22845400
C	0.24303100	0.06109700	-0.08978700
C	0.91233100	0.03935900	-1.37634700
C	0.43839500	1.63211200	-0.18350000
C	1.47084400	2.27763600	0.52987400
C	1.55812300	3.66734800	0.53026700
C	0.64554000	4.43076400	-0.20185300
C	-0.36550700	3.80066500	-0.93733800
C	-0.46823700	2.41683100	-0.93605300
H	2.09989600	-1.68837500	3.92754500
H	4.19737200	-2.21291800	2.71988500
H	4.41781300	-1.71401900	0.29860800
H	0.17455600	-0.64165800	2.72004000
H	0.44504300	0.35635400	-2.29876000
H	3.44404300	1.34294000	-1.22432600
H	3.20527400	0.72327000	-2.87268300
H	4.36914100	-0.06179700	-1.79269000
H	1.50330900	-2.49972200	-1.92145600
H	3.26075100	-2.28777000	-2.13985900
H	2.12046700	-1.53116700	-3.27683200
H	2.17075100	1.69172000	1.11301200
H	2.33693400	4.15497600	1.10911500
H	0.71735600	5.51471800	-0.19682200
H	-1.08116300	4.39172800	-1.50061700
H	-1.27231200	1.92336800	-1.47263800
Pt	-1.65144500	-0.55030000	0.00921900
Cl	-2.23927600	0.58260000	1.97614500
Cl	-1.31981200	-1.79707300	-1.98128500

3-c-IN3

C	-4.08050400	0.92860200	-1.64143100
C	-4.24142000	1.72370400	-0.49926700
C	-3.15373000	2.03392700	0.32715200
C	-1.90037500	1.53094700	0.00232000
C	-1.74685300	0.71527600	-1.13453600
C	-2.82708200	0.41352800	-1.96871700
C	-0.55566600	1.79356700	0.67180000
C	-0.57349200	1.71731700	2.20631800
C	-0.10256300	3.23034200	0.26114500
C	-0.35661800	0.26847700	-1.21855600
C	0.38641900	0.80994500	-0.08865900
C	1.85491300	1.03813900	-0.07983200
C	2.52070800	1.40716900	-1.26030300
C	3.88647800	1.68345200	-1.24693900
C	4.61148600	1.58264300	-0.05818500
C	3.96123600	1.20780700	1.12001100
C	2.59341300	0.94433900	1.11243100
H	-4.93902500	0.70490500	-2.26773500
H	-5.22631200	2.11025400	-0.25194400
H	-3.29898100	2.65941700	1.20361800
H	-2.69561400	-0.22446900	-2.83824900
H	0.10981000	-0.02523400	-2.15441200
H	-0.86148500	0.72606600	2.55847400
H	0.40628100	1.97723500	2.61891700
H	-1.29137700	2.44739600	2.59723600
H	-0.05306200	3.34783700	-0.82631700
H	-0.83053000	3.95237600	0.64522100
H	0.87880100	3.46456000	0.68293700
H	1.96720200	1.48397100	-2.19122800
H	4.38491200	1.97079500	-2.16839400
H	5.67810800	1.78871300	-0.05079700
H	4.52111100	1.11311300	2.04606300
H	2.10098600	0.62275700	2.02408000
Pt	-0.02841400	-1.33652100	0.14308800
Cl	-1.68784300	-1.55989100	1.78609100
Cl	1.67063200	-2.08988300	-1.30472700

3P-C₆H₅

C	4.21230700	-1.20773700	-0.03915400
C	4.31857100	0.17426300	0.15198500
C	3.17119200	0.97933100	0.19661500
C	1.92495900	0.38272400	0.05713300
C	1.81839200	-1.00850000	-0.13285400
C	2.96081500	-1.81233700	-0.18515600
C	0.53618000	1.01413900	0.03947300
C	0.45978900	1.96229900	-1.18693000
C	0.25956400	1.78596700	1.34836400
C	0.40633800	-1.34097700	-0.22999200
C	-0.37097500	-0.23184500	-0.10473500
C	-1.84469600	-0.24417400	-0.05573400
C	-2.53025100	-1.44969100	0.21510200
C	-3.91905400	-1.50690000	0.25647000
C	-4.68113000	-0.35460100	0.04289800
C	-4.02777900	0.85106500	-0.20690500
C	-2.63418500	0.90622700	-0.25300700
H	5.11209300	-1.81649500	-0.07330300
H	5.29914900	0.62854200	0.26670600
H	3.26758700	2.05303600	0.34205400
H	2.87981400	-2.88652700	-0.33241700

H	0.04378500	-2.35246200	-0.38010400
H	0.61823500	1.40680800	-2.11682800
H	-0.49980300	2.48104500	-1.25929700
H	1.24124400	2.72680100	-1.11177000
H	0.38101000	1.13224300	2.21824500
H	0.95797900	2.62432900	1.45300700
H	-0.75788100	2.18950400	1.36730200
H	-1.96207300	-2.35145300	0.41934600
H	-4.40940100	-2.45334800	0.46950400
H	-5.76615900	-0.39673400	0.08076600
H	-4.60198600	1.75962500	-0.36918600
H	-2.16382900	1.85956900	-0.45545800

3P'-C₆H₅

C	-1.77136200	2.81754900	-0.33490500
C	-3.02985800	2.21635900	-0.24841000
C	-3.14313100	0.82892400	-0.08317900
C	-1.98808700	0.06277100	0.00489700
C	-0.71708900	0.67020600	-0.06654500
C	-0.60445200	2.05016200	-0.24918800
C	-1.83121100	-1.44529100	0.15291800
C	-2.46165100	-2.20348000	-1.03900200
C	-2.43482900	-1.95979500	1.48052600
C	0.31114800	-0.39170000	0.03542700
C	-0.32072700	-1.58215500	0.15270200
H	-1.69660400	3.89283000	-0.47510300
H	-3.92652400	2.82672000	-0.31625000
H	-4.12606100	0.36593000	-0.02996600
H	0.36871600	2.52395400	-0.33640600
H	-2.05382300	-1.84829500	-1.99080200
H	-2.26444000	-3.27936000	-0.95969300
H	-3.54873300	-2.06191800	-1.05789800
H	-2.00355100	-1.43416200	2.33847500
H	-3.52057400	-1.80860000	1.49676800
H	-2.24285900	-3.03262100	1.60231500
H	0.17227800	-2.54237600	0.27292200
C	1.77347500	-0.18189600	0.01597700
C	2.37000300	0.86751600	0.73701000
C	2.60853200	-1.05093100	-0.70737600
C	3.75451200	1.03776900	0.73711700
H	1.74545400	1.53628900	1.32173600
C	3.99223700	-0.88099200	-0.70648300
H	2.15916300	-1.85303400	-1.28649300
C	4.57138300	0.16568500	0.01478000
H	4.19587700	1.85099300	1.30752000
H	4.61876800	-1.56205400	-1.27669500
H	5.64955700	0.30149900	0.01198100

3-IN1-tBu

Pt	-1.02617500	-1.64388900	-0.34612000
Cl	-1.06584700	-2.66919600	1.76726800
Cl	-1.07368300	-0.99695900	-2.60846600
H	-1.21699900	4.09259600	-2.12499600
C	-1.65733500	3.84749500	-1.15173100
C	-2.32038600	2.45585200	-1.20378300
H	-0.86126000	3.88337700	-0.39953600
H	-2.38580400	4.62986200	-0.90649700
C	-2.87895900	2.06747600	0.15721700
C	-3.39334300	2.38656500	-2.30648800

H	-1.54737300	1.72814500	-1.46861400
C	-3.98804900	2.73464400	0.69211000
C	-2.29831000	1.04084000	0.94791100
H	-2.94068900	2.60882400	-3.27906700
H	-3.83476100	1.38658200	-2.36296500
H	-4.19988600	3.11101400	-2.14149800
C	-4.51699500	2.39980000	1.93781200
H	-4.45050200	3.53253100	0.11846300
C	-2.84485700	0.69215700	2.20404300
C	-1.13501100	0.33011000	0.50937900
C	-3.94828200	1.37171200	2.69779500
H	-5.38189000	2.93879600	2.31536400
H	-2.39502300	-0.12583800	2.75766600
C	0.07115600	0.01594800	0.25581700
H	-4.36749600	1.10201900	3.66236400
C	1.49766100	0.20385000	0.24923300
C	2.18687000	0.38497200	1.45912000
C	2.21937000	0.21182400	-0.95916400
C	3.56406100	0.59376000	1.45451300
H	1.64012800	0.35644600	2.39632200
C	3.59162800	0.41793300	-0.94215300
H	1.69167100	0.04759800	-1.89368400
C	4.30024100	0.61400500	0.25965700
H	4.06367300	0.73313700	2.40596900
H	4.12431200	0.42021500	-1.88817000
C	5.82267600	0.82810700	0.22270300
C	6.49596300	-0.40705300	-0.42397100
H	6.14658900	-0.57493100	-1.44800000
H	7.58295200	-0.26727400	-0.46118400
H	6.28927400	-1.31502800	0.15368600
C	6.14154600	2.08714000	-0.61991200
H	5.68096100	2.98033400	-0.18251100
H	7.22539400	2.24870600	-0.66005800
H	5.78089500	1.99381500	-1.64952200
C	6.42329400	1.02428900	1.62781100
H	6.00664900	1.90396300	2.13170000
H	6.25968100	0.15044600	2.26863900
H	7.50554700	1.17406500	1.54636200

3-a-TS1-tBu

C	-0.18735900	4.42046100	-1.88833100
C	-1.18300700	5.09609100	-1.17614500
C	-1.96605300	4.41763300	-0.24372700
C	-1.78799400	3.05384500	0.02416200
C	-0.78088600	2.37651100	-0.71785100
C	0.00578700	3.06520100	-1.66421500
C	-2.67950100	2.32021500	1.01647800
C	-3.97863100	1.84822000	0.32724600
C	-2.99625000	3.14495100	2.27585900
C	-0.58436900	0.97135000	-0.52846800
C	-0.59393800	-0.27338000	-0.28373300
C	0.94697100	0.11337200	-0.14199500
C	1.49039600	0.38650300	1.13510600
C	2.86242300	0.40406000	1.30942900
C	3.74808400	0.14972600	0.23746200
C	3.19229700	-0.12312800	-1.02710900
C	1.81750700	-0.13765400	-1.22408800
H	0.42610600	4.94614100	-2.61379100
H	-1.34938300	6.15618200	-1.34727200
H	-2.73301300	4.96387100	0.29603000

H	0.77270600	2.52110600	-2.20677100
H	-2.14994900	1.41908600	1.34433300
H	-3.76599500	1.21023200	-0.53698800
H	-4.58481700	1.26685800	1.03007900
H	-4.57307800	2.70297500	-0.01869700
H	-2.08495200	3.52394200	2.75191100
H	-3.64770200	4.00011300	2.06007600
H	-3.51937100	2.51369800	3.00179300
H	0.81769400	0.56140700	1.96877400
H	3.25874900	0.61082900	2.29832700
H	3.83832900	-0.33260900	-1.87103900
H	1.39490200	-0.37773300	-2.19481400
Pt	-1.36085400	-1.99087000	-0.07626900
Cl	-1.97354800	-1.60958500	2.16418800
Cl	-0.91181800	-2.72363900	-2.26233200
C	5.26299800	0.16936800	0.48603700
C	6.07575900	-0.11481800	-0.79140900
H	7.14489200	-0.08483500	-0.55606100
H	5.85831800	-1.10641900	-1.20364500
H	5.88966000	0.63264500	-1.57107100
C	5.61443200	-0.91253800	1.53793200
H	6.69370500	-0.90760500	1.72952000
H	5.10602400	-0.74014900	2.49194000
H	5.33612000	-1.91134600	1.18427600
C	5.67302800	1.56358200	1.02256400
H	5.44044900	2.35041700	0.29602700
H	5.16597900	1.81044600	1.96072300
H	6.75227500	1.58599700	1.21253600

3-c-TS1-tBu

C	4.85932800	1.38862300	-0.25600000
C	4.69353200	2.77634100	-0.18982200
C	3.41718800	3.32535700	-0.08301700
C	2.29136000	2.49272600	-0.07788500
C	2.46048000	1.08464400	-0.09867900
C	3.75389100	0.54690900	-0.20248100
C	0.90445200	3.02721700	-0.03947200
C	0.19392300	3.13331600	-1.38279700
C	0.63782600	4.20457100	0.88897400
C	1.26164300	0.26435800	0.08275300
C	0.08136600	0.82577500	0.39443800
C	-1.34006200	0.65894200	0.26142500
C	-1.90018300	-0.03652400	-0.83184300
C	-3.27863100	-0.19856800	-0.92672100
C	-4.15541300	0.33424300	0.03334100
C	-3.58554600	1.04295800	1.11157100
C	-2.21396500	1.20108100	1.23004800
H	5.85549500	0.96341100	-0.33360400
H	5.55894600	3.43184300	-0.22913000
H	3.29527700	4.40421300	-0.04724300
H	3.87149700	-0.53052300	-0.22297300
H	0.33210100	2.07622100	0.63435500
H	0.42548700	2.28950300	-2.03609100
H	-0.89220100	3.19966800	-1.25607200
H	0.53037200	4.05426300	-1.87731500
H	1.09424300	4.06071300	1.87185300
H	1.05647600	5.11821200	0.44551000
H	-0.43773100	4.37002300	1.01058400
H	-1.24270900	-0.47337100	-1.57740800
H	-3.66844400	-0.75395700	-1.77167300

H	-4.22624300	1.46500300	1.87979400
H	-1.79897500	1.72861000	2.08478100
Pt	1.29155100	-1.67750400	0.04099600
Cl	0.99849800	-1.83450100	-2.29813000
Cl	1.59983400	-1.97881300	2.34209000
C	-5.68044000	0.16341800	-0.04757500
C	-6.35067900	1.55851900	-0.09278500
H	-7.44053200	1.44969000	-0.14187800
H	-6.11697900	2.15632600	0.79436500
H	-6.02649000	2.12306300	-0.97461900
C	-6.11907800	-0.62273400	-1.29780300
H	-5.81961800	-0.11947700	-2.22420500
H	-5.70657400	-1.63773700	-1.30900800
H	-7.21081800	-0.71160000	-1.30944100
C	-6.17106200	-0.60331100	1.20529100
H	-5.71412400	-1.59751200	1.26111600
H	-5.93122600	-0.07158400	2.13195800
H	-7.25939700	-0.73050400	1.16558000

3-IN1-OMe

Pt	0.47548300	-1.58238300	0.54648200
Cl	0.37446200	-2.88175100	-1.41535000
Cl	0.60535000	-0.62022600	2.68748500
H	0.93468800	4.45687400	1.35644900
C	1.42783300	3.99974500	0.49060700
C	1.95245100	2.59647900	0.85526200
H	0.70306700	3.95524100	-0.33028200
H	2.24232800	4.66554400	0.18088600
C	2.58518200	1.91466500	-0.34962700
C	2.92006100	2.65179900	2.05263900
H	1.09681400	1.99122600	1.16977700
C	3.76954600	2.41354800	-0.90800600
C	2.01443100	0.77057000	-0.96086900
H	2.41861100	3.10175300	2.91692500
H	3.24569000	1.64698600	2.33900800
H	3.80946500	3.25434000	1.83244200
C	4.37778200	1.80810100	-2.00628500
H	4.22902400	3.29498600	-0.46961200
C	2.63951800	0.14630600	-2.06139900
C	0.77367900	0.20405000	-0.49271600
C	3.81480300	0.66634800	-2.58511500
H	5.29840300	2.22380800	-2.40721700
H	2.18893300	-0.74954300	-2.47731200
C	-0.48691300	0.11882300	-0.35289000
H	4.29195500	0.18477800	-3.43335500
C	-1.88427100	0.37737800	-0.44974500
C	-2.61977000	-0.09477400	-1.56231100
C	-2.55199700	1.09338900	0.56195400
C	-3.97097700	0.17288400	-1.66661000
H	-2.11112400	-0.67644900	-2.32408300
C	-3.91117300	1.36356300	0.46027300
H	-1.99509000	1.42430100	1.43262900
C	-4.62850900	0.90556800	-0.65853100
H	-4.55233600	-0.17764600	-2.51291200
H	-4.40348100	1.91824800	1.24999700
O	-5.95030200	1.10945400	-0.85634700
C	-6.69373900	1.82015000	0.12864000
H	-6.31502300	2.84197400	0.25350600
H	-7.71826300	1.85543900	-0.24378200
H	-6.67338100	1.30040200	1.09419800

3-a-TS1-OMe

C	1.16164000	0.63225900	0.12405400
C	-0.53258400	0.82234300	-0.48400000
C	-0.03765200	-0.32007900	-0.22242500
C	-2.50523600	2.25446200	-0.07311100
C	-1.26787000	2.02279600	-0.73523400
C	-0.76684600	2.95156700	-1.67297700
C	-3.09542800	1.25323100	0.90970900
C	-4.16829000	0.38440700	0.21896100
C	-3.65743100	1.92053200	2.17800700
C	-1.47030400	4.11043800	-1.96396200
C	-2.69509300	4.34331600	-1.32970500
C	-3.19737000	3.42633300	-0.40860900
C	1.37495400	1.06254300	1.46184800
C	2.56614300	1.65187700	1.82098600
C	3.58923000	1.82124300	0.85942600
C	3.39598000	1.39510500	-0.47125500
C	2.19216600	0.81327300	-0.83001700
H	-1.07615600	4.82303900	-2.68222900
H	-3.26104800	5.24323600	-1.55487800
H	-4.15240700	3.62826400	0.06673000
H	0.18305200	2.74793800	-2.15753500
H	-2.29674500	0.57455200	1.22569100
H	-3.75711900	-0.14039400	-0.64964500
H	-4.54462500	-0.37014600	0.91784900
H	-5.01436500	0.99495800	-0.12029100
H	-2.91105500	2.56054500	2.66207800
H	-4.54219700	2.53295900	1.96767000
H	-3.95759300	1.14862000	2.89457800
H	0.59052200	0.90588900	2.19532800
H	2.75423500	1.98568500	2.83589800
H	4.17878100	1.50813100	-1.21141500
H	2.03582700	0.44830600	-1.84035000
Pt	-0.09104100	-2.21383300	-0.13304600
Cl	-1.20399600	-2.25185700	1.93931000
Cl	1.00585800	-2.56167500	-2.18599600
O	4.71275700	2.39946200	1.31389200
C	5.81690300	2.58651900	0.42662500
H	6.59791600	3.05235200	1.02780000
H	6.17507500	1.62723100	0.03671900
H	5.54789700	3.24918400	-0.40383400

3-c-TS1-OMe

C	4.51390500	1.06497200	-0.39534900
C	4.46637100	2.46194500	-0.31905700
C	3.24470000	3.11348100	-0.16854900
C	2.05335700	2.37690500	-0.13145600
C	2.10417500	0.95870700	-0.15398500
C	3.34586000	0.31739300	-0.30460900
C	0.72072500	3.02463400	-0.04988100
C	-0.04038100	3.16459100	-1.36136400
C	0.58588000	4.23149500	0.86803200
C	0.85363800	0.23796000	0.08550300
C	-0.26377900	0.89983000	0.44650100
C	-1.69094900	0.82789700	0.35890300
C	-2.32905000	0.14403000	-0.70248700
C	-3.71317900	0.06056400	-0.76605700
C	-4.49782400	0.68460900	0.21992700
C	-3.87763300	1.38728400	1.27377000

C	-2.50062300	1.44968000	1.34264600
H	5.46823400	0.55931500	-0.50861100
H	5.38149800	3.04350500	-0.38634000
H	3.21266800	4.19841700	-0.12682900
H	3.37403400	-0.76600300	-0.32968200
H	0.09583100	2.11581900	0.66869800
H	0.10852100	2.30314400	-2.01574400
H	-1.11379700	3.29951000	-1.18760200
H	0.32910500	4.05936600	-1.88011900
H	1.07235700	4.06700000	1.83319500
H	1.05232700	5.10513100	0.39221900
H	-0.46744600	4.48131800	1.03331300
H	-1.72087400	-0.35036800	-1.45404700
H	-4.17227500	-0.48975100	-1.57872700
H	-4.50684000	1.85226000	2.02544600
H	-2.02436300	1.96690400	2.17092500
Pt	0.74009600	-1.70110200	0.05505500
Cl	0.37157100	-1.83948200	-2.27707400
Cl	1.08029400	-2.01961500	2.34852200
O	-5.84727500	0.66897900	0.24887700
C	-6.55275500	-0.04599800	-0.76306200
H	-7.60996000	0.06902200	-0.52119200
H	-6.35667700	0.37408300	-1.75684200
H	-6.28793200	-1.10976100	-0.75456700

4-Me

C	1.58666800	-2.48942200	-0.00048900
C	2.53033500	-1.45959000	-0.00049200
C	2.10641100	-0.13155300	0.00004300
C	0.74836300	0.21232100	0.00053700
C	-0.20491900	-0.83666000	0.00033300
C	0.23197300	-2.17781800	-0.00008000
C	0.32311500	1.67507500	0.00084100
C	-1.61393300	-0.57820200	0.00052200
C	-2.81416200	-0.40210000	0.00066100
C	0.79426000	2.40514500	-1.27178200
C	0.80119700	2.40724300	1.26962600
H	1.90499100	-3.52836400	-0.00081500
H	3.59263000	-1.68933800	-0.00087200
H	2.85137100	0.66036400	0.00005500
H	-0.51353200	-2.96729700	-0.00004800
H	-0.77188300	1.69408400	0.00388200
H	0.42826400	3.43898600	-1.27804700
H	0.42347300	1.90678200	-2.17413600
H	1.88865100	2.43983000	-1.33417100
H	0.43461100	3.44086500	1.27640500
H	0.43584500	1.91006000	2.17484500
H	1.89588400	2.44282000	1.32580100
C	-4.25799900	-0.18576300	0.00095000
H	-4.55967700	0.49982000	-0.80085100
H	-4.80071600	-1.12744400	-0.14662700
H	-4.59777700	0.24677800	0.95055500

4-IN1

Pt	-1.52797000	-0.08263200	-0.28938000
Cl	-2.21578400	2.15767200	-0.12602400
Cl	-1.12316400	-2.35212000	-0.72393100
H	3.49856800	-3.03953300	1.39111100
C	3.58567700	-1.95407300	1.26859700
C	2.63510700	-1.46908200	0.15487000

H	3.35067900	-1.48319200	2.22989700
H	4.63207400	-1.72681700	1.03184500
C	2.68077900	0.04475600	0.01832700
C	2.93635600	-2.17036800	-1.18356000
H	1.61618500	-1.74925400	0.43971700
C	3.84087200	0.68859700	-0.42763700
C	1.56875800	0.86822300	0.34808500
H	2.84488900	-3.25524200	-1.06263800
H	2.22935800	-1.85933700	-1.95889600
H	3.95255700	-1.95742900	-1.53624000
C	3.90628300	2.07533400	-0.55928000
H	4.71214200	0.09207200	-0.68177300
C	1.63479900	2.27558800	0.20153300
C	0.35797200	0.31300900	0.84558400
C	2.80008500	2.87543500	-0.24777000
H	4.82463000	2.53623800	-0.91327800
H	0.75049600	2.86247200	0.42803300
C	-0.62242000	-0.12034200	1.52684000
H	2.85017200	3.95388800	-0.36175000
C	-1.20272000	-0.54059000	2.81724600
H	-1.52349200	-1.58584400	2.76600800
H	-0.45178700	-0.43307000	3.60845500
H	-2.07201100	0.07704300	3.06337600

4-a-TS1

Pt	-2.02589700	0.13387900	-0.11918300
Cl	-3.04454100	-1.96520100	0.16274700
Cl	-1.42608400	2.36974900	-0.44452400
H	2.66626900	3.51605600	-0.47270800
C	3.03649400	2.52493000	-0.75609500
C	2.81913200	1.53183500	0.40300600
H	2.49679400	2.20943800	-1.65475800
H	4.09885300	2.62083200	-1.01089000
C	3.25270600	0.12549500	0.01322900
C	3.52608300	2.00912100	1.68702800
H	1.74368300	1.51088700	0.60584700
C	4.59812000	-0.14908300	-0.27171400
C	2.33890900	-0.95219900	-0.09677700
H	3.14512900	2.99377500	1.97930700
H	3.35607900	1.31857800	2.52091300
H	4.60923100	2.10095800	1.54420500
C	5.02878700	-1.42234100	-0.63802500
H	5.32482700	0.65519700	-0.20457300
C	2.77462900	-2.23960000	-0.47493000
C	0.93479800	-0.75856600	0.15282100
C	4.11598700	-2.47672900	-0.74144600
H	6.08104100	-1.59329400	-0.84835200
H	2.04463600	-3.03867100	-0.56508000
C	-0.28170400	-0.46966500	0.16240800
H	4.44725300	-3.46794200	-1.03539200
C	0.13404100	-1.33624600	1.74697100
H	1.03922300	-1.91618900	1.93603000
H	0.01910700	-0.54021900	2.47949900
H	-0.71939200	-2.01101100	1.69358100

4-a-IN2

Pt	1.78414400	0.06533900	-0.03571500
Cl	1.55963300	2.35712800	-0.34074700
Cl	2.93644700	-1.92847800	0.29049700
H	-0.98341700	2.75237500	1.70600000

C	-1.75220200	1.97769300	1.62010200
C	-1.91266900	1.54497300	0.14943600
H	-1.46179000	1.13514300	2.25687600
H	-2.69612300	2.38141800	2.00597300
C	-2.87623600	0.38279900	0.02101500
C	-2.26440300	2.74025900	-0.75328800
H	-0.92445000	1.19940200	-0.19551300
C	-4.25624500	0.61773100	0.04827300
C	-2.42635900	-0.95679800	-0.08930900
H	-1.45983200	3.48068900	-0.71416400
H	-2.39443200	2.42974400	-1.79527900
H	-3.18759300	3.23351600	-0.42699600
C	-5.18554800	-0.41746000	-0.03530700
H	-4.61166900	1.63960100	0.13882900
C	-3.37383000	-1.99473900	-0.17526600
C	-0.98950300	-1.32664600	-0.10751900
C	-4.74002200	-1.73262100	-0.15084200
H	-6.24878800	-0.19556900	-0.01116600
H	-3.04622600	-3.02343500	-0.26511500
C	0.09122300	-0.57897800	-0.08553100
H	-5.44748000	-2.55361100	-0.22164700
C	-0.58773200	-2.81114500	-0.16108100
H	0.49486200	-2.94946100	-0.13955500
H	-1.01552200	-3.32958300	0.70288400
H	-0.97294700	-3.25411000	-1.08519000

4-a-TS2

Pt	1.74035700	-0.01108900	-0.07464500
Cl	1.80357300	2.08043600	-1.16604300
Cl	2.13486300	-1.98646000	1.10792300
H	-0.01131600	1.38637500	2.20046900
C	-1.04057300	1.03062800	2.09655500
C	-1.58936700	1.32399500	0.71334000
H	-1.07864300	-0.03100600	2.34457400
H	-1.66490600	1.58113400	2.81446100
C	-2.73962200	0.51866100	0.25267300
C	-1.52763600	2.78357000	0.30969800
H	-0.61998900	0.88224800	-0.20687200
C	-4.05258700	1.00430000	0.29687200
C	-2.47780000	-0.77791300	-0.25519100
H	-0.50084600	3.15719400	0.36606000
H	-1.91102700	2.94723200	-0.69977900
H	-2.13573300	3.36413500	1.01846600
C	-5.11449000	0.17645600	-0.06179800
H	-4.24692000	2.00993000	0.65833200
C	-3.56054900	-1.59828500	-0.61180100
C	-1.07513000	-1.15713900	-0.46115100
C	-4.86585400	-1.12701700	-0.50496200
H	-6.13383600	0.54301700	0.01419400
H	-3.37859900	-2.59914600	-0.98819200
C	-0.12658900	-0.21340500	-0.28913300
H	-5.69418200	-1.77175000	-0.78415000
C	-0.72741200	-2.54619900	-0.94184500
H	0.35186600	-2.67958200	-1.00739000
H	-1.12218200	-3.29960700	-0.25012200
H	-1.16928900	-2.72873400	-1.92923500

4-b-TS1

Pt	-1.71583100	0.12658400	-0.00884100
Cl	-1.48927800	1.39989100	1.95390300

Cl	-2.28972100	-0.87827500	-2.05222100
H	3.12101700	-2.61196800	1.99948300
C	3.38044100	-1.58145400	1.73642900
C	3.22542100	-1.31839100	0.25702300
H	2.79553900	-0.88337500	2.33874200
H	4.44292200	-1.43627400	1.98633500
C	3.11307700	0.10401600	-0.18084400
C	3.88364900	-2.30192500	-0.67374400
H	1.79377200	-1.55870200	0.04099000
C	4.13741800	0.98184200	-0.52909400
C	1.76707500	0.51007700	-0.17799200
H	3.77317600	-3.33480500	-0.33116800
H	3.51145700	-2.20502300	-1.69690400
H	4.96093200	-2.07219600	-0.69306800
C	3.79640100	2.30849900	-0.80605900
H	5.17599200	0.66281600	-0.54725400
C	1.42896200	1.84543600	-0.42943200
C	0.94483300	-0.66261400	0.06537500
C	2.46006600	2.72936300	-0.74723500
H	4.57642600	3.02184100	-1.05525600
H	0.39559900	2.16841800	-0.39330700
C	-0.27622200	-1.10558100	0.37769300
H	2.21757900	3.76537100	-0.96542200
C	-0.61711100	-2.47508900	0.88169900
H	-1.28031500	-2.97867700	0.17055300
H	0.28255900	-3.08679500	1.03072800
H	-1.15288600	-2.39671800	1.83361900

4-c-TS1

C	2.18966200	2.82377400	-0.99955000
C	3.50467100	2.38255900	-0.83087500
C	3.75692400	1.09431000	-0.35853800
C	2.69558000	0.22754600	-0.08082000
C	1.36311300	0.68219000	-0.23205600
C	1.12222500	1.98264200	-0.69717400
C	2.91549300	-1.17838800	0.37917000
C	3.96843400	-1.37938200	1.46510800
C	2.97852200	-2.21674800	-0.73708200
C	0.30168700	-0.24534500	0.17143300
C	0.55963500	-1.39356700	0.78308200
H	1.99491700	3.83076000	-1.35598900
H	4.33644200	3.03956900	-1.06837400
H	4.78229000	0.75735500	-0.23495900
H	0.09905600	2.32510800	-0.79564500
H	1.87349100	-1.37639100	1.03818400
H	3.84393100	-0.66901100	2.28643000
H	3.93732000	-2.39924300	1.86120800
H	4.96488300	-1.22912700	1.02947000
H	2.18324700	-2.07676500	-1.47295300
H	3.94259300	-2.10745300	-1.25003500
H	2.93118700	-3.23770000	-0.34193800
Pt	-1.60986500	0.10256300	-0.01501700
Cl	-1.90669100	-1.53499900	-1.68070300
Cl	-1.73609100	1.79685900	1.59750600
C	0.09479100	-2.76857600	1.06287200
H	-0.90236100	-2.88196000	0.62577600
H	0.74446800	-3.50679500	0.57511700
H	0.06092800	-2.98594800	2.13594800

4-c-IN2

C	-2.36129900	2.83158600	-0.89550400
C	-3.61815400	2.20659700	-0.79984200
C	-3.74456600	0.86376800	-0.43229900
C	-2.59229300	0.13161700	-0.16001100
C	-1.32545900	0.75516000	-0.27716100
C	-1.20336400	2.11519700	-0.63418900
C	-2.46806300	-1.30346300	0.31977400
C	-3.28500200	-2.28775000	-0.53790100
C	-2.93915700	-1.37725200	1.79228000
C	-0.30432600	-0.20977200	-0.01215500
C	-0.92107400	-1.57023200	0.17836600
H	-2.30247000	3.87858800	-1.17589100
H	-4.51362400	2.78527300	-1.01120400
H	-4.72871100	0.41050100	-0.35466800
H	-0.22223800	2.57267700	-0.69407300
H	-0.75386800	-2.04241600	-0.80754700
H	-3.01510800	-2.21633000	-1.59721800
H	-3.10725200	-3.31821600	-0.20970200
H	-4.35990300	-2.09399700	-0.44698200
H	-2.36461200	-0.70233700	2.43501400
H	-3.99453900	-1.09268300	1.86481900
H	-2.83800600	-2.39499500	2.18219700
Pt	1.53420400	0.11161700	-0.02304700
Cl	1.63185800	1.81622800	1.57299600
Cl	2.07044700	-1.48403200	-1.65305100
C	-0.25931500	-2.48484000	1.21832700
H	-0.24609500	-2.02931200	2.21239700
H	-0.79930400	-3.43592900	1.27860300
H	0.77103100	-2.69800800	0.92475000

4-c-TS2

C	-2.52688000	-2.72346300	-1.04020000
C	-3.76019900	-2.11543100	-0.77802400
C	-3.82672600	-0.79507500	-0.31996400
C	-2.63756500	-0.09734100	-0.12939000
C	-1.40626400	-0.70938600	-0.40230500
C	-1.33217100	-2.02257900	-0.85745400
C	-2.42811200	1.32359800	0.37607600
C	-3.14266500	2.38655900	-0.48769500
C	-2.86427700	1.45688700	1.86630000
C	-0.31198200	0.27806500	-0.15112600
C	-0.91577500	1.46422200	0.35719600
H	-2.49799900	-3.75183400	-1.38810600
H	-4.67821300	-2.67691900	-0.92738900
H	-4.79066100	-0.33597500	-0.11429500
H	-0.36886800	-2.48403200	-1.04719300
H	-0.27000100	1.02401500	-1.08225100
H	-2.83154800	2.32202900	-1.53530400
H	-2.94356000	3.39986800	-0.12397500
H	-4.22396100	2.22143000	-0.44600000
H	-2.34736900	0.73111900	2.50127900
H	-3.93938300	1.26237900	1.93310500
H	-2.67123500	2.46575700	2.24498900
Pt	1.58872400	-0.17813800	0.01309100
Cl	1.40478400	-1.67468900	1.79155600
Cl	2.09915400	1.32914600	-1.74889900
C	-0.18079900	2.67191000	0.80164300
H	-0.77437100	3.58573600	0.71261400
H	0.76430300	2.76592300	0.25636800
H	0.08593300	2.53168200	1.85954100

4-c-IN3

C	-3.29520200	-1.86044300	-1.37511700
C	-3.96764000	-1.21906500	-0.32662200
C	-3.40749400	-0.11136100	0.32288900
C	-2.15914900	0.34177800	-0.08278300
C	-1.47579600	-0.31941300	-1.12178400
C	-2.03761100	-1.41615700	-1.78149500
C	-1.37812200	1.56469400	0.38583800
C	-2.07757600	2.82042700	-0.22647200
C	-1.29738400	1.75935800	1.90900100
C	-0.16616500	0.30856900	-1.30782700
C	-0.02427600	1.39210500	-0.34962100
H	-3.75254300	-2.71453300	-1.86573700
H	-4.94249100	-1.58389700	-0.01499600
H	-3.94882700	0.37836100	1.12779500
H	-1.49747900	-1.92198900	-2.57691800
H	0.38110200	0.26908500	-2.24559300
H	-2.09748300	2.78598900	-1.32109600
H	-1.58434500	3.74445000	0.09079300
H	-3.11320700	2.85190700	0.12586500
H	-0.89947500	0.87604200	2.40913400
H	-2.29552200	1.96955300	2.30994900
H	-0.66105200	2.61819100	2.15077900
Pt	1.17145700	-0.37746200	0.20535500
Cl	0.13120900	-1.42439500	2.02344900
Cl	2.93626700	0.03644500	-1.30394700
C	0.88338900	2.58362000	-0.51117800
H	0.34348500	3.38274200	-1.03560200
H	1.78045600	2.33852600	-1.07718700
H	1.18477400	2.97811000	0.46464300

4P-Me

C	-3.09825200	0.51350400	0.00000800
C	-2.82959000	-0.85854600	-0.00000500
C	-1.50668900	-1.32504000	-0.00000700
C	-0.46787400	-0.40389500	0.00000500
C	-0.73900000	0.98047500	-0.00000500
C	-2.05509100	1.44592700	0.00001100
C	1.04016200	-0.62645600	-0.00004600
C	1.56704900	0.81524800	-0.00013200
C	0.54016400	1.69106900	-0.00007600
C	1.49469500	-1.38829300	1.26583200
C	1.49470600	-1.38857100	-1.26565300
H	-4.12877400	0.85952000	0.00001000
H	-3.65170900	-1.56938400	-0.00001600
H	-1.30811900	-2.39477400	-0.00002000
H	-2.26897700	2.51206600	0.00000100
H	0.63744500	2.77320100	-0.00009500
H	2.58577300	-1.49595900	1.28844700
H	1.06030400	-2.39433800	1.28721800
H	1.18120800	-0.86321500	2.17417200
H	1.18126400	-0.86376300	-2.17417400
H	2.58578900	-1.49622200	-1.28827900
H	1.06035600	-2.39464000	-1.28682300
C	3.02697800	1.14844000	-0.00002900
H	3.53961900	0.73605700	-0.88016400
H	3.18292200	2.23204800	-0.00008800
H	3.53934300	0.73622600	0.88039100