Supporting Information

Pronounced Electronic Modulation of Geometrically Regulated Metalloenediyne Cyclization

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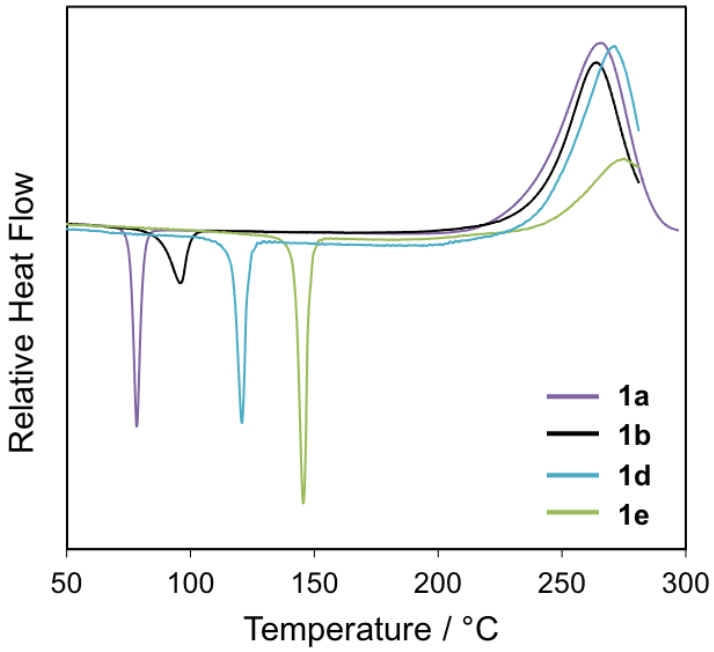

Figure 1S. Differential scanning calorimetry traces of enediyne ligands **1a**–**1b** and **1d**–**1e** showing endothermic melting and subsequent exothermic Bergman cyclization.

Table 1S. Selected crystallographically determined bond lengths (Å) and angles (°) for phosphine enediyne ligands **1d**–**1e** and phosphine oxide derivatives **2d**–**2e**.

	1d	**1e**	**2d**	**2e**
P1–C1	1.77	1.76	1.76	1.74
P2–C10	1.77	1.76	1.757	1.75
P1–O1	---	---	1.48	1.47
P2–O2	---	---	1.48	1.47
interalkynyl	4.09	4.20	4.21	3.94
C3–C2≡C1	179.26	177.12	177.18	178.10
C8–C9≡C10	174.85	177.12	177.97	176.35
C2≡C1–P1	170.18	172.72	179.24	169.36
C9≡C10–P2	175.88	172.72	173.99	169.26

Table 2S. Selected crystallographically determined bond lengths (Å) and angles (°) for the Pt(II) phosphine enediyne-bridged dimer **5d**.

	5d
Pt1–P1	2.23
Pt1–P2	2.24
Pt1–Cl1	2.35
Pt1–Cl2	2.34
interalkynyl	4.53
P1–Pt–P2	92.71
P1–Pt–Cl1	88.84
P1–Pt–Cl2	173.48
P2–Pt–Cl1	174.23
P2–Pt–Cl2	174.23
Cl1–Pt–Cl1	90.14
$C–C{\equiv}C_{avg}$	168.64
$C{\equiv}C–P_{avg}$	163.34

Table 3S. Selected crystallographically determined bond lengths (Å) and angles (°) for Pt(II) phosphine enediyne dichloride complexes **3e** and **3f**.

	3e	**3f**
Pt1–P1	2.24	2.25
Pt1–P2	2.24	2.26
Pt1–Cl1	2.33	2.35
Pt1–Cl2	2.33	2.36
interalkynyl	3.13	3.10
P1–Pt–P2	105.24	104.36
P1–Pt–Cl1	83.36	84.94
P1–Pt–Cl2	172.55	172.33
P2–Pt–Cl1	171.11	170.52
P2–Pt–Cl2	81.80	83.26
Cl1–Pt–Cl1	89.52	87.48
C2≡C1–P1	173.73	173.41
C9≡C10–P2	174.34	174.29

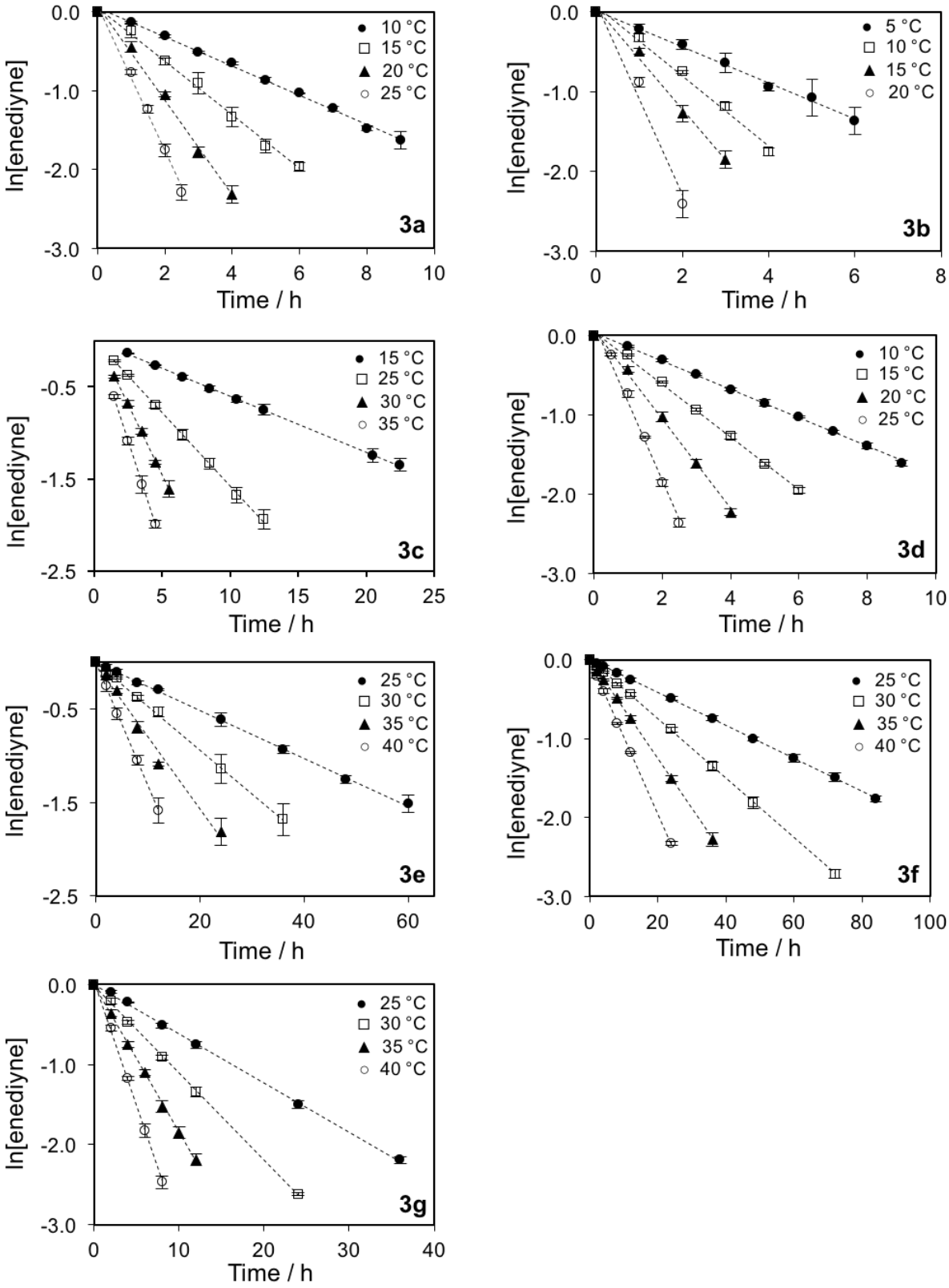

Figure 2S. Summary of temperature-dependent Bergman cyclization kinetics (via ^{31}P NMR) for complexes **3a**–**3g**.

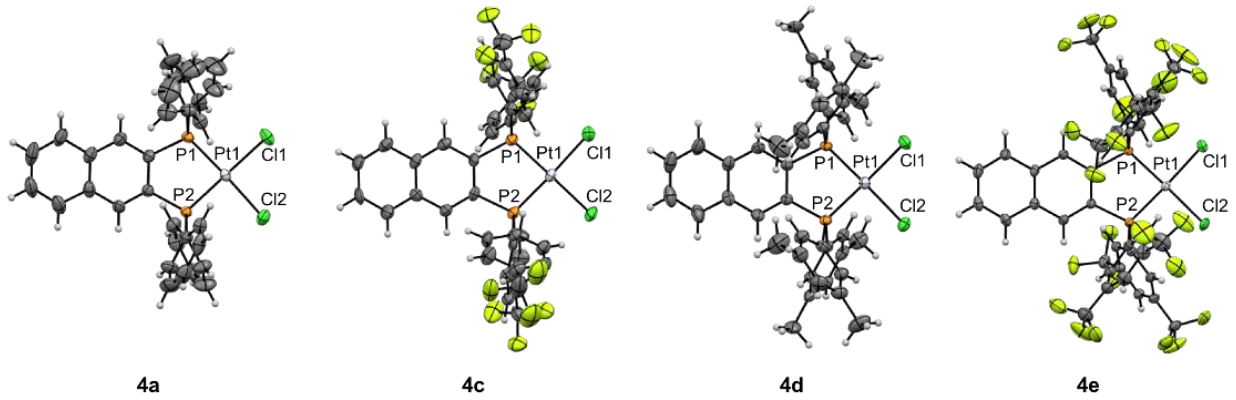

Figure 3S. X-ray crystallographic structures of cyclized Pt(II) phosphine dichloride complexes **4a** and **4c**–**4e**, isolated from cyclization reactions of the corresponding metalloenediyne. Thermal ellipsoids for all complexes are illustrated at 50% probability.

Table 4S. Selected crystallographically determined bond lengths (Å) and angles (°) for Bergman cyclized Pt(II) phosphine enediyne products **4a** and **4c**–**4f**.

	4a	4c	4d	4e	4f
Pt1–P1	2.22	2.26	2.21	2.20	2.22
Pt1–P2	2.22	2.26	2.21	2.21	2.22
Pt1–Cl1	2.35	2.41	2.35	2.33	2.35
Pt1–Cl2	2.36	2.41	2.35	2.34	2.35
P1–Pt–P2	88.60	87.88	88.48	88.07	88.44
P1–Pt–Cl1	91.93	89.51	89.97	89.55	92.14
P1–Pt–Cl2	177.35	171.95	178.18	172.64	175.78
P2–Pt–Cl1	176.94	174.17	178.18	175.72	177.34
P2–Pt–Cl2	88.76	91.78	89.97	90.11	90.40
Cl1–Pt–Cl1	90.72	91.44	91.62	92.68	88.84

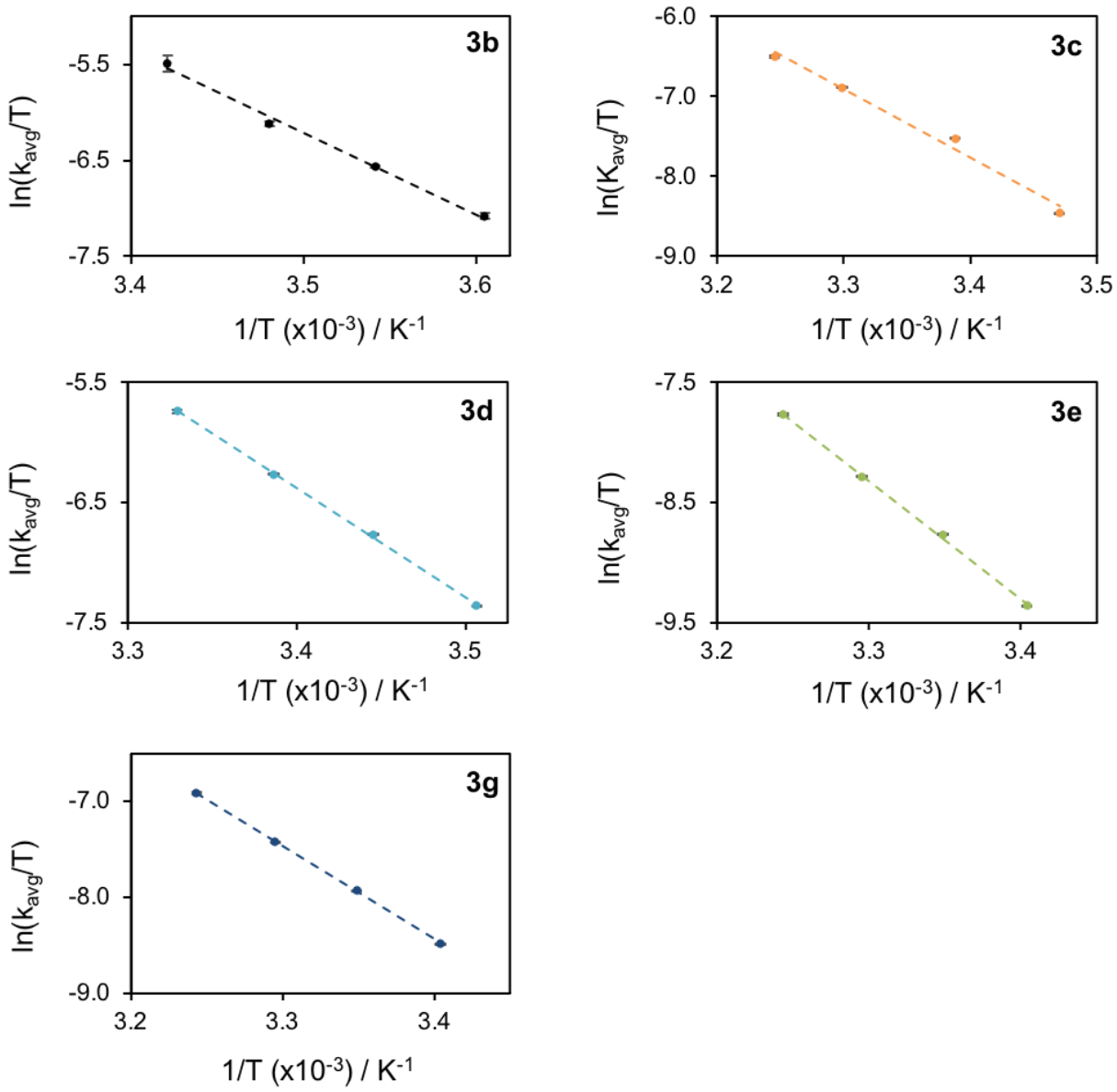

Figure 4S. Eyring plots for complexes **3b** – **3e** and **3g** used to derive activation parameters $\Delta H^{\ddagger}$, $T\Delta S^{\ddagger}$, and $\Delta G^{\ddagger}$.

Data collection, structure solution, and refinement. Data collections were performed at IUMSC using a Bruker APEX II Kappa Duo diffractometer equipped with an APEX II detector using Mo Kα radiation (graphite monochromator). Final cell constraints were calculated from the xyz centroids of strong reflections in the actual data after integration (SAINT).[1] The intensity data were corrected for absorption (SADABS).[2] Space groups were determined based on intensity statistics and systematic absences. Structures were solved and refined using Superflip[3] and the Oxford University Crystals for Windows system[4] or the SHELX suite of programs.[5] Full-matrix least squares / difference Fourier cycles were performed, which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were placed in ideal positions and refined as riding atoms.

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[1] SAINT, Bruker Analytical X-Ray Systems, Madison, WI, current version.
[2] SADABS, Bruker Analytical X-Ray Systems, Madison, WI, current version.
[3] Palatinus L., Chapuis G. (2007): Superflip - a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions. J. Appl. Cryst. 40, 786-790.
[4] Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. J. Appl. Cryst. 2003, 36, 1487.
[5] A short history of *SHELX*, G. M. Sheldrick, *Acta Cryst*. A64, 112 - 122 (2008).

Table 5S. Crystal data and structure refinement for **1d**.

Empirical formula	C42 H40 P2	
Formula weight	606.73	
Crystal color, shape, size	colorless plate, 0.350 x 0.300 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 9.1022(6) Å	α= 91.7747(18)°.
	b = 9.6658(7) Å	β= 92.4701(18)°.
	c = 20.7479(13) Å	γ = 102.405(2)°.
Volume	1779.6(2) $Å^3$	
Z	2	
Density (calculated)	1.132 Mg/m^3	
Absorption coefficient	0.149 mm^{-1}	
F(000)	644	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.967 to 32.238°.
Index ranges	-13<=h<=13, -14<=k<=14, 0<=l<=30
Reflections collected	11401
Independent reflections	11401 [R(int) = 0.000]
Observed Reflections	8541
Completeness to theta = 25.146°	97.9 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.99 and 0.96
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.111, B = 0.628
Data / restraints / parameters	11374 / 0 / 397
Goodness-of-fit on F^2	1.0066
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1728
R indices (all data)	R1 = 0.0788, wR2 = 0.1878
Largest diff. peak and hole	0.48 and -0.43 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 6S. Crystal data and structure refinement for **1e**.

Empirical formula	C42 H16 F24 P2	
Formula weight	1038.49	
Crystal color, shape, size	colorless rod, 0.300 x 0.100 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 18.2822(14) Å	α= 90°.
	b = 17.4936(12) Å	β= 124.678(3)°.
	c = 15.4479(18) Å	γ = 90°.
Volume	4063.0(7) $Å^3$	
Z	4	
Density (calculated)	1.698 Mg/m^3	
Absorption coefficient	0.251 mm^{-1}	
F(000)	2056	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.786 to 30.189°.
Index ranges	-25<=h<=25, -24<=k<=24, -21<=l<=21
Reflections collected	22482
Independent reflections	5994 [R(int) = 0.037]
Observed Reflections	4958
Completeness to theta = 29.585°	99.9 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.98 and 0.98
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.086, B = 8.675
Data / restraints / parameters	5976 / 60 / 320
Goodness-of-fit on F^2	0.9940
Final R indices [I>2sigma(I)]	R1 = 0.0634, wR2 = 0.1648
R indices (all data)	R1 = 0.0754, wR2 = 0.1765
Largest diff. peak and hole	0.95 and -0.78 $e.Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 7S. Crystal data and structure refinement for **2d**.

Empirical formula	C43 H42 Cl2 O2 P2	
Formula weight	723.60	
Crystal color, shape, size	colorless block, 0.32 × 0.31 × 0.31 mm^3	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 8.7241(4) Å	α= 90°.
	b = 18.1674(9) Å	β= 90.885(2)°.
	c = 24.8336(12) Å	γ = 90°.
Volume	3935.5(3) $Å^3$	
Z	4	
Density (calculated)	1.221 Mg/m^3	
Absorption coefficient	0.281 mm^{-1}	
F(000)	1520	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.389 to 30.146°.
Index ranges	-11<=h<=12, -25<=k<=25, -35<=l<=26
Reflections collected	36046
Independent reflections	11598 [R_{int} = 0.0273]
Observed Reflections	9575
Completeness to theta = 25.242°	99.9 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7460 and 0.6394
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.0604, B = 2.4590
Data / restraints / parameters	11598 / 25 / 475
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1220
R indices (all data)	R1 = 0.0592, wR2 = 0.1316
Largest diff. peak and hole	0.733 and -0.585 $e.Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 8S. Crystal data and structure refinement for **2e**.

Empirical formula	C47 H28 F24 O2 P2	
Formula weight	1142.63	
Crystal color, shape, size	colourless block, 0.31 × 0.28 × 0.23 mm^3	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 10.2044(5) Å	α= 90°.
	b = 19.1296(8) Å	β= 90.207(3)°.
	c = 24.2065(12) Å	γ = 90°.
Volume	4725.2(4) $Å^3$	
Z	4	
Density (calculated)	1.606 Mg/m^3	
Absorption coefficient	0.227 mm^{-1}	
F(000)	2288	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.357 to 27.534°.
Index ranges	-11<=h<=13, -22<=k<=24, -31<=l<=31
Reflections collected	44739
Independent reflections	10870 [R(int) = 0.0307]
Observed Reflections	8547
Completeness to theta = 25.242°	100.0 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6601
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.0927, B = 5.9186
Data / restraints / parameters	10870 / 337 / 746
Goodness-of-fit on F^2	1.018
Final R indices [I>2σ(I)]	R1 = 0.0630, wR2 = 0.1679
R indices (all data)	R1 = 0.0802, wR2 = 0.1821
Largest diff. peak and hole	0.872 and -0.599 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

R1 = $\Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. *w*R2 = $[\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 9S. Crystal data and structure refinement for **3e**.

Empirical formula	C42 H16 Cl2 F24 P2 Pt1	
Formula weight	1304.48	
Crystal color, shape, size	colorless plate, 0.300 x 0.300 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions	a = 12.3782(10) Å	α= 90°.
	b = 21.2832(16) Å	β= 90.947(4)°.
	c = 17.4143(15) Å	γ = 90°.
Volume	4587.1(6) $Å^3$	
Z	4	
Density (calculated)	1.889 Mg/m^3	
Absorption coefficient	3.375 mm^{-1}	
F(000)	2504	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.511 to 30.132°.
Index ranges	-17<=h<=17, -30<=k<=30, -24<=l<=23
Reflections collected	97743
Independent reflections	13502 [R(int) = 0.040]
Observed Reflections	12096
Completeness to theta = 30.132°	99.7 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.71 and 0.71
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.026, B = 11.510
Data / restraints / parameters	13460 / 177 / 705
Goodness-of-fit on F^2	1.0357
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0694
R indices (all data)	R1 = 0.0339, wR2 = 0.0723
Largest diff. peak and hole	1.11 and -0.85 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 10S. Crystal data and structure refinement for **3f**.

Empirical formula	C22 H32 Cl2 P2 Pt1	
Formula weight	624.44	
Crystal color, shape, size	colorless plate, 0.350 x 0.250 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P 1 21/c 1	
Unit cell dimensions	a = 19.6329(7) Å	α= 90°.
	b = 14.5514(5) Å	β= 113.8290(10)°.
	c = 18.4286(7) Å	γ = 90°.
Volume	4816.0(3) $Å^3$	
Z	8	
Density (calculated)	1.722 Mg/m^3	
Absorption coefficient	6.188 mm^{-1}	
F(000)	2448	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.897 to 30.175°.
Index ranges	-26<=h<=27, -20<=k<=20, -25<=l<=26
Reflections collected	56005
Independent reflections	14194 [R(int) = 0.036]
Observed Reflections	10189
Completeness to theta = 29.572°	99.9 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.54 and 0.21
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.009, B = 10.530
Data / restraints / parameters	14139 / 0 / 487
Goodness-of-fit on F^2	1.0081
Final R indices [I>2sigma(I)]	R1 = 0.0236, wR2 = 0.0501
R indices (all data)	R1 = 0.0417, wR2 = 0.0615
Largest diff. peak and hole	1.55 and -1.96 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 11S. Crystal data and structure refinement for **4a**.

Empirical formula	C35 H28 Cl4 P2 Pt	
Formula weight	847.40	
Crystal color, shape, size	colorless needle, 0.35 × 0.17 × 0.15 mm^3	
Temperature	253(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions	a = 8.9321(4) Å	α= 90°.
	b = 25.8402(11) Å	β= 95.622(2)°.
	c = 16.2519(7) Å	γ = 90°.
Volume	3733.0(3) $Å^3$	
Z	4	
Density (calculated)	1.508 Mg/m^3	
Absorption coefficient	4.152 mm^{-1}	
F(000)	1656	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.485 to 27.535°.
Index ranges	-11<=h<=7, -33<=k<=33, -14<=l<=21
Reflections collected	36500
Independent reflections	8547 [R_{int} = 0.0399]
Observed Reflections	7052
Completeness to theta = 25.242°	99.8 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.4735
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.0588, B = 18.5772
Data / restraints / parameters	8547 / 205 / 410
Goodness-of-fit on F^2	1.118
Final R indices [I>2σ(I)]	R1 = 0.0443, wR2 = 0.1265
R indices (all data)	R1 = 0.0563, wR2 = 0.1315
Largest diff. peak and hole	1.638 and -1.953 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 12S. Crystal data and structure refinement for **4c**.

Empirical formula	C39 H24 Cl4 F12 P2 Pt1	
Formula weight	1119.44	
Crystal color, shape, size	colorless plate, 0.300 x 0.300 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions	a = 10.297(3) Å	α= 90°.
	b = 21.652(5) Å	β= 104.527(10)°.
	c = 19.471(5) Å	γ = 90°.
Volume	4202.2(18) $Å^3$	
Z	4	
Density (calculated)	1.769 Mg/m^3	
Absorption coefficient	3.752 mm^{-1}	
F(000)	2168	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.432 to 24.682°.
Index ranges	-11<=h<=12, -18<=k<=25, -22<=l<=21
Reflections collected	21368
Independent reflections	6984 [R(int) = 0.085]
Observed Reflections	4816
Completeness to theta = 23.942°	99.6 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.69 and 0.32
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.091, B = 29.530
Data / restraints / parameters	6947 / 79 / 551
Goodness-of-fit on F^2	1.0016
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1374
R indices (all data)	R1 = 0.0952, wR2 = 0.1642
Largest diff. peak and hole	2.63 and -3.48 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 13S. Crystal data and structure refinement for **4d**.

Empirical formula	C42 H42 Cl2 P2 Pt	
Formula weight	874.68	
Crystal color, shape, size	colorless needle, 0.31 × 0.08 × 0.07 mm^3	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Orthorhombic, Pnma	
Unit cell dimensions	a = 16.5978(13) Å	α= 90°.
	b = 19.5096(13) Å	β= 90°.
	c = 18.9329(14) Å	γ = 90°.
Volume	6130.8(8) $Å^3$	
Z	4	
Density (calculated)	0.948 Mg/m^3	
Absorption coefficient	2.446 mm^{-1}	
F(000)	1744	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.499 to 30.145°.
Index ranges	-23<=h<=21, -27<=k<=16, -26<=l<=16
Reflections collected	58454
Independent reflections	9289 [R(int) = 0.0581]
Observed Reflections	6832
Completeness to theta = 25.242°	100.0 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7460 and 0.5627
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.0299, B = 3.7323
Data / restraints / parameters	9289 / 0 / 218
Goodness-of-fit on F^2	1.080
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0698
R indices (all data)	R1 = 0.0543, wR2 = 0.0775
Largest diff. peak and hole	1.426 and -0.774 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 14S. Crystal data and structure refinement for **4e**.

Empirical formula	C42 H18 Cl2 F24 P2 Pt	
Formula weight	1306.49	
Crystal color, shape, size	colorless needle, 0.23 × 0.08 × 0.05 mm^3	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 13.4013(13) Å	α = 90°.
	b = 23.743(2) Å	β = 99.623(4)°.
	c = 14.4223(13) Å	γ = 90°.
Volume	4524.4(7) $Å^3$	
Z	4	
Density (calculated)	1.918 Mg/m^3	
Absorption coefficient	3.422 mm^{-1}	
F(000)	2512	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.541 to 30.062°.
Index ranges	-16<=h<=18, -33<=k<=32, -20<=l<=14
Reflections collected	35328
Independent reflections	13121 [R_{int} = 0.0340]
Observed Reflections	10711
Completeness to theta = 25.242°	100.0 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7460 and 0.5481
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.0229, B = 7.8136
Data / restraints / parameters	13121 / 1020 / 690
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0338, wR2 = 0.0691
R indices (all data)	R1 = 0.0480, wR2 = 0.0740
Largest diff. peak and hole	1.272 and -1.421 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 15S. Crystal data and structure refinement for **4f**.

Empirical formula	C22 H34 Cl2 P2 Pt1	
Formula weight	626.45	
Crystal color, shape, size	colorless block, 0.150 x 0.100 x 0.100 mm^3	
Temperature	173 K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P 1 21/n 1	
Unit cell dimensions	a = 7.5197(6) Å	α= 90°.
	b = 17.6155(13) Å	β= 95.268(2)°.
	c = 17.7459(13) Å	γ = 90°.
Volume	2340.8(3) $Å^3$	
Z	4	
Density (calculated)	1.778 Mg/m^3	
Absorption coefficient	6.366 mm^{-1}	
F(000)	1232	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.632 to 28.718°.
Index ranges	-10<=h<=10, 0<=k<=23, 0<=l<=23
Reflections collected	5928
Independent reflections	5928 [R(int) = 0.000]
Observed Reflections	4787
Completeness to theta = 25.272°	99.1 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.53 and 0.53
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + AP^2 + BP]^{-1}$, with
	$P = (Fo^2 + 2\,Fc^2)/3$, A = 0.045, B = 41.870
Data / restraints / parameters	5910 / 0 / 244
Goodness-of-fit on F^2	1.0824
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1268
R indices (all data)	R1 = 0.0688, wR2 = 0.1448
Largest diff. peak and hole	2.67 and -2.13 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 16S. Crystal data and structure refinement for **5d**.

Empirical formula	C92 H96 Cl20 P4 Pt2	
Formula weight	2424.74	
Crystal color, shape, size	colorless plate, 0.21 × 0.19 × 0.05 mm^3	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Orthorhombic, Pbcn	
Unit cell dimensions	a = 22.317(3) Å	α = 90°.
	b = 21.114(2) Å	β = 90°.
	c = 21.952(3) Å	γ = 90°.
Volume	10344(2) $Å^3$	
Z	4	
Density (calculated)	1.557 Mg/m^3	
Absorption coefficient	3.322 mm^{-1}	
F(000)	4816	

Data Collection

Diffractometer	APEX II Kappa Duo, Bruker
Theta range for data collection	1.328 to 30.215°.
Index ranges	-31<=h<=31, -29<=k<=29, -30<=l<=30
Reflections collected	192734
Independent reflections	15230 [R_{int} = 0.0627]
Observed Reflections	11540
Completeness to theta = 25.242°	100.0 %

Solution and Refinement

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7460 and 0.4889
Solution	Intrinsic methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2 Fo^2 + BP]^{-1}$, with $P = (Fo^2 + 2\,Fc^2)/3$, B = 124.6135
Data / restraints / parameters	15230 / 821 / 740
Goodness-of-fit on F^2	1.176
Final R indices [I>2σ(I)]	R1 = 0.0598, wR2 = 0.1282
R indices (all data)	R1 = 0.0856, wR2 = 0.1403
Largest diff. peak and hole	2.476 and -1.738 e.$Å^{-3}$

Goodness-of-fit = $[\Sigma[w(F_o^2 - F_c^2)^2]/N_{observns} - N_{params})]^{1/2}$, all data.

$R1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.

Table 17S. Summary of computational results for **3a**–**3e**.

3a

Imaginary frequencies: n/a
Total Energy = –3032.24383746 a.u.
Zero-point vibrational energy = 288.86275 kcal/mol
Sum of electronic and zero-point Energies = –3031.783505
Sum of electronic and thermal Energies = –3031.745938
Sum of electronic and thermal Enthalpies = –3031.744994
Sum of electronic and thermal Free Energies = –3031.858598

Pt	-0.00000400	-1.33533200	-0.47501000
P	1.83470200	-0.03150300	0.03671400
P	-1.83470100	-0.03149100	0.03671400
C	2.55901100	-0.43388900	1.68790600
C	3.09769300	0.58111400	2.50552800
H	3.07800000	1.62005500	2.16885900
C	3.64603800	0.25892200	3.75507600
H	4.05934200	1.05155100	4.38392900
C	3.65709100	-1.07214100	4.19708700
H	4.08099300	-1.32066000	5.17343500
C	3.11765500	-2.08209300	3.38624500
H	3.12013000	-3.12036600	3.72676400
C	2.56579100	-1.77108000	2.13590600
H	2.14916400	-2.55553000	1.49995100
C	3.19772600	-0.10861200	-1.20740700
C	4.54307000	0.01353000	-0.81616700
H	4.80520000	0.07663800	0.24210300
C	5.55106000	0.03935400	-1.79120800
H	6.59671800	0.12201800	-1.48424700
C	5.21983600	-0.04721700	-3.15102500
H	6.00816300	-0.02978300	-3.90779800
C	3.87618600	-0.16680500	-3.53937700
H	3.61477500	-0.24846700	-4.59715500
C	2.86452000	-0.20266900	-2.57201500
H	1.82006100	-0.33002600	-2.86545600
C	-2.55901500	-0.43387700	1.68790400
C	-3.09769000	0.58112500	2.50553100
H	-3.07798800	1.62006700	2.16886700
C	-3.64603700	0.25893100	3.75507700
H	-4.05933500	1.05156000	4.38393400
C	-3.65710100	-1.07213400	4.19708100
H	-4.08100600	-1.32065600	5.17342700
C	-3.11767300	-2.08208700	3.38623400
H	-3.12015600	-3.12036100	3.72674800
C	-2.56580600	-1.77107200	2.13589600
H	-2.14918500	-2.55552100	1.49993800
C	-3.19772500	-0.10859200	-1.20740800
C	-4.54306800	0.01356100	-0.81616900
H	-4.80519900	0.07667200	0.24210100
C	-5.55105800	0.03938900	-1.79121100
H	-6.59671500	0.12206200	-1.48425100
C	-5.21983300	-0.04718700	-3.15102700
H	-6.00815900	-0.02974800	-3.90780100
C	-3.87618300	-0.16678500	-3.53937800
H	-3.61477100	-0.24845200	-4.59715600
C	-2.86451800	-0.20265500	-2.57201500
H	-1.82006000	-0.33002100	-2.86545500
Cl	-1.66029900	-3.00455200	-0.98516800
Cl	1.66027500	-3.00456400	-0.98517600
C	-0.71999000	4.19645500	0.08608600
C	0.72001800	4.19645000	0.08608600
C	1.41236800	5.42355800	0.07505900
C	0.70276800	6.63071300	0.06557800
C	-0.70272500	6.63071800	0.06557800
C	-1.41233200	5.42356700	0.07506000
H	2.50393800	5.41823500	0.07034600
H	1.24804400	7.57707500	0.05547600
H	-1.24799500	7.57708300	0.05547600
H	-2.50390300	5.41825100	0.07034700
C	-1.34446900	2.91914200	0.09841900
C	1.34448800	2.91913300	0.09841800
C	1.60576900	1.71611700	0.12706300
C	-1.60575700	1.71612800	0.12706500

3a-TS

Imaginary frequencies: –404.46 cm^{-1}
Total Energy = –3032.21620282 a.u.
Zero-point vibrational energy = 288.05573 kcal/mol
Sum of electronic and zero-point Energies = –3031.757157
Sum of electronic and thermal Energies = –3031.720506
Sum of electronic and thermal Enthalpies = –3031.719562
Sum of electronic and thermal Free Energies = –3031.830842

Pt	0.00000000	-1.61500300	-0.37197400
P	1.63647300	-0.09793800	0.02571700
P	-1.63647300	-0.09793800	0.02571700
C	0.98993200	1.59664300	0.00969700
C	1.36880500	2.81856100	-0.04584300
C	0.74652400	4.07479500	-0.09625000
C	1.40854000	5.32198800	-0.14453800
H	2.49938500	5.32281400	-0.14976700
C	0.70318400	6.52520600	-0.18925600
H	1.25071800	7.46951000	-0.22687000
C	-0.70318400	6.52520600	-0.18925600
H	-1.25071700	7.46951000	-0.22687000
C	-1.40853900	5.32198800	-0.14453800
H	-2.49938500	5.32281400	-0.14976700
C	-0.74652400	4.07479500	-0.09625000
C	-1.36880500	2.81856100	-0.04584300
C	-0.98993200	1.59664300	0.00969700
C	2.43297700	-0.25597700	1.68269400
C	3.42249000	0.68717500	3.69654500
H	2.59734500	1.87320700	2.08292800
C	3.67425300	-0.60511500	4.18017000
H	3.70271400	1.56119200	4.28994200
C	3.30345600	-1.72207300	3.41643200
H	4.15333400	-0.74090800	5.15315300
C	4.25477400	0.49185400	-0.88709000
H	3.49278300	-2.73138700	3.78969000
C	2.68015400	-1.55662000	2.17218800
H	2.38946200	-2.42425300	1.57350000
C	2.98539400	-0.01632000	-1.22236000
C	5.24700900	0.58675000	-1.87209200
H	4.47076100	0.80198900	0.13759400
C	4.97591600	0.18001300	-3.18767400
H	6.23496500	0.97261100	-1.60870500
C	3.71174100	-0.32999300	-3.51919200
H	5.75372200	0.25212700	-3.95209700
C	-2.80197400	0.86586000	2.45171600
H	3.50226600	-0.66202900	-4.53872500
C	2.71577000	-0.43476200	-2.53933500
H	1.73977800	-0.86154100	-2.77956700
C	-2.43297700	-0.25597700	1.68269400
C	-3.42249000	0.68717500	3.69654400
H	-2.59734500	1.87320800	2.08292800
C	-3.67425300	-0.60511400	4.18017000
H	-3.70271400	1.56119200	4.28994200
C	-3.30345500	-1.72207200	3.41643300
H	-4.15333400	-0.74090800	5.15315300
C	-2.68015300	-1.55662000	2.17218800
H	-1.73977700	-0.86153800	-2.77956700
C	-4.97591600	0.18001400	-3.18767400
H	-2.38946200	-2.42425300	1.57350100
C	-2.98539400	-0.01632000	-1.22236000
C	-4.25477500	0.49185300	-0.88709000
H	-4.47076200	0.80198700	0.13759400
C	-5.24701000	0.58674900	-1.87209100
H	-6.23496600	0.97260900	-1.60870500
C	-3.71174000	-0.32999100	-3.51919200
H	-5.75372200	0.25212700	-3.95209800
C	2.80197400	0.86586000	2.45171600
H	-3.50226400	-0.66202600	-4.53872600
C	-2.71577000	-0.43476000	-2.53933500
H	-3.49278200	-2.73138700	3.78969000
Cl	-1.69548800	-3.27923900	-0.76968900
Cl	1.69548800	-3.27924000	-0.76968900

3b

Imaginary frequencies: n/a
Total Energy = –3490.29308795 a.u.
Zero-point vibrational energy = 368.47106 kcal/mol
Sum of electronic and zero-point Energies = –3489.705892
Sum of electronic and thermal Energies = –3489.657666
Sum of electronic and thermal Enthalpies = –3489.656722
Sum of electronic and thermal Free Energies = –3489.794680

Pt	0.00000400	-0.40291000	-1.34756800
P	-1.83707300	-0.10090300	0.01902500
P	1.83707200	-0.10090400	0.01903600
C	-2.57477100	1.57743300	-0.13251000
C	-3.10713100	2.24198800	0.98838700
H	-3.07499800	1.76390400	1.97016300
C	-3.67077500	3.52069200	0.87195000
H	-4.07118100	4.00923400	1.76094700
C	-3.70180800	4.15426600	-0.38555800
C	-3.16484900	3.49572500	-1.51295700
H	-3.19292400	4.00413100	-2.47864900
C	-2.60541700	2.22587800	-1.38971200
H	-2.19616000	1.71993000	-2.26722500
C	-3.17374600	-1.33669700	-0.24073800
C	-4.52513600	-0.99610100	-0.07353500
H	-4.80750700	0.03658400	0.14314200
C	-5.53031500	-1.96681500	-0.19718500
H	-6.57324800	-1.67204800	-0.07650600
C	-5.17865400	-3.29981800	-0.48347900
C	-3.81987100	-3.64686700	-0.64972500
H	-3.56964600	-4.68231600	-0.88799200
C	-2.83051900	-2.67410700	-0.53541700
H	-1.78355800	-2.93916600	-0.69939300
C	2.57476900	1.57743100	-0.13250100
C	3.10711000	2.24200100	0.98839500
H	3.07496300	1.76392800	1.97017700
C	3.67075400	3.52070500	0.87195100
H	4.07114400	4.00925900	1.76094900
C	3.70180500	4.15426300	-0.38556400
C	3.16486600	3.49570700	-1.51296400
H	3.19295500	4.00410000	-2.47866100
C	2.60543500	2.22586000	-1.38971200
H	2.19619200	1.71990000	-2.26722400
C	3.17374900	-1.33669400	-0.24072200
C	4.52513700	-0.99609400	-0.07350500
H	4.80750300	0.03659000	0.14318000
C	5.53032000	-1.96680600	-0.19715200
H	6.57325000	-1.67203700	-0.07646200
C	5.17866500	-3.29980800	-0.48345700
C	3.81988500	-3.64685900	-0.64971900
H	3.56966400	-4.68230700	-0.88799500
C	2.83052800	-2.67410200	-0.53541400
H	1.78357000	-2.93916300	-0.69940200
Cl	1.65988800	-0.65435600	-3.07939900
Cl	-1.65986600	-0.65436300	-3.07941300
C	0.72018600	-0.66408100	4.21184400
C	-0.72021400	-0.66407600	4.21184000
C	-1.41178300	-0.85472200	5.42478100
C	-0.70277900	-1.04048700	6.61790900
C	0.70273600	-1.04049200	6.61791200
C	1.41174700	-0.85473300	5.42478800
H	-2.50342900	-0.85946000	5.41856900
H	-1.24827400	-1.18951200	7.55249400
H	1.24822600	-1.18952200	7.55250000
H	2.50339300	-0.85947800	5.41858200
C	1.34568000	-0.46544300	2.95056500
C	-1.34570000	-0.46543700	2.95055700
C	-1.60017000	-0.25988700	1.76314800
C	1.60015700	-0.25989000	1.76315700
O	-4.22038300	5.39751000	-0.61957600
O	-6.06970300	-4.32853800	-0.62568600
O	6.06971800	-4.32852500	-0.62566200
O	4.22038200	5.39750500	-0.61958900
C	4.76948400	6.11158300	0.48910600
H	5.12160000	7.06812800	0.08266400
H	4.00955000	6.30437400	1.26661700
H	5.62136100	5.57267600	0.93992600
C	7.46015100	-4.02671900	-0.50311300
H	7.98676100	-4.97618400	-0.66302800
H	7.78707900	-3.29665600	-1.26412300
H	7.70723500	-3.63912700	0.50117800
C	-7.46013800	-4.02673400	-0.50315100
H	-7.78706000	-3.29667700	-1.26416900
H	-7.98674500	-4.97620100	-0.66306600
H	-7.70723200	-3.63913700	0.50113500
C	-4.76950600	6.11157300	0.48911900
H	-4.00958400	6.30435500	1.26664500
H	-5.12161800	7.06812200	0.08268400
H	-5.62138800	5.57265700	0.93991900

3b-TS

Imaginary frequencies: –404.32 cm^{-1}
Total Energy = –3490.26625318 a.u.
Zero-point vibrational energy = 367.65140 kcal/mol
Sum of electronic and zero-point Energies = –3489.680363
Sum of electronic and thermal Energies = –3489.633027
Sum of electronic and thermal Enthalpies = –3489.632083
Sum of electronic and thermal Free Energies = –3489.767803

Pt	0.00000000	-0.35196500	-1.66739700
P	-1.64055600	-0.09510400	-0.12423500
P	1.64055600	-0.09510400	-0.12423500
C	-2.44103200	1.55846100	-0.13420400
C	-2.84025500	2.21691600	1.04301700
H	-2.65538700	1.75567100	2.01575900
C	-3.46660800	3.47065100	0.99169300
H	-3.75945800	3.95777000	1.92244700
C	-3.69641900	4.08337700	-0.25571100
C	-3.29288100	3.43001000	-1.44034500
H	-3.47392000	3.92203700	-2.39789000
C	-2.66913900	2.18595800	-1.38310100
H	-2.36110600	1.68324700	-2.30398900
C	-2.96677600	-1.35560200	-0.16270100
C	-4.25335900	-1.08260600	0.33209300
H	-4.49564000	-0.08659200	0.70945300
C	-5.24488200	-2.07273900	0.33600400
H	-6.23875600	-1.83106400	0.71400000
C	-4.94624300	-3.35848900	-0.15834500
C	-3.65564900	-3.63640900	-0.65907600
H	-3.45105600	-4.63261100	-1.05536100
C	-2.67963700	-2.64353300	-0.66650100
H	-1.69281100	-2.84872300	-1.08670100
C	2.44103200	1.55846100	-0.13420400
C	2.84025500	2.21691600	1.04301700
H	2.65538800	1.75567000	2.01575900
C	3.46660900	3.47065100	0.99169300
H	3.75945900	3.95776900	1.92244700
C	3.69641900	4.08337700	-0.25571100
C	3.29288100	3.43001000	-1.44034500
H	3.47391900	3.92203700	-2.39789000
C	2.66913900	2.18595800	-1.38310100
H	2.36110500	1.68324800	-2.30398900
C	2.96677600	-1.35560200	-0.16270100
C	4.25335900	-1.08260600	0.33209400
H	4.49563900	-0.08659300	0.70945400
C	5.24488200	-2.07274000	0.33600400
H	6.23875600	-1.83106500	0.71400100
C	4.94624300	-3.35849000	-0.15834600
C	3.65564900	-3.63640900	-0.65907800
H	3.45105600	-4.63261000	-1.05536300
C	2.67963700	-2.64353300	-0.66650200
H	1.69281100	-2.84872300	-1.08670300
Cl	1.69790700	-0.59510800	-3.36236400
Cl	-1.69790700	-0.59510800	-3.36236400
C	0.74595800	-0.54691100	4.02992100
C	-0.74595700	-0.54691000	4.02992100
C	-1.40810600	-0.69280800	5.26966800
C	-0.70323500	-0.83119400	6.46607500
C	0.70323500	-0.83119500	6.46607500
C	1.40810600	-0.69280800	5.26966800
H	-2.49904900	-0.69873600	5.26987800
H	-1.25085800	-0.94296900	7.40457400
H	1.25085800	-0.94297000	7.40457400
H	2.49904900	-0.69873700	5.26987800
C	1.36934900	-0.39945000	2.78128700
C	-1.36934900	-0.39945000	2.78128700
C	-0.99207000	-0.24845600	1.56711700
C	0.99207000	-0.24845600	1.56711700
O	-4.29253200	5.30144200	-0.42754100
O	-5.83111000	-4.39916700	-0.20463800
O	5.83111000	-4.39916700	-0.20463800
O	4.29253300	5.30144200	-0.42754100
C	4.71494000	6.00956900	0.73903100
H	5.15977900	6.94440100	0.37529300
H	3.86479700	6.24553500	1.40292500
H	5.47342000	5.44325100	1.30765000
C	7.16304800	-4.16604200	0.25693500
H	7.69600000	-5.11537800	0.11970000
H	7.66528400	-3.37833000	-0.33121400
H	7.18202600	-3.88990300	1.32595900
C	-7.16304800	-4.16604200	0.25693500
H	-7.66528400	-3.37833000	-0.33121500
H	-7.69600100	-5.11537800	0.11970100
H	-7.18202700	-3.88990200	1.32595900
C	-4.71493800	6.00956900	0.73903100
H	-3.86479500	6.24553500	1.40292500
H	-5.15977700	6.94440200	0.37529300
H	-5.47341800	5.44325300	1.30765000

3c

Imaginary frequencies: n/a
Total Energy = –4380.26441007 a.u.
Zero-point vibrational energy = 299.45343 kcal/mol
Sum of electronic and zero-point Energies = –4379.787201
Sum of electronic and thermal Energies = –4379.734378
Sum of electronic and thermal Enthalpies = –4379.733434
Sum of electronic and thermal Free Energies = –4379.889583

C	0.70267800	-1.52837300	6.64633400
C	1.41316900	-1.26763700	5.46809400
C	0.71983400	-1.00152200	4.27101900
C	-0.71993600	-1.00154700	4.27100600
C	-1.41328200	-1.26768600	5.46806900
C	-0.70280500	-1.52839600	6.64632100
H	1.24760100	-1.73563800	7.56978800
H	2.50463600	-1.27157700	5.46241600
H	-2.50475000	-1.27167300	5.46236900
H	-1.24773600	-1.73568300	7.56976400
C	-1.34298500	-0.72433300	3.02339100
C	1.34289500	-0.72425000	3.02342300
C	1.61334600	-0.44745800	1.85440400
C	-1.61343300	-0.44756800	1.85436600
P	-1.83291800	-0.18476000	0.12602800
P	1.83288300	-0.18478600	0.12605200
C	-2.55371100	1.51685800	0.05349900
C	-3.03902300	2.14367000	1.21899900
C	-2.60831200	2.19741700	-1.18024800
C	-3.57823800	3.43394800	1.15220000
H	-2.98971100	1.62635400	2.17938700
C	-3.15025900	3.48638400	-1.24172700
H	-2.23601800	1.71103800	-2.08491800
C	-3.63475000	4.10688000	-0.07842900
H	-3.95833400	3.91565100	2.05454800
H	-3.19927300	4.00865000	-2.19857500
C	-3.20623100	-1.37714100	-0.20553600
C	-4.54908300	-1.00898300	-0.01132400
C	-2.88369900	-2.69741400	-0.57197900
C	-5.56467700	-1.95831300	-0.18112300
H	-4.80858300	0.01622400	0.25954000
C	-3.89860100	-3.64532400	-0.73190200
H	-1.84273200	-2.97004900	-0.75749600
C	-5.24072200	-3.27673200	-0.53681000
H	-6.60902700	-1.67168100	-0.04786000
H	-3.65192900	-4.66560600	-1.02957200
C	3.20610800	-1.37728800	-0.20542400
C	4.54898500	-1.00922200	-0.01122300
C	2.88347700	-2.69754900	-0.57182000
C	5.56450600	-1.95863900	-0.18096300
H	4.80856100	0.01597900	0.25959100
C	3.89830700	-3.64554600	-0.73168600
H	1.84249100	-2.97011100	-0.75734300
C	5.24045300	-3.27705100	-0.53659000
H	6.60887700	-1.67208000	-0.04770200
H	3.65155900	-4.66582100	-1.02931500
C	2.55381100	1.51676400	0.05336000
C	2.60846700	2.19717700	-1.18046400
C	3.03918100	2.14366400	1.21878700
C	3.15051300	3.48609300	-1.24209200
H	2.23613500	1.71072100	-2.08507900
C	3.57849400	3.43389200	1.15184100
H	2.98983300	1.62646000	2.17923200
C	3.63505400	4.10668300	-0.07886500
H	3.19956600	4.00824700	-2.19899900
H	3.95863200	3.91566700	2.05413500
Pt	-0.00000500	-0.42996800	-1.25123100
Cl	-1.65993300	-0.60779500	-2.98357600
Cl	1.66002000	-0.60790800	-2.98346600
C	-4.15905800	5.52492900	-0.13925200
C	-6.33212500	-4.31664900	-0.65470900
C	6.33177600	-4.31705800	-0.65443000
C	4.15947300	5.52468400	-0.13985000
F	4.73447600	5.79939100	-1.34226800
F	3.15508900	6.42896700	0.04234000
F	5.09064400	5.76028500	0.82709100
F	6.02007300	-5.27886000	-1.56553500
F	6.53836600	-4.94926400	0.53900200
F	7.52109300	-3.76610100	-1.02401500
F	-6.53879200	-4.94888100	0.53869600
F	-7.52139100	-3.76558400	-1.02429900
F	-6.02048200	-5.27844400	-1.56584200
F	-5.09020800	5.76049400	0.82771800
F	-3.15460100	6.42911200	0.04303800
F	-4.73404100	5.79981700	-1.34163800

3c-TS

Imaginary frequencies: –407.20 cm^{-1}
Total Energy = –4380.23551359 a.u.
Zero-point vibrational energy = 298.61669 kcal/mol
Sum of electronic and zero-point Energies = –4379.759638
Sum of electronic and thermal Energies = –4379.707717
Sum of electronic and thermal Enthalpies = –4379.706772
Sum of electronic and thermal Free Energies = –4379.860421

C	0.70310200	-1.33519900	6.47363500
C	1.40903900	-1.11046100	5.29113800
C	0.74722900	-0.87623000	4.06530400
C	-0.74726600	-0.87623400	4.06529600
C	-1.40908800	-1.11047000	5.29112200
C	-0.70316300	-1.33520400	6.47362700
H	1.25043800	-1.51420600	7.40149000
H	2.49978700	-1.11609600	5.29174800
H	-2.49983600	-1.11611200	5.29172000
H	-1.25050900	-1.51421400	7.40147600
C	-1.36814500	-0.63806300	2.83073500
C	1.36812100	-0.63805500	2.83075000
C	0.98714300	-0.40069600	1.63078200
C	-0.98715600	-0.40070000	1.63077100
P	-1.63381300	-0.14563000	-0.04147900
P	1.63381700	-0.14563800	-0.04146400
C	-2.99264900	-1.38485600	-0.13687500
C	-4.25105500	-1.12656800	0.43829800
C	-2.74077700	-2.62263300	-0.75718300
C	-5.24947600	-2.10575600	0.39893700
H	-4.45653100	-0.16444500	0.91176600
C	-3.73951600	-3.60226000	-0.78919000
H	-1.77374100	-2.80426000	-1.22980500
C	-4.99285400	-3.34538800	-0.21051400
C	-2.43587700	1.51669700	0.02996400
C	-2.72778100	2.16074300	-1.19127600
C	-2.75584200	2.14663700	1.24853700
C	-3.34898700	3.41475000	-1.18498800
H	-2.46845500	1.67608400	-2.13672600
C	-3.37399600	3.40304600	1.24767600
H	-2.51494000	1.66276400	2.19697400
C	-3.67219500	4.03784900	0.03164900
C	2.99263100	-1.38488800	-0.13685000
C	4.99279900	-3.34545800	-0.21048900
C	3.73941000	-3.60235800	-0.78904500
C	4.25108500	-1.12657300	0.43820300
C	5.24948900	-2.10578000	0.39884100
H	1.77361200	-2.80436400	-1.22956500
C	2.74069100	-2.62271300	-0.75703700
H	4.45661400	-0.16441700	0.91157900
C	2.43590200	1.51667800	0.02998200
C	2.75589300	2.14659800	1.24855900
C	2.72779400	2.16073700	-1.19125400
C	3.67224200	4.03781800	0.03168100
H	2.51500100	1.66271400	2.19699300
C	3.34901100	3.41473900	-1.18495800
C	3.37405600	3.40300100	1.24770500
H	2.46845000	1.67609300	-2.13670600
Pt	0.00000900	-0.32442200	-1.59898900
Cl	1.69548100	-0.48824500	-3.29674100
Cl	-1.69543400	-0.48824600	-3.29676900
H	-6.22623400	-1.91012200	0.84428700
H	-3.54646500	-4.56350300	-1.26760400
H	-3.61244300	3.89580600	2.19166000
H	-3.56903400	3.91493000	-2.12947600
H	3.61252100	3.89574600	2.19169300
H	3.56905000	3.91493100	-2.12944200
H	3.54630400	-4.56363800	-1.26736200
H	6.22628200	-1.91013300	0.84410600
C	-6.09349800	-4.38002900	-0.29828600
C	-4.39069200	5.36962600	0.03341600
C	4.39075800	5.36958500	0.03347300
C	6.09342700	-4.38011000	-0.29831600
F	-6.93724200	-4.30789300	0.77033800
F	-6.84967800	-4.20402300	-1.41791700
F	-5.59452400	-5.64608300	-0.34365800
F	5.59442500	-5.64615900	-0.34352700
F	6.84946600	-4.20420700	-1.41805800
F	6.93730900	-4.30790500	0.77019500
F	-5.74380000	5.19608500	0.01059300
F	-4.09993600	6.09873000	1.14730200
F	-4.06369200	6.12282100	-1.05095300
F	4.09983700	6.09876000	1.14727100
F	4.06394100	6.12272100	-1.05099200
F	5.74386800	5.19602300	0.01087900

3d

Imaginary frequencies: n/a
Total Energy = –3346.73568746 a.u.
Zero-point vibrational energy = 422.67411 kcal/mol
Sum of electronic and zero-point Energies = –3346.062113
Sum of electronic and thermal Energies = –3346.008703
Sum of electronic and thermal Enthalpies = –3346.007759
Sum of electronic and thermal Free Energies = –3346.163316

C	0.70291100	-2.87917400	6.07221600
C	1.41215300	-2.36635000	4.97939600
C	0.71989900	-1.84423600	3.86833900
C	-0.71983900	-1.84421500	3.86835500
C	-1.41208300	-2.36630900	4.97942800
C	-0.70283200	-2.87915200	6.07223200
H	1.24818400	-3.28137400	6.92902000
H	2.50377500	-2.36421500	4.97427500
H	-2.50370500	-2.36412400	4.97434000
H	-1.24809600	-3.28133000	6.92905100
C	-1.34478300	-1.30120800	2.71256800
C	1.34483300	-1.30132200	2.71250100
C	1.61536300	-0.79102000	1.62528500
C	-1.61532700	-0.79086000	1.62537600
P	-1.85847700	-0.02509400	0.05205700
P	1.85848900	-0.02510100	0.05203800
C	-2.88914200	1.43086300	0.51896000
C	-4.05553600	1.23776400	1.28907900
C	-2.49113400	2.72335800	0.15045600
C	-4.83527200	2.33526100	1.68378000
H	-4.35763500	0.22842100	1.58082300
C	-3.25688000	3.84184900	0.53941400
H	-1.59529900	2.85200400	-0.46110200
C	-4.41811200	3.62691600	1.29848400
H	-5.02113600	4.49012100	1.60017500
C	-2.97558200	-1.24851900	-0.76298400
C	-4.12001700	-0.83254500	-1.45975500
C	-2.63652800	-2.61401600	-0.70625300
C	-4.94233200	-1.77889600	-2.10237300
H	-4.36975800	0.22833400	-1.51461400
C	-3.44017200	-3.57449700	-1.34102000
H	-1.74516200	-2.93362600	-0.15984200
C	-4.58995000	-3.13687000	-2.02804900
H	-5.22755300	-3.87791800	-2.52177800
C	2.97565900	-1.24839700	-0.76310800
C	4.12006100	-0.83230000	-1.45985700
C	2.63667900	-2.61391900	-0.70649700
C	4.94241700	-1.77855100	-2.10257600
H	4.36974300	0.22859800	-1.51462600
C	3.44036200	-3.57429900	-1.34136400
H	1.74533700	-2.93362500	-0.16010400
C	4.59010700	-3.13654700	-2.02837300
H	5.22773900	-3.87751600	-2.52218400
C	2.88907300	1.43086300	0.51909600
C	2.49093700	2.72338700	0.15083100
C	4.05552200	1.23773400	1.28912300
C	3.25661200	3.84187700	0.53993100
H	1.59505600	2.85206100	-0.46065500
C	4.83519000	2.33523000	1.68396000
H	4.35772000	0.22836800	1.58068400
C	4.41790500	3.62691300	1.29889900
H	5.02087600	4.49011900	1.60069900
Pt	-0.00000100	0.48711100	-1.21241400
Cl	-1.67478900	1.16328200	-2.80928900
Cl	1.67476100	1.16350600	-2.80922300
C	-2.82378800	5.23566200	0.13985500
C	-6.09535000	2.14621300	2.50134800
C	-3.07183700	-5.04239300	-1.30820900
C	-6.16098300	-1.32724600	-2.87777700
C	3.07211900	-5.04222000	-1.30867200
C	6.16104200	-1.32676000	-2.87793900
C	6.09533000	2.14615000	2.50142700
C	2.82338500	5.23572100	0.14062400
H	6.73986800	-0.57470800	-2.31945900
H	6.82893800	-2.16954700	-3.10907100
H	5.86653600	-0.86198400	-3.83366500
H	6.27456800	1.08494100	2.72662100
H	6.03706300	2.68834400	3.45942800
H	6.98039800	2.53009900	1.96802100
H	3.95888500	-5.67827100	-1.16151800
H	2.35798600	-5.26214000	-0.50153200
H	1.89448400	5.52756100	0.65829800
H	3.59128800	5.98358800	0.38636700
H	2.62162800	5.29430300	-0.94031900
H	-2.62209300	5.29408300	-0.94110900
H	-3.59173900	5.98350700	0.38551400
H	-1.89488400	5.52766400	0.65743000
H	-3.95859700	-5.67850200	-1.16128200
H	-6.73967400	-0.57493700	-2.31950800
H	-5.86651700	-0.86284100	-3.83369600
H	-6.82899000	-2.17004400	-3.10855500
H	-6.98047700	2.53001300	1.96793300
H	-6.03706900	2.68856000	3.45926200
H	-6.27449600	1.08502600	2.72671700
H	2.60346100	-5.35366300	-2.25756500
H	-2.60290200	-5.35381400	-2.25697300
H	-2.35790000	-5.26225200	-0.50087800

3d-TS

Imaginary frequencies: –404.56 cm^{-1}
Total Energy = –3346.71070242 a.u.
Zero-point vibrational energy = 422.03629 kcal/mol
Sum of electronic and zero-point Energies = –3346.038145
Sum of electronic and thermal Energies = –3345.985703
Sum of electronic and thermal Enthalpies = –3345.984759
Sum of electronic and thermal Free Energies = –3346.138136

C	0.70331400	-1.76615300	6.32868900
C	1.40837800	-1.44668700	5.16756600
C	0.74636300	-1.11331900	3.96466300
C	-0.74622900	-1.11331600	3.96468800
C	-1.40820500	-1.44668300	5.16761300
C	-0.70310300	-1.76615100	6.32871200
H	1.25094600	-2.01948100	7.23918400
H	2.49927700	-1.45222400	5.16693200
H	-2.49910400	-1.45221500	5.16701500
H	-1.25070600	-2.01947700	7.23922600
C	-1.36922800	-0.77640000	2.75354000
C	1.36932400	-0.77640300	2.75349400
C	0.99132200	-0.44218100	1.57688200
C	-0.99126600	-0.44218000	1.57691500
P	-1.63655600	-0.03584000	-0.06969900
P	1.63655600	-0.03583100	-0.06975300
C	-2.98940300	-1.26469300	-0.27406000
C	-4.25774300	-1.04517900	0.29609100
C	-2.71843900	-2.44874800	-0.97659100
C	-5.26566500	-2.01423800	0.16848400
H	-4.46575000	-0.11523000	0.83097900
C	-3.71277600	-3.43700800	-1.11163300
H	-1.73867900	-2.58508500	-1.44100600
C	-4.97077800	-3.20191900	-0.53209500
H	-5.75160100	-3.96287600	-0.63621700
C	-2.42157400	1.61863800	0.15299100
C	-2.64559200	2.39220900	-1.00076600
C	-2.80370500	2.10515800	1.41896200
C	-3.26815600	3.65170300	-0.89937000
H	-2.34213500	2.00398600	-1.97755000
C	-3.41734500	3.36364300	1.54112800
H	-2.61241400	1.50849300	2.31412600
C	-3.64199000	4.11779200	0.37276000
H	-4.11700300	5.10099900	0.45921100
C	2.98939200	-1.26468500	-0.27417500
C	4.97073200	-3.20194100	-0.53226800
C	3.71268600	-3.43704200	-1.11170800
H	5.75153500	-3.96291700	-0.63639700
C	4.25777800	-1.04515400	0.29586700
C	5.26568300	-2.01422800	0.16823000
H	1.73856400	-2.58513200	-1.44094900
C	2.71836500	-2.44877300	-0.97662800
H	4.46583000	-0.11518600	0.83070500
C	2.42157300	1.61865000	0.15292800
C	2.80391500	2.10507100	1.41888200
C	2.64541100	2.39229800	-1.00080100
C	3.64207600	4.11775900	0.37268300
H	2.61277400	1.50833100	2.31402900
C	3.26800100	3.65179100	-0.89941000
C	3.41760100	3.36352500	1.54104000
H	2.34181600	2.00413800	-1.97756800
Pt	-0.00002500	-0.08519100	-1.63977700
H	4.11716000	5.10093100	0.45912400
Cl	1.69287800	-0.09778900	-3.35678100
Cl	-1.69296000	-0.09782600	-3.35674900
C	-3.42489800	-4.70638400	-1.88321800
C	-6.64663600	-1.78221600	0.74356500
C	-3.80273600	3.91178300	2.89880800
C	-3.53646200	4.46860800	-2.14469000
C	6.64669600	-1.78219300	0.74320100
C	3.42478400	-4.70640100	-1.88331100
C	3.53588400	4.46885700	-2.14471500
C	3.80324200	3.91156000	2.89869000
H	3.10989100	4.70798200	3.21797000
H	4.81325400	4.35055300	2.88417800
H	3.78407800	3.12878800	3.67092700
H	7.01857800	-2.67424600	1.27155000
H	7.37457400	-1.55112300	-0.05275300
H	6.65359300	-0.94024600	1.45063500
H	4.28897000	-5.38639900	-1.87945500
H	3.17535600	-4.48016900	-2.93248400
H	2.67392600	4.44939400	-2.82841000
H	3.75970300	5.51767600	-1.90036900
H	4.39663200	4.06474200	-2.70338900
H	2.56525600	-5.24898000	-1.45755500
H	-3.17418600	-4.48010100	-2.93206800
H	-2.56619500	-5.24963700	-1.45664000
H	-4.28953400	-5.38581400	-1.88041600
H	-2.67587200	4.44671500	-2.83001100
H	-4.39924500	4.06614500	-2.70143200
H	-3.75744500	5.51809100	-1.90059000
H	-6.65349600	-0.94023400	1.45095700
H	-7.37459200	-1.55121400	-0.05233600
H	-7.01844100	-2.67425400	1.27199500
H	-4.81272200	4.35084100	2.88443000
H	-3.78350600	3.12904900	3.67108200
H	-3.10928400	4.70817500	3.21794200

3e

Imaginary frequencies: n/a
Total Energy = –5728.27595526 a.u.
Zero-point vibrational energy = 309.52110 kcal/mol
Sum of electronic and zero-point Energies = –5727.782702
Sum of electronic and thermal Energies = –5727.714237
Sum of electronic and thermal Enthalpies = –5727.713292
Sum of electronic and thermal Free Energies = –5727.911206

C	-0.68412600	1.21539800	6.75737200
C	-1.39859400	1.01053000	5.57067700
C	-0.70705300	0.80136300	4.36138500
C	0.73191100	0.80082100	4.35770200
C	1.42979700	1.00959600	5.56340300
C	0.72156000	1.21498500	6.75374100
H	-1.22623200	1.37702900	7.69142700
H	-2.48997600	1.01058200	5.56897000
H	2.52115700	1.00890300	5.55597300
H	1.26855500	1.37633400	7.68499400
C	1.35002400	0.58229100	3.09630900
C	-1.33190700	0.58424000	3.10301200
C	-1.62659800	0.38333900	1.92468200
C	1.63729100	0.37966400	1.91645800
P	1.85640500	0.05085100	0.20140700
P	-1.85637800	0.06117800	0.20983100
C	2.90601000	-1.46834000	0.25206000
C	4.08770900	-1.47009500	1.01635000
C	2.49480500	-2.63435300	-0.41316800
C	4.86008100	-2.63694100	1.10048300
H	4.40592400	-0.57482700	1.55321000
C	3.26960900	-3.80051700	-0.31248700
H	1.58885800	-2.62224100	-1.02067500
C	4.45244500	-3.80516800	0.43858300
H	5.05218100	-4.71289100	0.50944600
C	2.97287700	1.44134200	-0.28990200
C	4.07328100	1.23323800	-1.13887300
C	2.66847700	2.73643200	0.16214100
C	4.86727100	2.32413300	-1.52350400
H	4.30212900	0.23800700	-1.51826400
C	3.46372700	3.82081600	-0.23587100
H	1.81190600	2.90948800	0.81563200
C	4.56589700	3.61869200	-1.07791500
H	5.17535100	4.46444900	-1.39673200
C	-2.96991800	1.45718400	-0.27289900
C	-4.05746200	1.25702800	-1.14038300
C	-2.68294600	2.74541500	0.20906900
C	-4.85623900	2.34853600	-1.51318600
H	-4.28223400	0.26481100	-1.52957500
C	-3.48530600	3.83002100	-0.17397500
H	-1.83941400	2.91192800	0.88092200
C	-4.57420400	3.63577300	-1.03494300
H	-5.19830800	4.47960400	-1.32958400
C	-2.91568300	-1.45149700	0.25804400
C	-2.52408800	-2.61121000	-0.42920700
C	-4.08712400	-1.45395300	1.03805800
C	-3.30949100	-3.77109200	-0.33758200
H	-1.62026700	-2.60151300	-1.03967000
C	-4.86667800	-2.61605600	1.11868700
H	-4.39767100	-0.55930500	1.58037900
C	-4.48020400	-3.77736300	0.43200000
H	-5.08725100	-4.68065400	0.49778300
Pt	-0.00326800	-0.12691700	-1.13907500
Cl	1.67111900	-0.38633900	-2.84088700
Cl	-1.67780700	-0.37260700	-2.84295800
C	2.78733600	-5.07949600	-0.96804200
C	6.16823000	-2.62258400	1.86347100
C	3.16496900	5.20469100	0.30037600
C	6.09471900	2.09559200	-2.38212300
C	-3.21537000	5.20196100	0.40610400
C	-5.99644000	2.14595700	-2.49064400
C	-6.09272400	-2.64254400	2.00702000
C	-2.91835000	-5.00352100	-1.12905300
F	-5.78360000	-3.09981000	3.25410200
F	-7.05671000	-3.46004100	1.50618000
F	-6.63268300	-1.40172600	2.15583600
F	-3.37151800	-6.14139200	-0.53244900
F	-1.56895500	-5.10756100	-1.25302800
F	-3.44346600	-4.96619100	-2.38284400
F	1.96769800	-5.77289600	-0.12678300
F	2.08770500	-4.82914800	-2.10263400
F	3.82624800	-5.89972800	-1.28551000
F	6.15383200	-1.69919800	2.86524700
F	7.21167600	-2.31441200	1.04509900
F	6.43524400	-3.83486900	2.42036900
F	1.83527700	5.37573900	0.53571800
F	3.56539600	6.17617600	-0.56177700
F	3.81233900	5.42091700	1.48223200
F	6.35188500	3.16646500	-3.18075600
F	7.19892600	1.89916900	-1.60418300
F	5.96035000	1.00235500	-3.17596600
F	-7.00888800	3.02887200	-2.26180800
F	-6.51380800	0.89051000	-2.40238900
F	-5.58348100	2.32835300	-3.77291400
F	-3.88519400	5.37602500	1.58246400
F	-3.61509800	6.19205300	-0.43502500
F	-1.89224400	5.38429800	0.66857700

3e-TS

Imaginary frequencies: –406.58 cm^{-1}
Total Energy = –5728.24809466 a.u.
Zero-point vibrational energy = 308.79840 kcal/mol
Sum of electronic and zero-point Energies = –5727.755993
Sum of electronic and thermal Energies = –5727.688539
Sum of electronic and thermal Enthalpies = –5727.687595
Sum of electronic and thermal Free Energies = –5727.882567

C	-0.67951700	0.32150000	6.61503300
C	-1.39049900	0.29555000	5.41467500
C	-0.73296200	0.25754000	4.16527300
C	0.76234800	0.24651700	4.16016900
C	1.42893700	0.27514600	5.40502900
C	0.72664300	0.31143100	6.61022300
H	-1.22331800	0.35074300	7.56145100
H	-2.48110400	0.30588600	5.42008500
H	2.51959100	0.26998200	5.40298600
H	1.27729500	0.33295100	7.55287500
C	1.37708700	0.20360600	2.90112200
C	-1.35678100	0.22413100	2.91041200
C	-0.98060000	0.17578000	1.68637600
C	0.99195800	0.16079600	1.67966400
P	1.63384700	0.15327100	-0.01019400
P	-1.63351800	0.17665400	0.00074400
C	2.97459600	1.41630500	0.05720500
C	4.22591300	1.11732500	0.62062900
C	2.70674500	2.70687400	-0.43052100
C	5.20595400	2.11752400	0.70211900
H	4.45156600	0.11420300	0.98510700
C	3.69230800	3.70005300	-0.33955300
H	1.74297400	2.92699300	-0.89171800
C	4.94211600	3.40981800	0.22559200
H	5.70720700	4.18392200	0.28967900
C	2.46432300	-1.49121800	-0.16976700
C	2.70701500	-1.98718900	-1.46591800
C	2.84532500	-2.24380800	0.95522700
C	3.34188200	-3.22858700	-1.62231700
H	2.40181000	-1.40444700	-2.33989900
C	3.47742600	-3.48457800	0.78279800
H	2.65095200	-1.87218800	1.96250700
C	3.72806500	-3.98057000	-0.50401800
H	4.21496100	-4.94692200	-0.63521700
C	-2.95266100	1.46174800	0.07466500
C	-4.88521500	3.48829100	0.25237600
C	-3.62035500	3.76669200	-0.28484800
H	-5.63712500	4.27502700	0.31870300
C	-4.21737800	1.17582900	0.61418200
C	-5.18098900	2.19189100	0.69759800
H	-1.68280100	2.96458300	-0.83636400
C	-2.65336900	2.75639700	-0.38357500
H	-4.46234100	0.17381000	0.96883000
C	-2.48923400	-1.45544100	-0.15174600
C	-2.88509900	-2.19483500	0.97698100
C	-2.73555600	-1.95611700	-1.44534900
C	-3.78946900	-3.92756600	-0.47380900
H	-2.68814000	-1.81970400	1.98246200
C	-3.38850000	-3.18890600	-1.59571700
C	-3.53547900	-3.42690500	0.81062100
H	-2.41980800	-1.38327800	-2.32205500
Pt	-0.00245600	0.52968700	-1.52538100
H	-4.29041700	-4.88736100	-0.60027800
Cl	-1.70659500	0.92119600	-3.17013700
Cl	1.69081200	0.90052000	-3.18621000
C	3.42925600	5.07672700	-0.91715500
C	6.53110800	1.81628400	1.37000500
C	3.82334100	-4.32011000	1.99749900
C	3.65245600	-3.73215400	-3.01950700
C	-6.56808600	1.87093300	1.21400700
C	-3.27832900	5.18167100	-0.70706400
C	-3.70194300	-3.69703200	-2.99063000
C	-3.89790000	-4.24956300	2.02932700
F	-2.70468600	-3.40420500	-3.86212400
F	-4.84413500	-3.13023700	-3.46712300
F	-3.88377600	-5.04718000	-2.99962200
F	-4.19249000	-3.45609500	3.09759700
F	-2.86540800	-5.05682200	2.40178800
F	-4.97287000	-5.04803500	1.79560200
F	4.11267000	6.03770700	-0.23361500
F	3.82183000	5.14727900	-2.21606100
F	2.10789800	5.39338500	-0.86916800
F	6.87620300	0.50687500	1.23312900
F	7.53762500	2.57023700	0.85463800
F	6.47372800	2.07898300	2.70797600
F	2.77520400	-5.10883500	2.36593100
F	4.88272400	-5.13813400	1.76044700
F	4.13280700	-3.53752400	3.06970200
F	3.81477900	-5.08469700	-3.03686400
F	4.80442800	-3.17888200	-3.48855900
F	2.66258300	-3.41915500	-3.89233600
F	-2.79013900	5.89422800	0.34977800
F	-2.33535700	5.20334700	-1.68148900
F	-4.37512000	5.84376500	-1.16534200
F	-7.13397400	2.94572000	1.82754300
F	-6.54174900	0.84653200	2.11260300
F	-7.39785300	1.49857400	0.20183100