Supplementary Material (ESI) for Chemical Communications

Supporting Information

C-H Activation in Strongly Acidic Media. The Co-catalytic Effect of the Reaction Medium

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S.1 *Computational details and coordinates of calculated structures.*

All calculations were performed with the hybrid density functional B3LYP.

Geometry optimizations included solvation using the Poisson-Boltzmann reactive field (PBF) with a dielectric constant of 98.0 and a probe radius of 2.205 to simulate sulfuric acid.

For geometry optimizations the smaller LACVP** basis set augmented with an extra d-function on sulfur. For single point energies we used the LACV3P**++ basis set augmented with one f-function on platinum and two d-functions and an f-function on sulfur. Frequency calculations were performed numerically including the PBF-solver at the B3LYP/LACVP**(+d on S) level.

Free energies were calculated as the sum G = E(lacv3p**++ 2df(S) f(Pt)) + Gsolv + ZPE + ΔH(450) + Strans/rot. To account for the decrease in translational+rotational entropy of the products from the gas phase values calculated in the QM, to the values appropriate in the solvent (where these modes become librational modes), we decreased the gas phase values by 60%, which we have found empirically to describe the change in translational+rotational entropy when molecules are transferred from the gas phase to the solution phase.

All species were calculated at 1 M or 1 atm except sulfuric acid and methane, which were corrected to 18 M and 30 atm, respectively, to reflect typical experimental conditions.

S.2 *Solvation of ions*

We found that simple solvation of small ions by the PBF method did not yield good results. Inclusion of one solvent molecule improved the result, and further improvement was found when two explicit solvent molecules were used to solvate the ions. Table S.1 shows the calculated values for solvation of H_2SO_4 in H_2SO_4, solvation of H_2O in H_2SO_4 ($H_2O(g) + H_2SO_4(l) \rightarrow H_3O^+(solv) + HSO_4^-(solv)$), and finally the autoionization of sulfuric acid ($2\ H_2SO_4 \rightarrow HSO_4^- + H_3SO_4^+$). Hence, for all calculation of these ions in solution two explicit solvent molecules were used in addition to the PBF implicit solvation. All geometries were optimized including the PBF solver. The input geometries were constructed manually, but several geometries were tried. This strategy is usable for these small clusters, but inclusion of more than two explicit solvent molecules would most likely require a more elaborate conformational search such as one based on molecular dynamics.

# explicit solvent molecules:	0	1	2	Exp
H2SO4(g) -> H2SO4 (l)	-18.6	-12.4	-11.0	-10 kcal mol^{-1}
$H_2O(g) + H_2SO_4(l)$ -> $H_3O^+(solv) + HSO_4^-(solv)$	-2.9	-10.5	-11.2	-11 kcal mol^{-1}
2 H_2SO_4 -> HSO_4^- + $H_3SO_4^+$	21.1	13.0	10.7	+8.5 kcal mol^{-1}

Table S.1. Solvation of smaller ions is greatly improved by addition of explicit solvent molecules.

From Table S.1. we see that the inclusion of explicit solvent molecules are important to get accurate solvation energies of ions. For bisulfate the solvation energy is improved by 7.0 kcal mol^{-1}. This stabilization of the bisulfate ion also stabilizes the **9ts** relative to **8ts**. Further, in the previous studies the bisulfate ion has been positioned close to the hydrophobic methyl group which we found to be unfavorable. The total discrepancy is hence a combination of the removal of the very poor interaction between the methyl group and the bisulfate, plus the introduction of the favorable interaction with the solvent.

For the metal complexes, we tested the solvation of several complexes by inclusion of explicit solvent molecules (table S.2). No significant changes in relative energies were found. Thus even the 5-coordinate platinum(IV) hydride complex **10** seemed to be well described by the continuum model. Coordination of a sulfuric acid molecule trans to the hydride did not alter the energy significantly. This is likely due to a combination of the very large trans-influence of the hydride and the weak coordinating ability of sulfuric acid. This can be contrasted to the sulfuric acid complex **5**, where exclusion of the sulfuric acid leads to a significantly different energy. The trans ligand in **5** is a nitrogen donor which is a relatively weakly trans-influencing ligand and therefore the coordination site must be occupied by an explicit ligand for a good description. Thus, all platinum complexes were solvated by the PBF solver only, except **5** and **6ts**.

Without explicit solvent	With explicit solvent	ΔE for adding one explicit solvent
$[(Hbpym)Pt^{II}Cl(CH_4)]^{2+}$	$[(Hbpym)Pt^{II}Cl(CH_4)]^{2+}H_2SO_4$	-0.1 kcal mol^{-1}
$[(Hbpym)Pt^{IV}ClH(CH_3)]^{2+}$	$[(Hbpym)Pt^{IV}ClH(CH_3)(H_2SO_4)]^{2+}$	0.9 kcal mol^{-1}
$[(Hbpym)Pt^{II}Cl(CH_3)]^{+}$	$[(Hbpym)Pt^{II}Cl(CH_3)]^{H+}H_2SO_4$	-1.5 kcal mol^{-1}
$[(Hbpym)Pt^{II}Cl(H_2SO_4)]^{2+}$	$[(Hbpym)Pt^{II}Cl(H_2SO_4)]^{2+}H_2SO_4$	-0.2 kcal mol^{-1}
$[(Hbpym)Pt^{II}Cl(HSO_4)]^{+}$	$[(Hbpym)Pt^{II}Cl(HSO_4)]^{+}H_2SO_4$	-2.0 kcal mol^{-1}
$[(Hbpym)Pt^{II}Cl]^{2+}$	$[(Hbpym)Pt^{II}Cl(H_2SO_4)]^{2+}$	-9.5 kcal mol^{-1}

Table S.2. Test calculations (B3LYP/LACVP** + PBF) show that most complexes are well described by the PBF solvation model. The exception is $[(Hbpym)Pt^{II}Cl]^{2+}$, since a free coordination site trans to a relatively weak donor is described by the electrostatic solvation model.

S.3 Detailed results from QM calculations

S.3.1 Structure 1

Gas Phase Energy = -1807.238786 = Eh

Free Energy of Solvation = -0.1685 = Eh

Zero Point Energy = 113.871 = kcal/mol

Hvib (Enthalpy) = 8.590 = kcal/mol

Geometry Coordinates

Pt1	-0.1974369198	0.2757412902	-0.2018467890
N2	1.8149185420	-0.0793723654	-0.0878986165
N3	0.4720619054	2.1930001671	-0.2083019236
C4	1.8237941322	2.3178918411	-0.1430888947
C5	2.5454986094	1.0420355722	-0.0819183316
N6	3.8825086323	0.9934432813	-0.0162389598
N7	2.4980497822	3.4495897670	-0.1268493935
C8	-0.2482907674	3.3317881494	-0.2608886718
C9	1.7858397917	4.5857814134	-0.1797703831
C10	2.4359201368	-1.2773304257	-0.0299980666
C11	4.5504154849	-0.1753375411	0.0470223301
C12	3.8221237328	-1.3568620050	0.0394205014
C13	0.3930061809	4.5666732510	-0.2482295606
H14	1.7995140044	-2.1555537472	-0.0391498804
H15	5.6321868176	-0.1243776487	0.1005021898
H16	-1.3263202240	3.2354298684	-0.3120555149
H17	2.3426173884	5.5184736336	-0.1658487137
H18	-0.1862852376	5.4824533424	-0.2899894666
H19	4.3190285152	-2.3191103760	0.0882172824
Cl20	-2.4912849371	0.8436486761	-0.3335714729
H21	4.3894422856	1.8850042908	-0.0142130799
S22	-1.7153950780	-2.5232219134	0.3829250299

O23	-1.9413901940	-2.0676569257	1.7329840333
O24	-1.4952039666	-3.9279770933	0.1660802259
O25	-0.5769226230	-1.7536417548	-0.2830484880
O26	-3.0012653484	-2.1875317190	-0.4946596888
H27	-3.1790230149	-1.2211466413	-0.4710131390

S.3.2 Structure 2

Gas Phase Energy = -1183.547219 = Eh

Free Energy of Solvation = -0.3077468 = Eh

Zero Point Energy = 112.140 = kcal/mol

Hvib (Enthalpy) = 6.914 = kcal/mol

Geometry Coordinates

Pt1	-0.2051463772	0.1319415513	-0.2134801509
N2	1.8253965126	-0.1469128237	-0.1124991506
N3	0.3926613473	2.0653225876	-0.1849221896
C5	1.7373732511	2.2478628790	-0.1136981127
C6	2.5108406111	1.0019424340	-0.0775108788
N7	3.8482546212	1.0075606613	-0.0131603250
N8	2.3601056390	3.4077239499	-0.0781761160
C9	-0.3788183164	3.1704496098	-0.2207568635
C10	1.5977447641	4.5122621527	-0.1163855299
C11	2.4952693538	-1.3197582185	-0.0829684077
C12	4.5638299688	-0.1333337819	0.0199118703
C13	3.8842578821	-1.3434003579	-0.0154800643
C14	0.2072902153	4.4325043737	-0.1878886620
H15	1.8968777037	-2.2244207554	-0.1133179298
H16	5.6428359313	-0.0382852240	0.0727534842

H17	-1.4509558700	3.0245125490	-0.2765855957
H18	2.1127671140	5.4685205262	-0.0886824752
H19	-0.4118354960	5.3224230731	-0.2176813774
H20	4.4221866502	-2.2842501330	0.0097371614
Cl36	-2.5144059721	0.5615035249	-0.3318766651
H37	4.3181058779	1.9191162351	0.0100372505
O22	-0.6215544400	-1.9291535629	-0.2275134318
H23	-1.1770197824	-2.1909761131	0.5303735120
H24	-1.1126914457	-2.1935619633	-1.0279175011

S.3.3 Structure 3ts

Gas Phase Energy = -1847.718078 = Eh

Free Energy of Solvation = -0.1650494 = Eh

Zero Point Energy = 141.373 = kcal/mol

Hvib (Enthalpy) = 9.340 = kcal/mol

Geometry Coordinates

C21	0.0000000000	0.0000000000	0.0000000000
Pt1	0.0000000000	0.0000000000	2.8672589557
O3	2.6634026010	0.0000000000	2.1143323131
N2	-0.8269383520	0.0708796197	4.6917570552
N3	0.0387212748	2.0388015327	3.1703878694
Cl4	-0.0776467305	-2.3248325000	2.6181961719
C5	-0.9040180384	1.3116925772	5.2449817017
C6	-0.4165894163	2.3885610275	4.3791119373
N7	-1.3748801613	1.5869089476	6.4418644176
C8	-1.8194177754	0.5590616645	7.1817375704
C9	-1.7842901443	-0.7495096793	6.7001860240

C10	-1.2719388398	-0.9704373756	5.4255945602
N11	-0.4456206349	3.6694590186	4.7653022186
C12	-0.0295850987	4.6640708610	3.9548274131
C13	0.4291935172	4.3383839219	2.6871314978
C14	0.4535188534	2.9975640095	2.3124142479
H15	-2.2067895149	0.7933851608	8.1692455129
H16	-2.1430388984	-1.5847250739	7.2920336625
H17	-1.2127336353	-1.9551784182	4.9794055809
H18	-0.0846495239	5.6748562797	4.3442592905
H19	0.7569119876	5.1110808087	2.0011789318
H20	0.7726246815	2.6812303847	1.3267302096
H22	0.8659201179	-0.0061628510	0.6862248536
H23	-0.9634519593	0.1380718812	0.4955210141
H24	0.1598655976	0.8204335811	-0.7050042726
H25	-0.0050540207	-0.9654787272	-0.5111406238
H26	-0.8003795308	3.8759014736	5.7057557620
S5	3.7548688987	0.9819686887	2.2138123644
O6	4.6397170371	0.7537104800	0.8766629164
O7	4.6411584439	0.7308634625	3.3404413382
O8	3.3181550427	2.3626911309	2.0678023024
H32	5.0416513000	-0.1344569888	0.8917435225

S.3.4 Structure 4ts

Gas Phase Energy = -1224.050025 = Eh

Free Energy of Solvation = -0.2858675 = Eh

Zero Point Energy = 139.345 = kcal/mol

Hvib (Enthalpy) = 9.312 = kcal/mol

Geometry Coordinates

C21	0.0000000000	0.0000000000	0.0000000000
Pt1	0.0000000000	0.0000000000	2.6961810464
O27	2.5683487302	0.0000000000	2.0375935185
N2	-0.9100466210	-0.0673738199	4.5077886593
N3	-0.2805896204	2.0535199920	3.0270987208
C14	0.2039998232	-2.2870687598	2.4942753406
C5	-1.2444374817	1.1401722115	5.0324203665
C6	-0.8912706094	2.2852213619	4.1991609484
N7	-1.8402319270	1.3586813580	6.1892363203
C8	-2.1506644997	0.2816551295	6.9260426107
C9	-1.8499159453	-1.0087303736	6.4756665208
C10	-1.2178094343	-1.1594978633	5.2414637029
N11	-1.1757037615	3.5359486463	4.6074865600
C12	-0.8660502599	4.6216169321	3.8666667084
C13	-0.2285317205	4.4219129839	2.6485334873
C14	0.0550721786	3.1141749824	2.2551239754
H15	-2.6415600390	0.4596642368	7.8784928821
H16	-2.0992944279	-1.8843128747	7.0659571111
H17	-0.9504700162	-2.1215973116	4.8178063615
H18	-1.1332518575	5.5942116893	4.2676939704
H19	0.0416459059	5.2638628594	2.0204637539
H20	0.5551815843	2.8925536164	1.3178515436
H22	0.7392386027	0.1760321730	0.8382187312
H23	-1.0544810056	-0.0555225164	0.2722788067
H24	0.1722138472	0.8439109016	-0.6724510965
H25	0.3110373278	-0.9468167061	-0.4419954503
H26	-1.6451807736	3.6131987736	5.5180942945
H28	3.2434045227	0.2557594548	2.6829006702
H29	2.7266404201	-0.9430084131	1.8712933308

S.3.5 Structure 5

Gas Phase Energy = -1807.499355 = Eh

Free Energy of Solvation = -0.3053939 = Eh

Zero Point Energy = 120.877 = kcal/mol

Hvib (Enthalpy) = 9.007 = kcal/mol

Geometry Coordinates

Pt1	0.0351670254	0.2504820086	0.1567683063
N2	2.0391097883	-0.0493770334	-0.2183639240
N3	0.5815864542	2.1520142805	-0.2107817432
C4	1.8849410792	2.3152712791	-0.5632862485
C5	2.6704819797	1.0789415156	-0.5617803630
N6	3.9693126458	1.0770830789	-0.8877729162
N7	2.4607480855	3.4531857041	-0.8904215944
C8	-0.1907589453	3.2579400849	-0.1816187167
C9	1.6958990448	4.5557855726	-0.8735949387
C10	2.7317948159	-1.2090134399	-0.1910317255
C11	4.7017226049	-0.0533186139	-0.8838960362
C12	4.0817035949	-1.2418649054	-0.5239109388
C13	0.3498708390	4.4965395698	-0.5144177967
H14	2.1873254589	-2.1014515155	0.0974466738
H15	5.7446303534	0.0331554125	-1.1671575815
H16	-1.2279902545	3.1301847307	0.1019897175
H17	2.1727472022	5.4916529729	-1.1514565786
H18	-0.2722830007	5.3847694624	-0.4950991835
H19	4.6346879141	-2.1736724855	-0.5042861064
Cl20	-2.2358096512	0.7532315839	0.5130956843
H21	4.3938116472	1.9749028249	-1.1455418586
S22	-1.4325833131	-2.6380824275	0.8587174736

O23	-2.1434539141	-2.2618610249	2.0279392961
O24	-0.7981373164	-4.0576484711	0.9529740630
O25	-0.2670712199	-1.8518642526	0.4170580351
O26	-2.4731192035	-2.7083627984	-0.3022250531
H27	-2.0820178807	-2.9384155554	-1.1714157343
H28	-1.3949468736	-4.7021733810	1.3916435457

6ts

Gas Phase Energy = -1848.008802 = Eh

Free Energy of Solvation = -0.2931775 = Eh

Zero Point Energy = 148.726 = kcal/mol

Hvib (Enthalpy) = 9.960 = kcal/mol

Geometry Coordinates

O3	0.1485734484	0.0914126995	-0.1114364620
Pt1	-0.1109954319	-0.0263165229	2.6197599415
H22	1.7846153738	-0.0608479291	1.6082307563
C21	2.8413355552	-0.0558954701	1.9583811043
N2	-1.3663377661	-0.0836470808	4.1865470967
N3	-0.3204339947	-2.0804167776	2.8135646591
C14	0.0819595569	2.3003908891	2.5230459547
C5	-1.7080921339	-1.3276466324	4.6165027297
C6	-1.1191637422	-2.4173035560	3.8349779305
N7	-2.4862165306	-1.5941650535	5.6429994855
C8	-2.9844914272	-0.5527701077	6.3275493076
C9	-2.6925242451	0.7610778211	5.9613729336
C10	-1.8643414681	0.9722656753	4.8623468586
N11	-1.3668738437	-3.6977542429	4.1349618991

C12	-0.8290495296	-4.7097777433	3.4282245383
C13	0.0039181768	-4.4006200405	2.3614434290
C14	0.2453213538	-3.0610073546	2.0711696262
H15	-3.6214187542	-0.7807168491	7.1781735119
H16	-3.0890888828	1.6086428912	6.5098564312
H17	-1.5860130466	1.9609230321	4.5203928798
H18	-1.0783606013	-5.7185841834	3.7394483417
H19	0.4569744593	-5.1877098826	1.7691047949
H20	0.9058806463	-2.7706946385	1.2567679048
H23	2.9116383141	-0.3854533163	2.9931649531
H24	3.3828971062	-0.7375600776	1.3000406377
H25	3.1983605846	0.9700619367	1.8544937213
H26	-1.9843017009	-3.8896434077	4.9324376779
S5	0.8495214594	-0.6669416360	-1.1108796337
O6	2.0228236398	0.1822398960	-1.7089330776
O7	-0.1681440536	-0.8242178886	-2.2850692891
O8	1.4231498649	-1.9214117734	-0.7351397817
H32	1.7466752138	1.0879263803	-1.9616498509
H33	0.1689195079	-1.4043143693	-2.9968227706

7

Gas Phase Energy = -1147.579782 = Eh

Free Energy of Solvation = -0.3013535 = Eh

Zero Point Energy = 124.970 = kcal/mol

Hvib (Enthalpy) = 6.848 = kcal/mol

Geometry Coordinates

Pt1	-0.0198781279	-0.0289158607	0.0106850468

N2	-0.0273205197	-0.0249337819	2.0340019871
N3	2.0172610361	0.0248868729	0.3555717119
C14	-2.3567540888	-0.0846001515	-0.2261507526
C5	1.2020819823	-0.0002658319	2.6110818859
C6	2.3175611017	0.0275577131	1.6595395655
N7	1.4437667996	0.0041616227	3.9040334320
C8	0.3826413457	-0.0160420883	4.7269880979
C9	-0.9200319757	-0.0362845146	4.2309975784
C10	-1.0996696604	-0.0410469521	2.8505838708
N11	3.5878609406	0.0592664841	2.0804366069
C12	4.6233309507	0.0898272824	1.2200986894
C13	4.3508407731	0.0874103590	-0.1407659401
C14	3.0221390402	0.0522954578	-0.5474649665
H15	0.5862002635	-0.0147780301	5.7940919014
H16	-1.7796549771	-0.0488906296	4.8921288270
H17	-2.0787712369	-0.0582721560	2.3876809349
H18	5.6208926668	0.1134376991	1.6446294759
H19	5.1519852034	0.1120784544	-0.8706646886
H20	2.7540621349	0.0456423055	-1.5980591755
C21	0.0202406377	0.3165211670	-2.4559616852
H22	0.0833356218	-0.6032756383	-1.7729426578
H23	0.0694897574	1.3192373098	-2.0241532925
H24	0.8796120590	0.1633869867	-3.1116701133
H25	-0.9337600798	0.1890866232	-2.9670688304
H26	3.7496242085	0.0589475887	3.0940480819

8ts

Gas Phase Energy = -1847.728243 = Eh

Free Energy of Solvation = -0.1530777 = Eh

Zero Point Energy = 139.165 = kcal/mol

Hvib (Enthalpy) = 10.118 = kcal/mol

Geometry Coordinates

C22	0.0000000000	0.0000000000	0.0000000000
H23	0.0000000000	0.0000000000	1.3846004347
O2	0.7054707347	0.0000000000	2.5869443832
Pt1	-1.9112507284	-0.1593963092	1.0947426117
S1	1.3291355826	1.2812252467	3.0636218271
O4	2.8571473507	1.2287952397	2.5666860981
O5	1.3561203759	1.3317858707	4.5096119839
O6	0.7910767428	2.4299433445	2.3650440312
N2	-3.7932829971	-0.2368516729	2.0099563580
N3	-2.3804529229	1.8614778509	1.1572743867
N4	-5.4730721521	1.2085905603	2.8891344357
N5	-4.0116788691	3.3636223217	1.8946875214
C17	-1.5941723878	-2.4871816598	1.1111330974
C8	-4.3419751203	0.9746735600	2.2501779957
C9	-3.5572693443	2.1110886683	1.7488985995
C10	-6.1355263426	0.1382311626	3.3545863307
C11	-5.6480651529	-1.1564096098	3.1712633376
C12	-4.4504544114	-1.3134302181	2.4800396987
C13	-3.3246222136	4.4321823571	1.4471640317
C14	-2.1084544897	4.2135582771	0.8185679698
C15	-1.6561581135	2.9038309616	0.6901724111
H16	-7.0652498992	0.3264992588	3.8840287899
H17	-6.1775565005	-2.0210448815	3.5557492659
H18	-4.0028189996	-2.2832999075	2.2941469808
H19	-3.7690416078	5.4085690502	1.6055273274
H20	-1.5229547742	5.0413923266	0.4346990729
H21	-0.7141201974	2.6773384728	0.2087865786

H24	-0.6012177875	-0.0100643210	-0.9153248639
H25	0.5868770063	0.9220706089	-0.0075037002
H26	0.6466763048	-0.8791296162	-0.0312739584
H33	-4.9155244949	3.4814369010	2.3662546950
H32	3.3741773905	0.6195286846	3.1278282311

9ts

Gas Phase Energy = -1147.563265 = Eh

Free Energy of Solvation = -0.3012988 = Eh

Zero Point Energy = 123.448 = kcal/mol

Hvib (Enthalpy) = 6.036 = kcal/mol

Geometry Coordinates

C1	0.0000000000	0.0000000000	0.0000000000
H2	0.0000000000	0.0000000000	1.6923738592
Pt4	1.5440267323	0.0000000000	1.5261773486
N9	3.5247932370	-0.1741232618	2.3926982876
N10	1.7428629243	-2.0554676899	1.6249472919
N11	5.0423226413	-1.7839390953	3.1099282797
N12	3.2567664292	-3.7589040253	2.3116865276
Cl13	1.5378410495	2.3493645923	1.5330677707
C14	3.8599476171	-1.4500308037	2.5755815053
C15	2.9105142663	-2.4974582508	2.1565751038
C16	5.9449962802	-0.8513447060	3.4739795981
C17	5.6356841775	0.4870274287	3.2798447544
C18	4.3961736146	0.7983412550	2.7276469096
C19	2.3814724951	-4.6928065926	1.9066541779
C20	1.1553990059	-4.3414888961	1.3446232693

C21	0.8597421663	-2.9872171670	1.2192817911
H22	6.8760652878	-1.2084905575	3.9001684245
H23	6.3395253167	1.2663909399	3.5483005546
H24	4.0822313243	1.8211089307	2.5415637686
H25	2.6741581368	-5.7303862293	2.0386056550
H26	0.4450308778	-5.0903997469	1.0118425626
H27	-0.0776562804	-2.6464845174	0.7953954737
H28	0.5555113146	-0.5919469927	-0.7297053313
H29	-0.9711992805	-0.4528546129	0.2088790124
H30	-0.1029551089	1.0418304656	-0.2920864959
H32	5.2435334059	-2.7826919864	3.2306755407

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Gas Phase Energy = -1147.560143 = Eh

Free Energy of Solvation = -0.3169348 = Eh

Zero Point Energy = 124.475 = kcal/mol

Hvib (Enthalpy) = 7.051 = kcal/mol

Geometry Coordinates

Pt4	-0.0124361444	-0.0004466131	-0.0400920562
H2	0.1674508145	0.0863152595	1.4580980345
N9	2.3317727725	0.0198439682	-0.0148842934
N10	0.4765883703	-2.0280379919	0.0782432136
N11	4.0756031240	-1.5041452062	0.2233265423
N12	2.2846047348	-3.5652653368	0.2153372754
Cl13	-0.3311635330	2.3332573225	0.0763486157
C14	2.7664693346	-1.2271966328	0.0881354871
C15	1.7949989517	-2.3435147593	0.1128148127

C16	5.0002934421	-0.5274182149	0.2878213903
C17	4.5780090350	0.7929501205	0.2244550917
C18	3.2146398679	1.0327934340	0.0651573221
C19	1.4139959852	-4.5809691472	0.3081590717
C20	0.0396408676	-4.3551768595	0.3168096997
C21	-0.4022836180	-3.0423560776	0.1964323252
H22	6.0357553857	-0.8325136535	0.3946726726
H23	5.2888990190	1.6080451731	0.2974316712
H24	2.8105688276	2.0398996042	0.0176630763
H25	1.8296629960	-5.5818726247	0.3847105196
H26	-0.6722511588	-5.1668802887	0.4172010478
H27	-1.4573847083	-2.7977310343	0.1991870040
H32	4.3462986141	-2.4915442858	0.2886476711
C1	-1.9947856780	-0.2783028679	0.5284566923
H28	-2.5128171693	-0.7241960690	-0.3239297159
H29	-1.9896606707	-0.9470074391	1.3939488892
H30	-2.4221057690	0.6851088248	0.8051960088

11ts

Gas Phase Energy = -1847.753958 = Eh

Free Energy of Solvation = -0.147596 = Eh

Zero Point Energy = 140.443 = kcal/mol

Hvib (Enthalpy) = 10.183 = kcal/mol

Geometry Coordinates

O3	0.0000000000	0.0000000000	0.0000000000
H2	0.0000000000	0.0000000000	1.5669239778
Pt4	0.1414150075	0.0000000000	3.1524290805

N9	2.3540579195	0.3880504822	2.6312836010
N10	0.2283198710	2.0728409796	3.0999303458
N11	3.6683277428	2.1811308859	1.9356193828
N12	1.6607185977	3.9139735920	2.6311108753
C113	0.2522718409	-2.3490795349	3.0839123311
C14	2.5243528420	1.6902544596	2.4446157647
C15	1.4175470929	2.6224287890	2.7523855564
C16	4.6659220551	1.3709952798	1.5322657374
C17	4.5008054456	0.0000110246	1.6599133964
C18	3.3170748340	-0.4624860608	2.2297645702
C19	0.6450919114	4.7591097177	2.8584701129
C20	-0.6207261733	4.2925975829	3.2063991191
C21	-0.7966290241	2.9180385724	3.3210153826
H22	5.5487604759	1.8440697931	1.1163257862
H23	5.2687749790	-0.6860583775	1.3217376736
H24	3.1200353460	-1.5221438985	2.3648003833
H25	0.8537590736	5.8202030938	2.7538073393
H26	-1.4501754415	4.9696179342	3.3772318976
H27	-1.7568089710	2.4874063402	3.5790410213
H32	3.7508325833	3.1997103806	1.8525505185
C1	-1.9223997283	-0.0991248259	3.1499028121
H28	-2.2761194981	0.1352376129	4.1584837571
H29	-2.2948061256	0.6282400056	2.4232366906
H30	-2.2352761364	-1.1019319559	2.8561476761
S5	0.8646979514	1.0415518546	-0.6292673032
O6	0.3453778938	1.1529288470	-2.1488713733
O7	2.2630796578	0.6440865207	-0.6770358402
O8	0.6108594091	2.3644989394	-0.0903939190
H31	0.6476727274	0.3888329178	-2.6752438008

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Gas Phase Energy = -1147.349555 = Eh

Free Energy of Solvation = -0.1193964 = Eh

Zero Point Energy = 118.293 = kcal/mol

Hvib (Enthalpy) = 7.055 = kcal/mol

Geometry Coordinates

Pt1	-0.2258014263	0.0719565967	-0.2604873381
N2	1.8116165359	-0.1471361435	-0.0577701940
N3	0.4382519572	2.1849578985	-0.1477081066
C4	-0.6265338977	-1.9413833051	-0.3548751182
C5	1.7721454640	2.2886072956	-0.0140105472
C6	2.4963460418	1.0065778385	0.0335904844
N7	3.8322503878	1.0112502079	0.1689182394
N8	2.4763428649	3.4084648927	0.0761848588
C9	-0.2582447389	3.3337685043	-0.1938424525
C10	1.7815956086	4.5547609115	0.0292925088
C11	2.5082666098	-1.3087047112	-0.0090485767
C12	4.5600705546	-0.1189029829	0.2217133575
C13	3.8904226910	-1.3304399419	0.1309606256
C14	0.3915238945	4.5624948938	-0.1067136984
H15	1.9379699401	-2.2267080837	-0.0828502665
H16	5.6336112891	-0.0153664958	0.3324424695
H17	-1.3349596979	3.2498714997	-0.3014874616
H18	2.3493035017	5.4786636210	0.1018647585
H19	-0.1670317249	5.4914980166	-0.1429664958
H20	4.4261361062	-2.2717914251	0.1667243656
H26	-1.6948319073	-2.1251768695	-0.5020013027
H27	-0.3109523440	-2.4244363324	0.5793978770
H28	-0.0744350669	-2.3884726108	-1.1927246794

Cl36	-2.5187813886	0.5618186857	-0.4793803616
H37	4.2846813650	1.9296284737	0.2314256343

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Gas Phase Energy = -1147.539929 = Eh

Free Energy of Solvation = -0.3428968 = Eh

Zero Point Energy = 127.519 = kcal/mol

Hvib (Enthalpy) = 6.994 = kcal/mol

Geometry Coordinates

Pt1	-0.2144374643	0.0796851473	-0.2527294363
N2	1.8167441063	-0.1313275804	-0.0533134413
N3	0.4802438879	2.1722295315	-0.1381113628
C4	-0.6404977752	-1.9262119732	-0.3588346720
C5	1.8022245258	2.2759506107	-0.0172910840
C6	2.5432073116	1.0006051144	0.0339457754
N7	3.8837944649	0.9419760389	0.1645486034
N8	2.3945187564	3.4866955643	0.0533540382
C9	-0.2719423291	3.2916329720	-0.1881002364
C10	1.6822365347	4.6292399045	0.0065623267
C11	2.4682188390	-1.3222454176	-0.0015704451
C12	4.5602608815	-0.2183720595	0.2179262699
C13	3.8435844544	-1.4036298461	0.1353397256
C14	0.3020821136	4.5547955008	-0.1170977286
H15	1.8580972186	-2.2138817437	-0.0729922231
H16	5.6374800934	-0.1551829589	0.3226285823
H17	-1.3436265359	3.1452446148	-0.2860855880
H18	2.2410980318	5.5563021145	0.0692017344

H19	-0.3024430244	5.4537548333	-0.1562978072
H20	4.3415556878	-2.3655982024	0.1739238382
H21	-1.7108936897	-2.0977218772	-0.4985537849
H22	-0.3212922466	-2.4119714328	0.5721497045
H23	-0.0980890180	-2.3637605996	-1.2067487605
Cl24	-2.4967352898	0.5779710188	-0.4704737891
H25	4.4376744707	1.7965560283	0.2273694252
H26	3.4063443089	3.5814954766	0.1447340856
