Supporting Information:

The Mechanism by which Ionic Liquids enable Shilov-type CH Activation in an Oxidizing Media

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$[PtCl_4][HPzm]_2$ (A)
Mulliken charge 0
Gas phase Energy: -2413.74089573945 hartrees
Solvation Energy: -2413.76604725501 hartrees
Zero Point Energy: 108.287 kcal/mol
Coordinates:

Pt1	-0.0388539649	0.1577791857	-0.1027161066
Cl2	-2.2193607895	0.8778625971	-0.7713310970
Cl3	0.7843250456	0.8433604077	-2.2411852080
Cl4	2.1412807888	-0.5633968025	0.5657994070
Cl5	-0.8620005325	-0.5268907604	2.0359377638
C6	-2.8902827587	-3.8529912091	0.6241340601
C7	-3.6850558901	-4.1394084514	-0.4885746430
C8	-3.7771529664	-2.9387287652	-1.1967796176
N9	-3.0805987102	-2.0083053584	-0.5307228771
N10	-2.5456310610	-2.5597412469	0.5675387697
H11	-2.5508350404	-4.4778590131	1.4368342214
H12	-4.1290239278	-5.0876421429	-0.7484560368
H13	-4.2826087505	-2.6924807312	-2.1187451191
H14	-2.8737123632	-0.9903310920	-0.7351948496
H15	-1.9376976318	-1.9554767684	1.1891808203
N16	3.0048068288	2.3225784124	0.3259362385
N17	2.4726561906	2.8735531106	-0.7739234719
C18	2.8184372862	4.1664663511	-0.8309108919
C19	3.6113739983	4.4531389273	0.2829856527
C20	3.7010582540	3.2529557448	0.9923813922
H21	2.7969170643	1.3048382161	0.5307061322
H22	1.8647087547	2.2696736866	-1.3957893091
H23	2.4810462934	4.7908795970	-1.6448101678
H24	4.0557126870	5.4011889506	0.5428657858
H25	4.2045585098	3.0070374640	1.9155147706

Pt_6Cl_{12}
Mulliken charge 0
Gas phase Energy: -6237.79870450018 hartrees
Solvation Energy: -6237.78272818435 hartrees
Zero Point Energy: 14.379 kcal/mol
Coordinates:

Pt1	40.9491020484	39.8312176628	38.9246616579
Cl2	42.8193015221	39.5782235851	40.3821823094
Cl3	42.0122196928	38.4340011243	37.3101493076
Cl4	39.1099523688	40.1425302279	37.4401428595
Cl5	39.9213465475	41.2841062898	40.5128500892
Pt6	40.1411433659	42.0362641808	36.4265815503
Cl7	41.2243476532	40.6054388194	34.8530130865
Cl8	41.2493884669	43.9205789747	35.4781078980
Cl9	39.1359717449	43.4555630425	38.0600727834
Pt10	43.1197770031	43.6675376464	36.9355063115
Cl11	44.1476414171	42.2147081801	35.3473229508
Cl12	44.9588528722	43.3560449399	38.4200167499
Cl13	42.0567476989	45.0647808082	38.5500957390
Pt14	43.9276449247	41.4623507002	39.4335353959
Cl15	44.9330269357	40.0429512099	37.8000835034
Cl16	42.8444845193	42.8932081740	41.0071691508
Pt17	43.1039090947	40.2906409879	36.2891147289
Pt18	40.9652723420	43.2080171993	39.5708956770

[HPzm][Cl]
Mulliken charge 0
Gas phase Energy: -687.02884769017 hartrees
Solvation Energy: -687.01596696956 hartrees
Zero Point Energy: 50.447 kcal/mol
Coordinates:

N1	-1.8465156190	1.7081977449	-0.1597147229
C2	-1.0851838053	0.6177254026	-0.0597788139
C3	0.2568028313	0.9050964233	-0.3908374692
C4	0.2637172490	2.2546460135	-0.7022490949
N5	-1.0108202640	2.6914857930	-0.5507125499
H6	-1.5296669105	-0.3198841528	0.2431837233
H7	1.0981356444	0.2291715766	-0.4018173891
H8	-1.3802892880	3.6212477731	-0.6912204215
H9	-3.4544695391	2.1957563480	0.0505150889
H10	1.0576534566	2.9182842611	-1.0116542993
Cl11	-4.6522163701	2.8029620720	0.1523431555

H_2SO_4
Mulliken charge 0
Gas phase Energy: -700.22683331272 hartrees
Solvation Energy: -700.23240676019 hartrees
Zero Point Energy: 23.924 kcal/mol
Coordinates:

S1	1.1162779222	0.9187392247	0.1787910997
O2	0.2055455950	1.5983197036	1.0765795641
O3	1.9126147520	-0.1608272900	1.1029716479
O4	2.0704576664	1.5859492600	-0.6824049970
O5	0.2538358808	-0.0558859589	-0.8010569004
H6	-0.5652474895	-0.3139934806	-0.3423848564
H7	2.7142722619	-0.4457930490	0.6296513659

$[PtCl_4][HPzm]_2[H_2O]$
Mulliken charge 0
Gas phase Energy: -2490.19218761895 hartrees
Solvation Energy: -2490.20954175899 hartrees
Zero Point Energy: 124.052 kcal/mol
Coordinates:

Pt1	-0.1539198841	0.1454721670	0.2594353374
Cl2	-2.3953095684	0.8836407915	0.0587759772
Cl3	0.2410504985	0.7434009689	-2.0403910009
Cl4	2.0985665048	-0.6717693597	0.4524487699
Cl5	-0.5763513859	-0.4819591097	2.5034669407
O6	0.0675504539	-3.1854574726	1.2664418056
H7	-0.0956265553	-2.4698952423	1.9255232562
H8	0.8612190397	-2.8747071557	0.8058058931
C9	-2.6815460182	-4.2994865681	-0.6980826897
C10	-3.8179356791	-3.9160012535	-1.4160444332
C11	-3.8475554799	-2.5172431873	-1.3509713104
N12	-2.7864762167	-2.1166509411	-0.6442204546
N13	-2.0796447285	-3.1911330431	-0.2412865623
H14	-2.2692527945	-5.2772182433	-0.4758006679
H15	-4.5205305103	-4.5615110931	-1.9152983322
H16	-4.5397930615	-1.7879042408	-1.7553766807
H17	-2.5140009876	-1.1344231420	-0.3917608544
H18	-1.1889308404	-3.1139030294	0.3537726209
N19	2.9115887329	2.2379084398	0.0847597363
N20	2.3295911571	2.6835316747	-1.0455615885
C21	2.8004222615	3.9117358929	-1.3311923298
C22	3.7306126044	4.2651235575	-0.3412654569
C23	3.7680187417	3.1742201408	0.5401251351
H24	2.6593240554	1.2828188338	0.4415661436
H25	1.5957315572	2.0691506699	-1.5161343304
H26	2.4494671857	4.4489805858	-2.2060546309
H27	4.2970446246	5.1877924072	-0.2703762906
H28	4.3376510853	3.0085654624	1.4470390399

$[Pt(H_2O)Cl_3][HPzm]_2[Cl]$
Mulliken charge 0
Gas phase Energy: -2490.18421931974 hartrees
Solvation Energy: -2490.20705642547 hartrees
Zero Point Energy: 123.911 kcal/mol
Coordinates:

Pt1	0.0388108155	-0.2711865235	-0.1799919960
Cl2	-1.9967578143	0.8383177326	-0.6081739316
Cl3	1.0267216296	0.5989664471	-2.1638060666
O4	1.8489089300	-1.2886420804	0.1460448042
Cl5	-0.7659274262	-1.2074555253	1.8585724728
Cl6	3.9126368833	0.3331908846	1.5242589704
H7	2.4811106589	-0.7632556512	0.7394799826
H8	2.3021444225	-1.3304227058	-0.7120267829
C9	-3.5448972986	-3.8498555099	0.2833947513
C10	-4.4714701789	-3.8051552217	-0.7614614924
C11	-4.3546975937	-2.5248938464	-1.3066485819
N12	-3.4159736088	-1.8632280602	-0.6155851005
N13	-2.9271213917	-2.6627686849	0.3436147182
H14	-3.2892998110	-4.6389108553	0.9750890729
H15	-5.1348445762	-4.5935278376	-1.0810887806
H16	-4.8689866792	-2.0514379624	-2.1297754707
H17	-3.0192380565	-0.8926803673	-0.7156743232
H18	-2.1591951509	-2.2855180172	0.9676851604
N19	3.2411676855	2.9032518190	0.3371314131
N20	2.3889652140	3.0235172781	-0.6917522477
C21	2.2624793707	4.3193039586	-1.0231713358
C22	3.0716517375	5.0615743918	-0.1648597014
C23	3.6711542064	4.1212475150	0.6805996431
H24	3.4842398858	1.9247637713	0.7779197708
H25	1.9442645557	2.1899169584	-1.1270980872
H26	1.6133203129	4.6181362707	-1.8325866471
H27	3.2049717757	6.1319334843	-0.1533546261
H28	4.3678337785	4.2386158905	1.4977723508

$[PtCl_4][HPzm]_2[H_2SO_4]$
Mulliken charge 0
Gas phase Energy: -3113.99570212904 hartrees
Solvation Energy: -3114.00547762585 hartrees
Zero Point Energy: 133.701 kcal/mol
Coordinates:

C1	3.9433453090	2.8753966992	0.6963498291
N2	3.1179619337	2.1322024092	-0.0547797757
N3	2.3135780175	2.9390123430	-0.7631058456
C4	2.6114903104	4.2127242324	-0.4773170698
C5	3.6543161954	4.2188052752	0.4528802292
Cl6	2.2669550965	-0.7836606439	-0.5838029618
Pt7	0.0175501087	0.0628552120	-0.4164152238
Cl8	-0.3273173426	-1.1446680989	1.6258985336
Cl9	-2.2059961773	0.8614984051	-0.2763800884
Cl10	0.3291440040	1.3336526982	-2.4023419933
N11	-2.4101420806	-3.0242735585	0.0626751463
C12	-2.9150552087	-4.2233966114	-0.2552032180
C13	-4.0791161099	-4.0100881250	-0.9970779284
C14	-4.2144643794	-2.6240205078	-1.0955129923
N15	-3.1934616644	-2.0556125955	-0.4383442978
O16	1.7303108698	-3.4004393711	1.7079988842
H17	1.1079661445	-2.6216428044	1.7744532991
S18	1.1447043787	-4.4891730409	0.6912929382
H19	-2.4028258088	-5.1196023036	0.0611455852
H20	-4.7320114504	-4.7610036915	-1.4134967959
H21	-4.9565743004	-2.0129527018	-1.5873726125
H22	-2.9162906007	-1.0459926403	-0.3522082973
H23	-1.5720335029	-2.7711324558	0.6019011029
H24	2.9902400380	1.1009325200	-0.1339801995
H25	1.5806460100	2.5064510082	-1.3912058563
H26	2.0688488060	5.0215011159	-0.9438254185
H27	4.1320018108	5.0795333533	0.8939401771
H28	4.6679557295	2.4079413118	1.3464843355
O29	2.1557785392	-5.5165104122	0.5633635599
O30	0.9875042929	-3.6459940993	-0.6814266821
O31	-0.2315325840	-4.8395298392	1.0455591180
H32	1.6487690215	-2.9165883440	-0.7472265977

$[Pt(HSO_4)Cl_3][HPzm]_2[HCl]$
Mulliken charge 0
Gas phase Energy: -3113.97653824015 hartrees
Solvation Energy: -3113.98547859030 hartrees
Zero Point Energy: 133.204 kcal/mol
Coordinates:

C1	1.8888759589	3.2255953506	-0.1001185103
N2	1.1038812014	2.2938728840	-0.6586082451
N3	0.2393171051	2.8961546231	-1.4895834672
C4	0.4439731021	4.2205434723	-1.4587132997
C5	1.5001777710	4.4761496154	-0.5838299893
Cl6	1.5754123116	-0.6074051550	0.0397912780
Pt7	-3.2849195016	1.5983811527	-1.0934049080
Cl8	-4.1655057397	0.8201991068	0.9799893388
Cl9	-5.0796829272	3.0760941982	-1.3067973846
Cl10	-2.4660585036	2.1207673920	-3.2559900101
N11	-6.3636196543	-0.4193762838	-0.7284599418
C12	-7.0678820419	-1.5364719699	-0.9490292693
C13	-7.9925819274	-1.2725167940	-1.9627979891
C14	-7.7819585917	0.0600895061	-2.3212648467
N15	-6.7956073760	0.5456013519	-1.5542887374
O16	-0.6227089293	-2.0184957155	-1.3830741935
H17	0.2801656924	-1.6862694630	-1.0685538602
S18	-1.7501971910	-1.2756050247	-0.5520392093
H19	-6.8646094909	-2.4342750509	-0.3845730747
H20	-8.7130772680	-1.9558898616	-2.3841041350
H21	-8.2588759817	0.6825824291	-3.0637543342
H22	-6.3150659748	1.4773900750	-1.5432577122
H23	-5.5854568341	-0.1916956573	-0.0610334617
H24	1.1525340218	1.2484106801	-0.5125632175
H25	-0.5195153755	2.4059861454	-2.0077140573
H26	-0.1785517370	4.8761838223	-2.0493890859
H27	1.9231569768	5.4356952847	-0.3317323478
H28	2.6623973109	2.9345047517	0.5951571324
O29	-1.6975451835	0.1561411445	-0.9978227032
O30	-1.2248567872	-1.3474413576	0.9477229594
O31	-2.9911082878	-2.0007140757	-0.6665904377
H32	-0.2694539484	-1.0306511345	0.9588768316

$[PtCl_4][HPzm]_2[CH_4][HCl]$ (B)
Mulliken charge 0
Gas phase Energy: -2915.07708702351 hartrees
Solvation Energy: -2915.09570283875 hartrees
Zero Point Energy: 142.095 kcal/mol
Coordinates:

Pt1	-0.0516622936	0.2089973685	0.0214596134
Cl2	-2.2987560197	0.9040851684	-0.3927093632
Cl3	0.5755228175	1.2153582200	-2.0506696985
Cl4	2.1812533303	-0.5418920968	0.4097216695
Cl5	-0.6961251575	-0.8518494399	2.0628692011
C6	-2.9652837811	-3.9560839482	0.4952434397
C7	-3.8865024844	-4.0883612241	-0.5465177249
C8	-4.0084750391	-2.8109267449	-1.0985813047
N9	-3.2072123382	-1.9837361224	-0.4139014077
N10	-2.5778305881	-2.6746247582	0.5474751679
H11	-2.5655117011	-4.6808254221	1.1888967442
H12	-4.3932476004	-4.9873970970	-0.8606944998
H13	-4.6025683129	-2.4448804165	-1.9227526816
H14	-2.9920239119	-0.9534965647	-0.5150086252
H15	-1.8921955805	-2.1609995999	1.1668465602
N16	3.4287361344	2.2180426125	0.1182315348
N17	2.7944314048	2.9064618242	-0.8410049216
C18	3.2793991431	4.1539932289	-0.8819850187
C19	4.2747706819	4.2639342907	0.0911963848
C20	4.3305461404	3.0128246951	0.7085677767
H21	3.1119125613	1.2349672357	0.3197308942
H22	2.0069806327	2.4351724523	-1.3572875763
H23	2.8880939591	4.8740028194	-1.5850274123
H24	4.8675124975	5.1344787333	0.3241501369
H25	4.9397892024	2.6459867364	1.5210283371
H26	0.8499556894	-4.4305958727	-2.2701510028
C27	1.8497552535	-3.9871604549	-2.2544427550
H28	2.5599653929	-4.7086122232	-1.8415323143
H29	2.1455143851	-3.7284254675	-3.2745944473
H30	1.8429587857	-3.0853122085	-1.6378505349
H31	0.1729205427	2.1257461060	1.2842277300
Cl32	0.4989448882	3.2530082220	1.9001996058

$[PtCl_3][HPzm]_2[Cl][CH_4][HCl]$ (TS1)
Mulliken charge 0
Gas phase Energy: -2915.03812562470 hartrees
Solvation Energy: -2915.05315775174 hartrees
Zero Point Energy: 141.264 kcal/mol
Coordinates:

Pt1	-0.0034622042	-1.3256066511	0.1077461134
Cl2	-0.1275388659	-1.3432336040	2.4716728845
Cl3	2.2892162476	-1.4854159263	0.1447626515
Cl4	-0.0755456096	-1.5606630289	-2.2477610987
Cl5	-1.8682701937	1.2458371933	-0.0208358031
C6	-3.1910547280	-2.4824962750	0.1693567301
H7	-3.4651643144	-1.4261298207	0.1522408562
H8	-3.6016775602	-2.9944499096	-0.7041873454
H9	-3.5487884365	-2.9513388014	1.0893499352
H10	0.4755821332	0.5044773979	2.7829225406
H11	-0.8079379614	1.9971233397	1.4302347111
H12	0.3065866705	0.2765197755	-2.8355308582
H13	-1.0178742746	1.8633503877	-1.6429911092
N14	0.3299519989	1.2910749326	-3.1303161648
N15	-0.4692547039	2.1682179411	-2.5070154278
C16	0.9626716080	1.9054785439	-4.1391604754
C17	-0.3501386850	3.3645615119	-3.1000516008
C18	0.5580910995	3.2422457697	-4.1542442276
H19	1.6473857626	1.3602150725	-4.7718248646
H20	-0.9123180818	4.2137376560	-2.7407025928
H21	0.8773010142	4.0144145602	-4.8367207742
N22	-0.1664495249	2.3802036240	2.1906034849
N23	0.6036327633	1.5456328671	2.9028444496
C24	0.1003230659	3.6410977579	2.5599469021
C25	1.3656739285	2.2543857054	3.7464847639
C26	1.0770091806	3.6079337653	3.5578765520
H27	-0.4154817233	4.4694116795	2.0973918183
H28	2.0524914722	1.7577952273	4.4159629811
H29	1.5145312845	4.4478930447	4.0745490644
H30	-2.0949434540	-2.5865383479	0.1393048620
H31	0.4392531522	-3.8053787395	0.2547959448
Cl32	0.3826328193	-5.1064850732	0.3229870872

$[PtCl_3(CH_4)][HPzm]_2[Cl]$ (C)
Mulliken charge 0
Gas phase Energy: -2915.05593609717 hartrees
Solvation Energy: -2915.06850034817 hartrees
Zero Point Energy: 142.469 kcal/mol
Coordinates:

Pt1	1.0016581004	-1.2282214773	-0.5615319214
Cl2	-0.7200071299	-2.8374051535	-0.8043114080
Cl3	-0.5247145309	0.5077564205	-0.7878149078
Cl4	2.7806952796	0.3075534666	-0.2617833369
Cl5	-2.9608974172	2.8067701580	1.7855386796
C6	2.6773451479	-3.0790432148	-0.6581122174
H7	2.3531253899	-4.1147573017	-0.5527049159
H8	2.0787274363	-2.5496024923	0.1625254013
H9	2.5539693392	-2.7680086114	-1.6965734610
H10	3.7075274703	-2.8994373800	-0.3493424384
C11	-5.2112444133	-0.3469834211	1.1520616730
C12	-5.2762512620	-1.6446303613	0.6366244234
C13	-4.0253910221	-1.8823544883	0.0675119278
N14	-3.2792928368	-0.7817278468	0.2460656658
N15	-3.9949928937	0.1508455229	0.8957406963
H16	-5.9402894615	0.2481262666	1.6817302697
H17	-6.1150587130	-2.3220315857	0.6725590537
H18	-3.6075299135	-2.7386984333	-0.4399899047
H19	-2.3226907350	-0.5802477898	-0.0764789961
H20	-3.5777622319	1.0976645364	1.1739553154
N21	-0.1169253396	3.6518962049	1.4415679624
N22	0.8374526424	2.9263877335	0.8357435329
C23	2.0150546436	3.5630722252	0.9236526923
C24	1.8050317485	4.7494456518	1.6260563245
C25	0.4423161506	4.7629234397	1.9371312055
H26	-1.1290386094	3.3090089542	1.5196749586
H27	0.6032285835	2.0481823753	0.3526814245
H28	2.8989474984	3.1219452599	0.4879873279
H29	2.5413362060	5.4967194833	1.8772071225
H30	-0.1598730708	5.4796554541	2.4756186110
H31	1.1366822324	-0.9404777477	-2.9975541421
Cl32	1.3785054792	-0.9791915429	-4.2793091907

$[PtCl_3(CH_3)(H)][HPzm]_2[Cl][HCl]$ (TS2)
Mulliken charge 0
Gas phase Energy: -2915.04726939117 hartrees
Solvation Energy: -2915.05675232041 hartrees
Zero Point Energy: 141.269 kcal/mol
Coordinates:

Pt1	1.0921957075	-1.1365609912	-0.6168886623
Cl2	-0.6290352340	-2.7887770858	-0.6025721482
Cl3	-0.5738741311	0.6211553477	-0.8619831287
Cl4	2.8217477115	0.4720783602	-0.5723231241
Cl5	-3.0517964649	2.9612120755	1.8641081208
C6	2.5643346474	-2.6565481074	-1.1025729326
H7	2.2864933023	-3.6666044956	-0.8034275582
H8	1.9884531185	-2.0861860363	0.2378615368
H9	2.4335573225	-2.5327848323	-2.1798692099
H10	3.5783924916	-2.3877362433	-0.8103583566
C11	-5.2491186255	-0.2382730755	1.1306310279
C12	-5.2539282719	-1.5146401161	0.5609260046
C13	-3.9907804996	-1.6722478840	-0.0089458439
N14	-3.2938623737	-0.5491895226	0.2214865629
N15	-4.0548153442	0.3223688687	0.9032540845
H16	-6.0067490532	0.3010973824	1.6796201419
H17	-6.0616447458	-2.2296044758	0.5630973039
H18	-3.5358373171	-2.4901916933	-0.5470478995
H19	-2.3452224475	-0.2827705513	-0.0961250281
H20	-3.6723199483	1.2725114373	1.2199847116
N21	-0.1702657197	3.6808666738	1.5532578881
N22	0.7188090678	2.9802529933	0.8298044784
C23	1.9362250398	3.5303893434	0.9555419890
C24	1.8200168974	4.6327763898	1.8019819439
C25	0.4699292595	4.6888056737	2.1588660091
H26	-1.1993190889	3.3921403481	1.6189069596
H27	0.4140977819	2.1672336114	0.2681249001
H28	2.7803276988	3.0901197326	0.4464204575
H29	2.6088064928	5.2979505169	2.1166658014
H30	-0.0716317506	5.3698130393	2.7985847237
H31	-0.1893793590	-3.9220434117	-2.4921246532
Cl32	0.1304498466	-4.5750169079	-3.5794008543

$[PtCl_3(CH_3)(H)][HPzm]_2[Cl][HCl]$ (D)
Mulliken charge 0
Gas phase Energy: -2915.05861943313 hartrees iterations: 11
Solvation Energy: -2915.07790891644 hartrees
Zero Point Energy: 142.074 kcal/mol
Coordinates:

Pt1	-0.9195738386	1.0461345273	-0.0590220514
Cl2	-0.8409526423	0.8983615370	2.2896575134
Cl3	1.7265542332	1.1968130408	-0.1770233971
Cl4	-1.0775806712	1.3886689498	-2.4121885838
Cl5	-0.3931343400	-2.4272677101	-0.3767789918
C6	-2.9762444809	0.9944658169	0.0301770814
H7	-3.2795593753	0.4462095813	0.9215586863
H8	-0.8811964525	-0.5163680975	-0.2032338310
H9	-3.2965862486	2.0398936444	0.0928150439
H10	-3.3570236224	0.5327662733	-0.8809179810
C11	1.5192934421	-2.5740748500	3.2488772381
C12	2.3782924512	-1.8395385862	4.0681299374
C13	2.6826893231	-0.6852492424	3.3438276968
N14	2.0483403974	-0.7524757246	2.1670136282
N15	1.3428614233	-1.8904443504	2.1099599091
H16	1.0274237024	-3.5232906184	3.4002462392
H17	2.7264615809	-2.1031898428	5.0544059987
H18	3.2923459960	0.1714098446	3.5896960377
H19	1.9662899914	-0.0436048707	1.3976556059
H20	0.7340935882	-2.0987375248	1.2792002185
N21	1.1048720266	-1.4846859181	-2.8932978986
N22	1.8008151865	-0.3377822299	-2.8558840505
C23	2.2875269605	-0.0750295718	-4.0756380293
C24	1.8935084050	-1.1073707651	-4.9295020234
C25	1.1397948183	-1.9765447452	-4.1396880243
H26	0.5947310410	-1.8305838569	-2.0429771498
H27	1.8221602610	0.2338212876	-1.9794877603
H28	2.8464628599	0.8309636331	-4.2565489577
H29	2.1141064244	-1.2033395742	-5.9809518363
H30	0.6295033822	-2.8975660635	-4.3790689735
H31	0.5007596633	2.7727496651	-3.1315348131
Cl32	1.4582650032	3.4486125832	-3.7257838670

$[PtCl_3(CH_3)(HCl)(HCl)][HPzm]_2$ (E)
Mulliken charge 0
Gas phase Energy: -2915.05609234862 hartrees
Solvation Energy: -2915.07149506880 hartrees
Zero Point Energy: 141.063 kcal/mol
Coordinates:

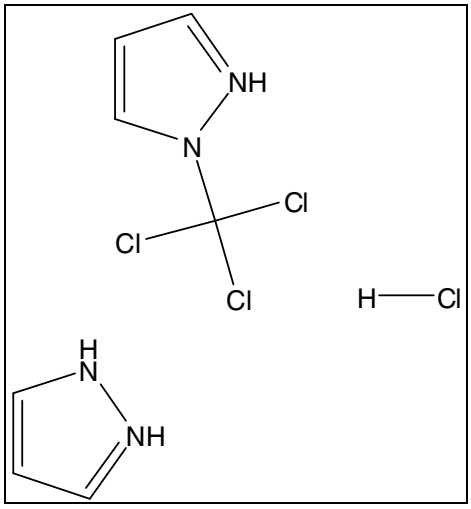
Pt1	0.4968728973	-0.9610688392	0.1072375185
Cl2	-0.2003305290	-2.2929848004	-1.7378526798

Cl3	-1.1315157451	1.0434881615	-0.7079664595
Cl4	1.1970513905	0.3138338821	1.9944788841
C6	1.7379465270	-2.4925255540	0.6699930563
H7	1.1405050657	-3.4026264376	0.7742006554
H8	-0.9784064643	-1.8365059985	1.5651619116
H9	2.4810154089	-2.6328759481	-0.1209151819
H10	2.2242066292	-2.2390019751	1.6136366236
C11	-4.1905168962	-2.8827164400	-0.9313274711
C12	-5.2709429087	-2.1745168616	-0.4007705894
C13	-4.8031281015	-0.8736930875	-0.2087766192
N14	-3.5277205820	-0.8270812959	-0.6160746095
N15	-3.1581523114	-2.0391326337	-1.0540420187
H16	-4.0899245481	-3.9190880553	-1.2171010965
H17	-6.2547727522	-2.5548574413	-0.1754984170
H18	-5.2865136250	0.0059071437	0.1894017839
H19	-2.8158391729	-0.0598899880	-0.5963245264
H20	-2.1558985281	-2.2017990384	-1.3427087264
N21	1.7989570183	2.9368180969	0.5853238321
N22	0.9451664600	3.2415021599	-0.4015955878
C23	1.3536837726	4.3635632380	-1.0093548554
C24	2.5187294027	4.7986886341	-0.3754148781
C25	2.7690317815	3.8585069083	0.6268938105
H26	1.6563122296	2.0443102215	1.1313261602
H27	0.1546244710	2.5839988653	-0.6033172292
H28	0.8008016794	4.7711760279	-1.8424864989
H29	3.1059568473	5.6712613359	-0.6147824285
H30	3.5664734866	3.7849248534	1.3511817477
Cl30	-1.9642590812	-2.3773577577	2.2807937785
H31	2.1466897010	-0.0700706602	-1.1247448814
Cl32	3.0986423062	0.5896622882	-1.7844130342

$[PtCl_3(CH_3)][HPzm]_2[HCl]$
Mulliken charge 0
Gas phase Energy: -2454.23819009965 hartrees
Solvation Energy: -2454.25462872990 hartrees
Zero Point Energy: 135.128 kcal/mol
Coordinates:

Pt1	0.8936787342	-0.1741380629	-2.1593615945
C2	1.3185824422	-2.1392984723	-2.5498067353
Cl3	-1.2394156490	-0.5252509546	-3.1930838327
Cl4	0.2825974886	2.3481083526	-1.6339541844
Cl5	3.0446578466	0.1186643680	-1.1942540451
H6	4.2507362318	-0.4455403561	-2.5653372833
N7	-2.3093122027	1.7167178559	-0.3616096601
N8	-2.8833058340	0.6352630056	-0.9066718168
C9	-4.0510274361	0.3933326688	-0.2926975688
C10	-4.2300190217	1.3666857257	0.6919594379
C11	-3.0986582977	2.1852236922	0.6123573973
H12	-1.3569384065	2.0378732923	-0.7517012932
H13	-2.3891363601	0.1495636908	-1.7011445703
H14	-4.6674397157	-0.4426687924	-0.5897769780
H15	-5.0625172068	1.4653632155	1.3711279318
H16	-2.8101411423	3.0569925292	1.1809094087
C17	1.3826767969	2.6766154103	-5.0700619308
C18	2.2760831408	3.2123847344	-6.0059719410
C19	3.4098310713	2.4052122061	-5.9434783368
N20	3.1827072182	1.4456363844	-5.0295826481
N21	1.9593750620	1.6136897720	-4.5054106227
H22	2.1243222802	4.0741175531	-6.6367765433
H23	4.3491734684	2.4484529423	-6.4746002179
H24	1.5940258901	0.9731124945	-3.7229150838
Cl25	5.0626003643	-0.7186305008	-3.6437224939
H26	0.3970139604	2.9808797352	-4.7497292679
H27	3.8097814573	0.7084172859	-4.6694809066
H28	1.0910571235	-2.3688372195	-3.5947269618
H29	0.6673222657	-2.7357104906	-1.9000777869
H30	2.3637053920	-2.3627475134	-2.3264411470

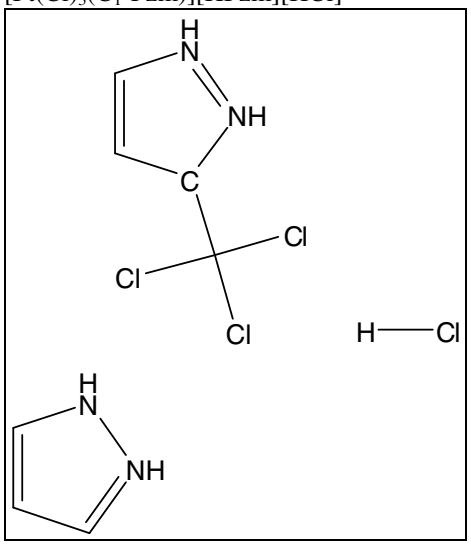
[$Pt(Cl)_3$(N-Pzm)][HPzm][HCl]



Gas phase Energy: -2413.74182112200 hartrees
Solvation Energy: -2413.75666511920 hartrees
Zero Point Energy: 106.674 kcal/mol
Coordinates:

Pt1	0.5758661915	-1.1419724283	0.1028507935
Cl2	-1.4995364275	-0.4969550732	-0.8719839034
Cl3	-0.3972855471	-3.2403062514	0.6633731053
Cl4	2.6900432023	-1.8202716937	1.0279069069
N5	0.7257259496	1.5482029029	-1.1809149777
C6	1.4050621090	2.7061510297	-1.3061846155
C7	2.5530780166	2.5912800003	-0.5357875484
C8	2.4853135036	1.3127632399	0.0428150366
N9	1.3663839666	0.6926792740	-0.3568613103
H10	-0.1899065243	1.2619008445	-1.5262997658
H11	1.0244422165	3.5117473617	-1.9162278469
H12	3.3281525068	3.3299678269	-0.4015446853
H13	3.1655818936	0.8093374598	0.7111741757
H14	2.9158854608	-3.4181952916	-0.1826446283
N15	2.8134209442	-4.2588473538	-0.8065587773
C16	3.6999840211	-4.9542407800	-1.5333985842
C17	3.0089743563	-5.9614959650	-2.2095885992
C18	1.6707751686	-5.8090687747	-1.8364816421
N19	1.5889175467	-4.7731498191	-0.9917475477
H20	4.7475507195	-4.6921010444	-1.5240428919
H21	3.4207468388	-6.7002359065	-2.8793142719
H22	0.7863785436	-6.3624541787	-2.1158258309
H23	0.7762339056	-4.3268107510	-0.4751260016
H24	-2.0986398038	1.1235546167	0.5838503070
Cl25	-2.3333436868	2.2256323500	1.2498112434

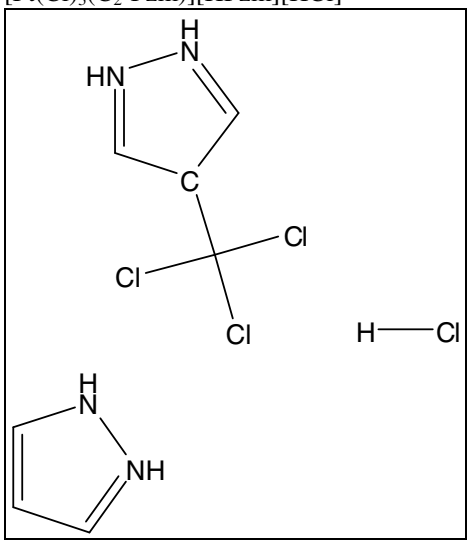
[$Pt(Cl)_3(C_1$-Pzm)][HPzm][HCl]



Gas phase Energy: -2413.72350878046 hartrees
Solvation Energy: -2413.75109155319 hartrees
Zero Point Energy: 106.288 kcal/mol
Coordinates:

Pt1	0.5679737444	-1.1746634649	0.1939181468
Cl2	-1.5757597773	-0.5172291616	-0.6351016536
Cl3	-0.3707665528	-3.3961515241	0.7338587625
Cl4	2.7417250776	-1.8389581592	0.9711876821
N5	0.6791726122	1.4294299356	-1.1154206413
N6	1.3304551258	2.6227645767	-1.2369005481
C7	2.3597715151	2.6009067231	-0.3434298792
C8	2.3904430285	1.3662802196	0.2643178601
C9	1.2795009023	0.6141340255	-0.2281958492
H10	-0.1745447817	1.2219384214	-1.6241679770
H11	0.8030217844	3.4354285387	-1.5305752387
H12	2.9922875971	3.4692531473	-0.2263459180
H13	3.1100129885	1.0128720071	0.9848329869
H14	2.8905031744	-3.4052010049	-0.2906749372
N15	2.7684242490	-4.2259540495	-0.9365668500
C16	3.6220513364	-4.8563487329	-1.7569281228
C17	2.9184364020	-5.8634513884	-2.4193720333
C18	1.6081597093	-5.7778222447	-1.9379826019
N19	1.5535671871	-4.7813475322	-1.0463158036
H20	4.6565171554	-4.5522149635	-1.8163829267
H21	3.3037761055	-6.5590517316	-3.1484435547
H22	0.7252493860	-6.3542167772	-2.1715955172
H23	0.7579276457	-4.3717434115	-0.4520099084
H24	-2.0561730986	1.5612446047	-0.1081001841
Cl25	-2.2065168478	2.8736839786	-0.0859586246

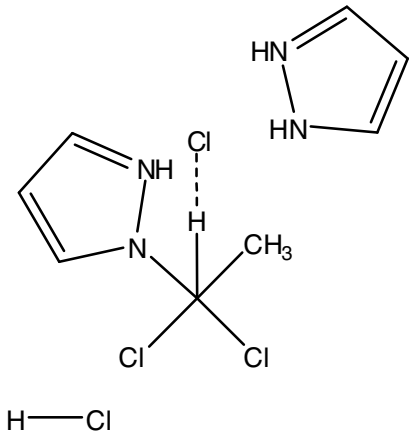
[$Pt(Cl)_3(C_2$-Pzm)][HPzm][HCl]



Gas phase Energy: -2413.69935126124 hartrees
Solvation Energy: -2413.74416180399 hartrees
Zero Point Energy: 105.902 kcal/mol
Coordinates:

Pt1	0.5578968785	-1.2551425480	0.2650129601
Cl2	-1.6571610523	-0.5655495715	-0.2524795699
Cl3	-0.2804380200	-3.5360450719	0.8096149880
Cl4	2.8420500978	-1.8625660814	0.7746024119
C5	0.7182384454	1.4345461666	-1.1627577453
N6	1.3583635816	2.6296938418	-1.0888071153
N7	2.1557814905	2.6036283834	0.0118132975
C8	2.1059626665	1.3610036895	0.5459884007
C9	1.1749704046	0.5780039985	-0.1535800724
H10	-0.0473116866	1.2773950278	-1.9077579264
H11	1.0151359188	3.5169807616	-1.4345640376
H12	2.8173226826	3.3472184433	0.1852540545
H13	2.7389857086	1.1008199690	1.3816891986
H14	2.9457754075	-3.5082829395	-0.3781619671
N15	2.8122617464	-4.3876405965	-0.9399510991
C16	3.6401310818	-5.0793750049	-1.7376313316
C17	2.9328192855	-6.1671021042	-2.2517670329
C18	1.6481173815	-6.0628450370	-1.7073095380
N19	1.6108035182	-4.9801065309	-0.9222169255
H20	4.6606014709	-4.7588248217	-1.8860019320
H21	3.2991422994	-6.9260181294	-2.9255461092
H22	0.7717807909	-6.6821067805	-1.8291801718
H23	0.8314907116	-4.5305751554	-0.3185377959
H24	-1.8734128041	1.4685281264	0.3053770148
Cl25	-1.9796898787	2.7807499858	0.5121831078

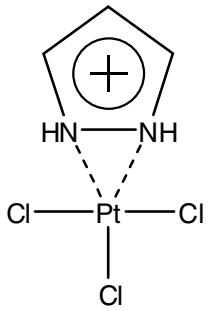
$[Pt(Cl)_2(N\text{-}Pzm)(CH_3)][Cl][HPzm][HCl]$



Gas phase Energy: -1532.61541665214 hartrees
Zero Point Energy: 122.925 kcal/mol
Coordinates:

Pt1	0.5348765645	-1.0933191832	0.0594902785
Cl3	-0.4088188615	-3.2445151167	0.4980791619
Cl4	2.9133061661	-1.8738935197	0.7603076063
N5	0.6885715680	1.6752995762	-1.0863553001
C6	1.3879093234	2.8331511164	-1.1400352895
C7	2.5066059072	2.6625375389	-0.3418875208
C8	2.4058596017	1.3542778079	0.1684290623
N9	1.2940235519	0.7658387779	-0.2906961487
H10	-0.1927798513	1.4303962047	-1.5149713446
H11	1.0421991144	3.6690998342	-1.7299168268
H12	3.2885695172	3.3812456924	-0.1506468377
H13	3.0646390173	0.8004150580	0.8190348107
H14	3.0289950224	-3.4929538857	-0.2169468326
N15	2.9130892611	-4.4169037575	-0.7550911467
C16	3.7841227424	-5.2203425511	-1.3783427457
C17	3.0736942909	-6.2892155531	-1.9330812721
C18	1.7381104917	-6.0579557147	-1.5965764613
N19	1.6794467979	-4.9215078185	-0.8878676882
H20	4.8381491864	-4.9853187172	-1.3877797063
H21	3.4718787004	-7.1165028289	-2.4997392930
H22	0.8415780916	-6.6199825506	-1.8125159715
H23	0.8698285376	-4.3998212158	-0.4440370026
C23	-1.3361574308	-0.4493002159	-0.4947295610
H24	-1.5895366868	0.4833433672	0.0262438387
H25	-1.3810449000	-0.2994945933	-1.5858371844
H26	-2.0832400840	-1.2030910435	-0.2364336678

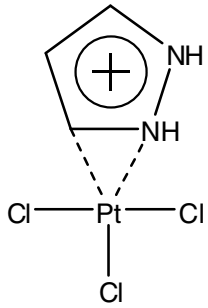
$[Pt(Cl)_3(N,N\text{-}HPzm)][Cl{:}HPzm]$



Gas phase Energy: -1726.64553342865
Zero Point Energy: 55.073 kcal/mol
Coordinates:

Pt1	2.5409932344	-2.1461112191	0.7722032546
Cl2	4.7997998674	-2.6016647122	0.8262695146
C3	1.0438788273	-0.8751141301	5.3668533315
N4	1.0208309509	-1.3168881820	4.1006216577
N5	0.3291134887	-0.4532151128	3.3411179884
C6	-0.0992544774	0.5575470530	4.1090632960
C7	0.3351091817	0.3261458855	5.4166147787
Cl8	1.9392302145	-3.7110551302	2.3447819269
H9	1.4223053468	-2.1685601518	3.6537089777
H10	0.2393222516	-0.6398104641	2.3052385082
H11	0.1612333148	0.9462270135	6.2819368904
H12	1.5558844584	-1.4332499307	6.1365308692
H13	-0.6749857003	1.3653974408	3.6823908672
Cl14	0.3337008968	-1.2890491471	0.4219585843

$[Pt(Cl)_3(N,C\text{-}HPzm)][Cl{:}HPzm]$

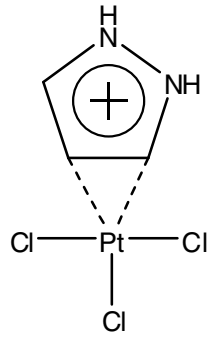


Gas phase Energy: -1726.62579579387 hartrees
Zero Point Energy: 55.758 kcal/mol
Coordinates:

Pt1	2.2055905382	-2.0621791464	1.3452012549
Cl2	3.9711447871	-0.6825318917	2.1231715352
C3	1.5975311818	-1.4174022038	4.4615419756
C4	0.9958108268	-1.9794238633	3.3016919779
N5	0.6904471865	-0.9159193190	2.4396661178
N6	0.9933240843	0.2725127456	3.0997769980
C7	1.6482518060	-0.0660771244	4.2616733511
Cl8	3.6328053192	-3.1873624076	-0.0402700324
H9	0.4525537578	-2.9100956498	3.2051472731
H10	-0.1498554767	-0.9372799119	1.8556069659
H11	2.1039690609	0.7134603350	4.8555482287
H12	1.9837621820	-1.9682490391	5.3045620535

H13	1.3513109340	1.0120166330	2.4995313170
Cl14	0.2767472246	-3.1942851589	0.5042408115

[$Pt(Cl)_3$(C,C-HPzm)][Cl:HPzm]



Gas phase Energy: -1726.63056842649 hartrees
Zero Point Energy: 55.822 kcal/mol
Coordinates:

Pt1	2.2023476658	-2.1162875597	1.4295470899
Cl2	4.0110834969	-0.7731852331	2.2595608007
C3	1.5014728603	-1.3325973966	4.2962093910
C4	0.7835501501	-1.8824144907	3.2049179863
C5	0.6438204113	-0.8100425796	2.2596928818
N6	1.1234203036	0.3501200475	2.8873487067
N7	1.7239504799	-0.0542989828	4.0574677205
Cl8	3.5192185919	-2.6954503807	-0.3761839276
H9	0.2249352765	-2.8064566101	3.2157182925
H10	-0.1085528776	-0.6995362716	1.4896921140
H11	2.3995226165	0.5498095373	4.5110350125
H12	1.8614113791	-1.8027115903	5.2004839438
H13	1.6631266073	1.0286361543	2.3547888471
Cl14	0.4327398112	-3.4466819103	0.5708513931