

Supporting Information

On the Nature of Hydrogen Bonds to Platinum(II) – Which Interaction can Predict their Strength?

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Platinum(II) complexes geometries

1. *trans*-[Pt(CH₃)₂(NH₃)₂]

Pt	-0.0001465911	0.0002742934	0.0000000000
N	-0.0005517122	-0.0019466310	2.0820325113
H	-0.8022798596	-0.5284820012	2.4220469262
H	0.8427292801	-0.4425024668	2.4431332241
H	-0.0653817331	0.9458885631	2.4469259503
N	-0.0005517122	-0.0019466310	-2.0820325113
H	0.8427292801	-0.4425024668	-2.4431332241
H	-0.8022798596	-0.5284820012	-2.4220469262
H	-0.0653817331	0.9458885631	-2.4469259503
C	-1.0998815863	1.8433310168	0.0000000000
H	-2.1879713456	1.6748982737	0.0000000000
H	-0.8806949790	2.4770564129	0.8755935313
H	-0.8806949790	2.4770564129	-0.8755935313
C	1.1054484347	-1.8403776599	0.0000000000
H	1.7669708981	-1.9466772710	-0.8758091803
H	1.7669708981	-1.9466772710	0.8758091803
H	0.4426901760	-2.7195978506	0.0000000000

2. *trans*-[Pt(CN)₂(CO)₂]

Pt	0.0000000000	0.0000000000	0.0003002069
O	3.0846755355	0.0000000000	-0.0005023242
C	1.9636346472	0.0000000000	0.0000795076
O	-3.0846755355	0.0000000000	-0.0005023242
C	-1.9636346472	0.0000000000	0.0000795076
N	0.0000000000	3.1942731606	-0.0007937249
C	0.0000000000	2.0371702729	-0.0009224797
N	0.0000000000	-3.1942731606	-0.0007937249
C	0.0000000000	-2.0371702729	-0.0009224797

3. *trans*-[Pt(CN)₂(NH₃)₂]

Pt	0.0020736736	-0.0006868236	0.0000000000
N	-0.0034604847	0.0077268551	2.0890675157
H	-0.9599453777	0.0353866143	2.4369548323
H	0.4625857883	-0.8163696020	2.4636173393
H	0.4728754852	0.8386596054	2.4346041887
N	-0.0034604847	0.0077268551	-2.0890675157
H	0.4625857883	-0.8163696020	-2.4636173393
H	-0.9599453777	0.0353866143	-2.4369548323
H	0.4728754852	0.8386596054	-2.4346041887
N	-1.8001455023	2.6287144918	0.0000000000
C	-1.1413308826	1.6724031671	0.0000000000
N	1.7853968878	-2.6397370481	0.0000000000
C	1.1370391216	-1.6761031045	0.0000000000

4. *trans*-[Pt(CN)₂(PH₃)₂]

Pt	0.0057938730	-0.0088518466	0.0000000000
P	-0.0180519545	0.0262918651	2.3249781833
H	-1.2890604426	-0.0129181281	2.9243337081
H	0.6547557719	-0.9987217551	3.0115548934
H	0.5198432375	1.1772981837	2.9265857249
P	-0.0180519545	0.0262918651	-2.3249781833
H	0.6547557719	-0.9987217551	-3.0115548934
H	-1.2890604426	-0.0129181281	-2.9243337081
H	0.5198432375	1.1772981837	-2.9265857249
N	-1.7095136227	2.6822539321	0.0000000000
C	-1.0865822663	1.7035445040	0.0000000000
N	1.7185301220	-2.6910214946	0.0000000000
C	1.0943429499	-1.7130490027	0.0000000000

5. *trans*-[Pt(OH)₂(NH₃)₂]

Pt	0.0108813259	0.0268264502	0.0000000000
N	-0.0404420238	-0.0153127196	2.0670902764
H	-0.9572904156	0.3184161075	2.3612314599
H	0.1089401380	-0.9796273992	2.3612144872
H	0.6731464328	0.5705066451	2.4929565707
N	-0.0404420238	-0.0153127196	-2.0670902764
H	0.1089401380	-0.9796273992	-2.3612144872
H	-0.9572904156	0.3184161075	-2.3612314599
H	0.6731464328	0.5705066451	-2.4929565707
O	1.1844253030	-1.6509473381	0.0000000000
H	2.1092883893	-1.3930324911	0.0000000000
O	-1.3886858938	1.5213110849	0.0000000000
H	-0.9449726985	2.3727785835	0.0000000000

6. *trans*-[Pt(Br)₂(NH₃)₂]

Pt	-0.4326669792	-0.3431008083	-0.4045881505
Br	-0.4218624711	2.1937386183	-0.1968439556
Br	-0.4434746020	-2.8822498384	-0.5809636070
N	1.6444419980	-0.3423591679	-0.4061836361
H	1.9968535805	-1.2943279351	-0.3064190034
H	1.9907645470	0.0470261001	-1.2811277908
H	1.9989476138	0.2354819873	0.3540982276
N	-2.5097693084	-0.3427273837	-0.4058788991
H	-2.8654866306	-1.0697204860	0.2126223607
H	-2.8620513823	0.5664157842	-0.1069540087
H	-2.8549679930	-0.5347543938	-1.3444302678

7. *trans*-[Pt(Br)₂(PH₃)₂]

Pt	0.0080398815	-0.0121497944	0.0000000000
Br	-1.3131677125	2.1858089739	0.0000000000
Br	1.3179186987	-2.1950022445	0.0000000000
P	-0.0264842246	0.0422253135	2.3166642410
H	-1.3008263106	0.0516395959	2.9136319230
H	0.6096416460	-0.9962987689	3.0222674373
H	0.5414555500	1.1820743833	2.9153428769
P	-0.0264842246	0.0422253135	-2.3166642410
H	0.6096416460	-0.9962987689	-3.0222674373
H	-1.3008263106	0.0516395959	-2.9136319230
H	0.5414555500	1.1820743833	-2.9153428769

8. *trans*-[Pt(Cl)₂(CO)₂]

Pt	0.0001073640	-0.0004390327	0.0000000000
Cl	-1.3469404074	1.9400823446	0.0000000000
Cl	1.3483699532	-1.9400613947	0.0000000000
O	-0.0016754819	0.0021855934	3.0816802374
C	-0.0007218083	0.0006227732	1.9591634833
O	-0.0016754819	0.0021855934	-3.0816802374
C	-0.0007218083	0.0006227732	-1.9591634833

9. *trans*-[Pt(Cl)₂(NH₃)₂]

Pt	-0.4332207532	-0.3436039484	-0.4056241940
Cl	-0.4309660155	2.0105118768	-0.3023591439
Cl	-0.4311850434	-2.6985161314	-0.4741649615
N	1.6416050352	-0.3428253210	-0.4076983423
H	1.9857109704	-1.3027024842	-0.3847551791
H	1.9922072134	0.1207811121	-1.2435285884
H	1.9920569472	0.1655251127	0.4018773987
N	-2.5086620826	-0.3408975667	-0.4030856740
H	-2.8618030885	-1.1333115632	0.1313136814
H	-2.8539457721	0.5320146272	-0.0048830364
H	-2.8569927476	-0.4215074986	-1.3563992852

10. *trans*-[Pt(Cl)₂(PH₃)₂]

Pt	0.0068031130	-0.0103662948	0.0000000000
Cl	-1.1528686839	2.0600957294	0.0000000000
Cl	1.1586730459	-2.0675527624	0.0000000000
P	-0.0205954854	0.0310347316	2.3183897609
H	-1.2905318088	-0.0035139409	2.9240311747
H	0.6482197360	-0.9987909878	3.0061624722
H	0.5165462159	1.1805608044	2.9267836622
P	-0.0205954854	0.0310347316	-2.3183897609
H	0.6482197360	-0.9987909878	-3.0061624722
H	-1.2905318088	-0.0035139409	-2.9240311747
H	0.5165462159	1.1805608044	-2.9267836622

11. *trans*-[Pt(F)₂(NH₃)₂]

Pt	-0.0030624103	0.0038422124	0.0000000000
F	-1.0511951880	1.7159053838	0.0000000000
F	1.0526052872	-1.7076377020	0.0000000000
N	0.0154602529	-0.0245176832	2.0684006730
H	-0.9268389706	-0.1177060449	2.4398803001
H	0.5762980665	-0.8236759983	2.3618877579
H	0.4186531075	0.8324727811	2.4397221581
N	0.0154602529	-0.0245176832	-2.0684006730
H	0.5762980665	-0.8236759983	-2.3618877579
H	-0.9268389706	-0.1177060449	-2.4398803001
H	0.4186531075	0.8324727811	-2.4397221581