

Supporting Information: Halogen Bonding involving I₂ and d⁸ Transition Metal Pincer Complexes

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Comparison of calculated and experimental geometries for complex 1

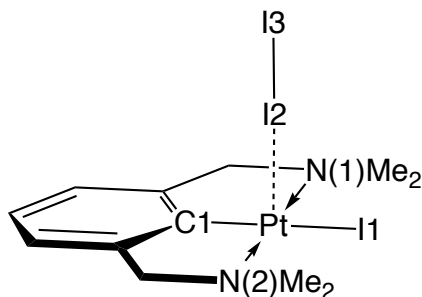


Figure S1: Labeling atoms in complex 1

Table S1: Comparison calculated geometry parameters of 1 with experiment.^a

Parameter	Exp. ^b	Calc. ^c
Pt-I1	2.727	2.707
Pt-I2	2.895	2.887
Pt-N1	2.116	2.099
Pt-N2	2.106	2.099
Pt-C1	1.937	1.933
I2-I3	2.822	2.787
Pt-I2-I3	179.4	175.6
N1-Pt-N2	160.7	161.9
C1-Pt-I1	172.4	170.4

^a Bond length is in Å, and bond angle is in Deg. ^b J. Am. Chem. Soc. 1986, **108**, 5010-5011. ^c PBE0-D3(BJ)/aug-cc-pVTZ/PP(M,I) level of theory.

NBO charges of the (M-I-I) unit of complexes 1 – 20

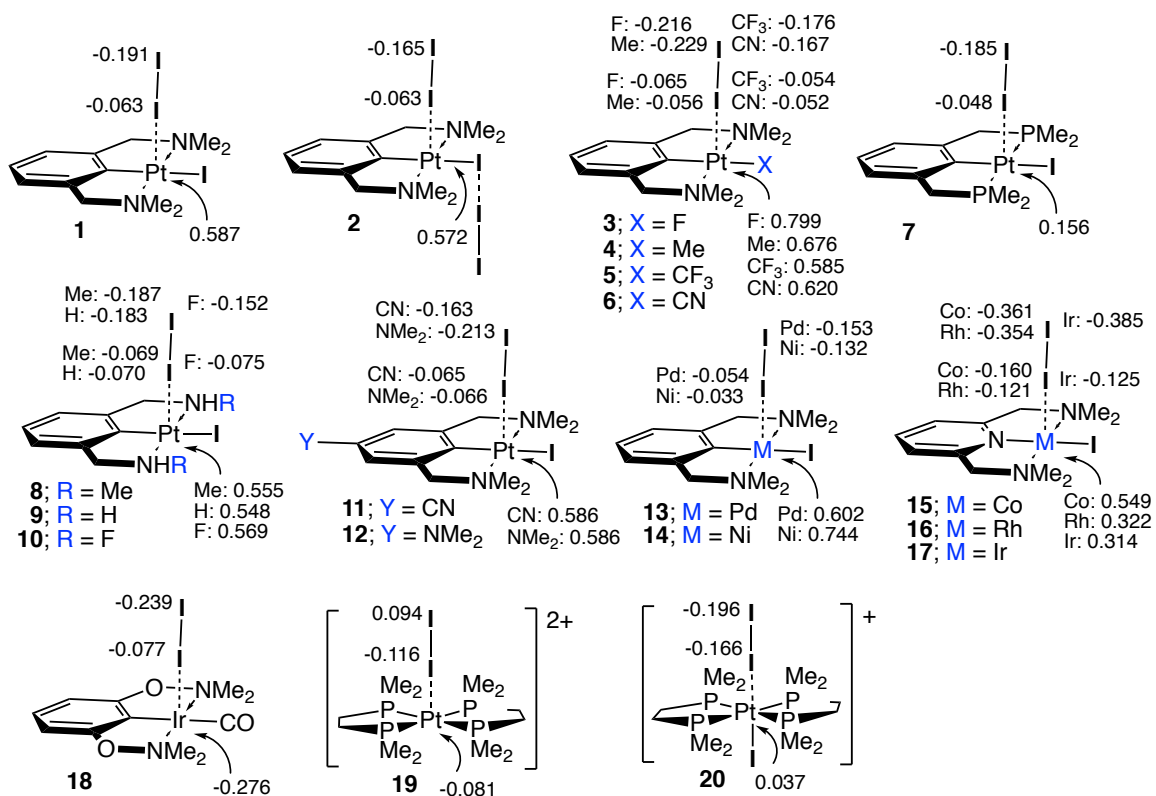


Figure S2: NBO charges of the (M-I-I) unit of complexes 1 – 20. PBE0-D3(BJ)/aug-cc-pVTZ/PP(M,I) level of theory.

Molecular electrostatic potential maps

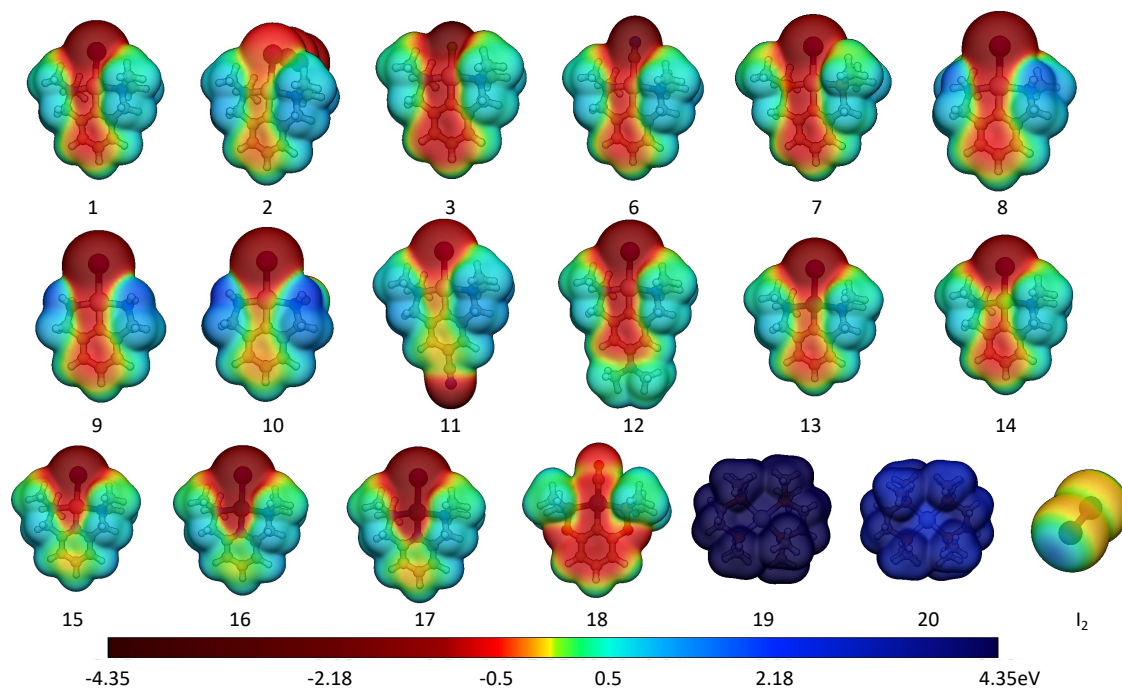


Figure S3: Molecular electrostatic potential of metal-pincer complexes **1** – **20** and I₂ mapped onto the 0.001 a.u electron density surface. Blue and red correspond, respectively, to the positive and negative potential. PBE0-D3(BJ)/aug-cc-pVTZ/PP(M,I) level of theory.

Binding energy ΔE versus sum of local M–I and I–I stretching force constants

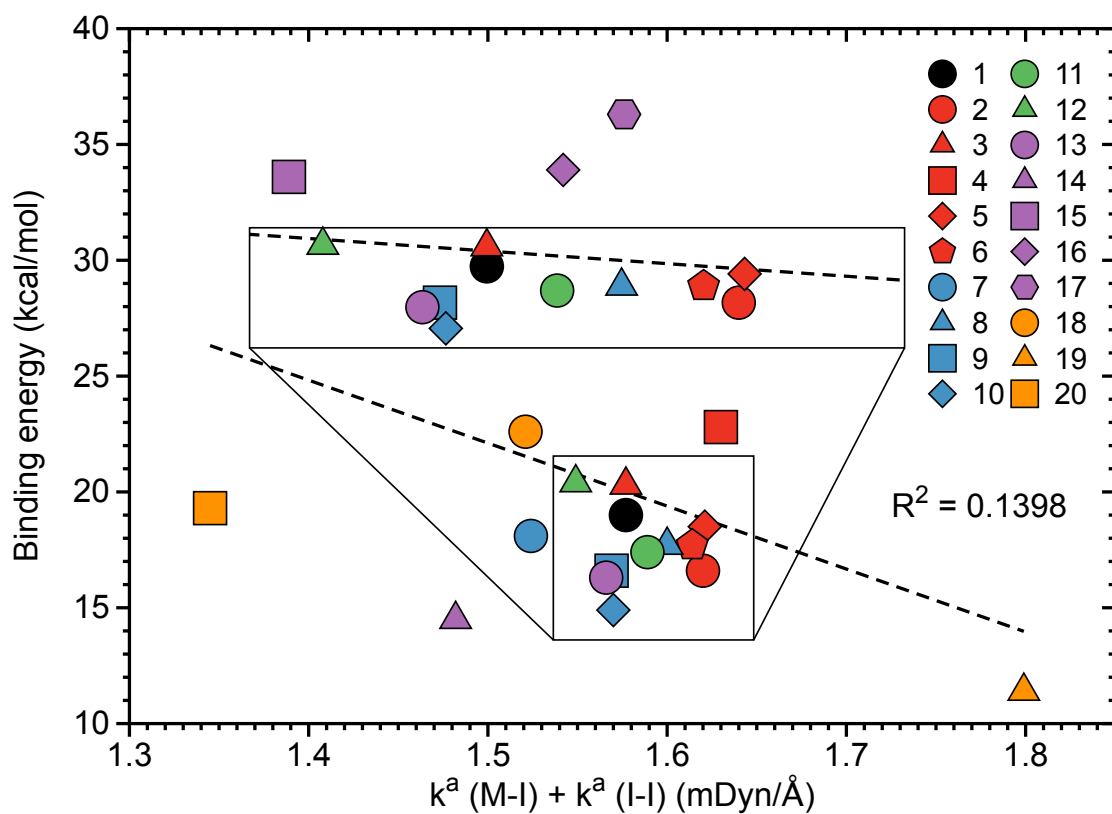


Figure S4: Correlation between binding energy ΔE and the sum of $k^a(\text{M-I}) + k^a(\text{I-I})$ for complexes 1 – 20. PBE0–D3(BJ)/aug–cc–pVTZ/PP(M,I) level of theory.

Charge transfer versus 3c–4e character

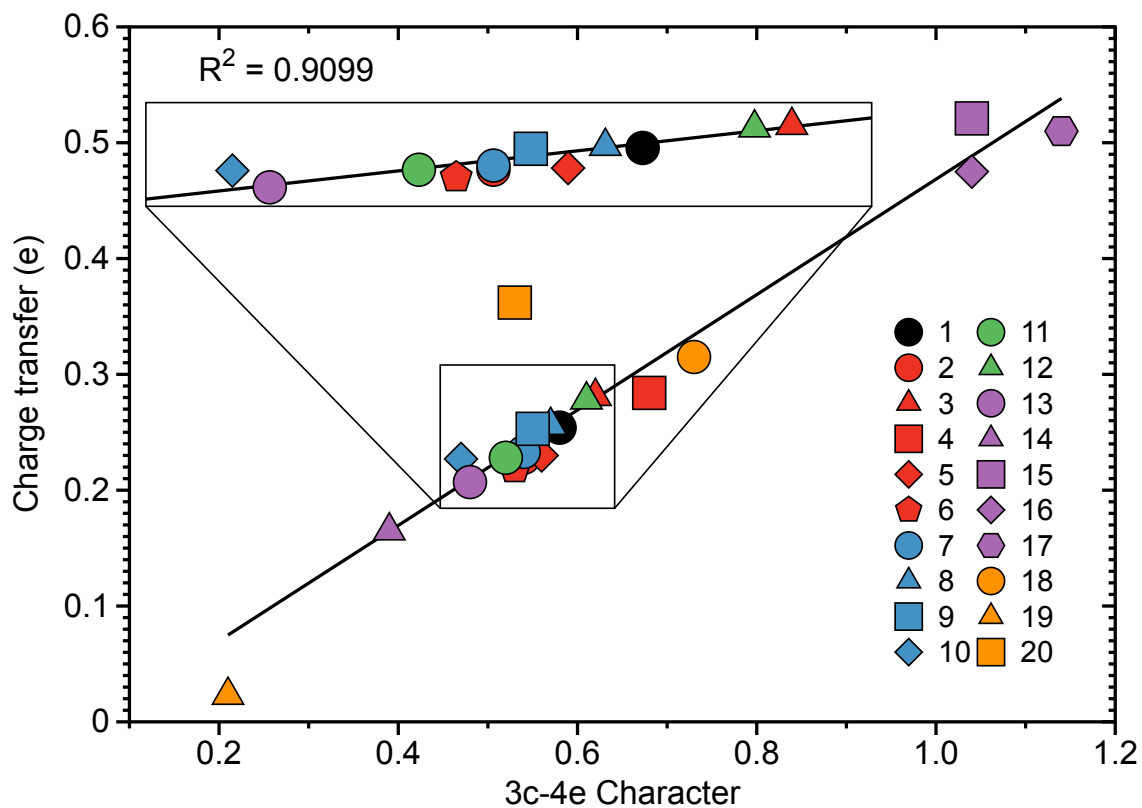


Figure S5: Correlation between charge transfer CT and the 3c–4e bond character of the M–I–I bonds given by $\text{BSO } n(\text{M–I})/\text{BSO } n(\text{I–I})$ for complexes **1** – **20**. PBE0–D3(BJ)/aug–cc–pVTZ/PP(M,I) level of theory.

Coordinates of complexes 1 – 20

PBE0/aug-cc-pVTZ

1

C	-2.625135	-0.779630	1.216740
C	-2.625135	-0.779630	-1.216740
C	-4.010106	-0.692583	-1.215521
H	-4.566972	-0.631546	-2.144027
C	-1.697463	-0.661655	2.384010
H	-1.491093	0.397529	2.557927
H	-2.086908	-1.085799	3.314357
C	-1.697463	-0.661655	-2.384010
H	-2.086908	-1.085799	-3.314357
H	-1.491093	0.397529	-2.557927
Pt	-0.062849	-1.196477	0.000000
I	0.131772	1.683901	0.000000
I	0.534156	4.442196	0.000000
N	-0.374435	-1.306081	-2.073221
N	-0.374435	-1.306081	2.073221
C	-4.690125	-0.666439	0.000000
H	-5.771093	-0.604267	0.000000
C	-1.966667	-0.859961	0.000000
C	-0.466140	-2.748156	-2.382576
H	-0.648443	-2.879528	-3.454255
H	0.467698	-3.231231	-2.101984
H	-1.288299	-3.185945	-1.819068
C	0.669229	-0.704608	-2.920150
H	1.612507	-1.210014	-2.725728
H	0.393229	-0.812423	-3.973981
H	0.771314	0.348902	-2.668944
C	-0.466140	-2.748156	2.382576
H	0.467698	-3.231231	2.101984
H	-0.648443	-2.879528	3.454255
H	-1.288299	-3.185945	1.819068
C	0.669229	-0.704608	2.920150
H	0.393229	-0.812423	3.973981
H	1.612507	-1.210014	2.725728
H	0.771314	0.348902	2.668944
I	2.486629	-2.107366	0.000000
C	-4.010106	-0.692583	1.215521
H	-4.566972	-0.631546	2.144027

2

C	2.847696	-1.113350	1.216444
C	2.847696	-1.113350	-1.216444
C	4.201455	-1.418007	-1.215140
H	4.740358	-1.568197	-2.143858
C	1.914379	-1.096864	2.383515
H	1.554208	-2.114604	2.554744
H	2.363006	-0.737320	3.314151
C	1.914379	-1.096864	-2.383515
H	2.363006	-0.737320	-3.314151
H	1.554208	-2.114604	-2.554744
Pt	0.374736	-0.329091	0.000000
I	-0.293810	-3.150470	0.000000
I	-1.109850	-5.802001	0.000000
N	0.703325	-0.261616	-2.075571
N	0.703325	-0.261616	2.075571
C	4.869031	-1.548683	0.000000
H	5.926959	-1.778884	0.000000
C	2.212395	-0.924506	0.000000
C	1.017204	1.150614	-2.381526
H	0.171362	1.779467	-2.113345
H	1.888711	1.461638	-1.808720
C	-0.409514	-0.697165	-2.935488
H	-1.263864	-0.046416	-2.766299
H	-0.103511	-0.642435	-3.984734
H	-0.682210	-1.719345	-2.681701
C	1.017204	1.150614	2.381526
H	0.171362	1.779467	2.113345
H	1.888711	1.461638	1.808720
C	-0.409514	-0.697165	2.935488
H	-0.103511	-0.642435	3.984734
H	-1.263864	-0.046416	2.766299
H	-0.682210	-1.719345	2.681701
C	4.201455	-1.418007	1.215140
H	4.740358	-1.568197	2.143858
I	-2.128671	0.764386	0.000000
I	-0.924486	3.682415	0.000000
I	0.265531	6.179591	0.000000
H	1.227960	1.251806	-3.450852
H	1.227960	1.251806	3.450852

3

C	-1.854559	-1.674075	1.220061
C	-1.854559	-1.674075	-1.220061
C	-3.204733	-1.994142	-1.217935

H	-3.757331	-2.107104	-2.144378
C	-0.980570	-1.324000	2.390884
H	-1.079836	-0.255189	2.596319
H	-1.222266	-1.867580	3.309357
C	-0.980570	-1.324000	-2.390884
H	-1.222266	-1.867580	-3.309357
H	-1.079836	-0.255189	-2.596319
Pt	0.695099	-1.355311	0.000000
I	0.095497	1.442186	0.000000
I	-0.211891	4.224998	0.000000
N	0.469767	-1.555105	-2.053737
N	0.469767	-1.555105	2.053737
C	-3.862755	-2.161082	0.000000
H	-4.915474	-2.414566	0.000000
C	-1.205924	-1.546824	0.000000
C	0.821469	-2.961231	-2.331869
H	0.755282	-3.152471	-3.408220
H	1.837131	-3.144519	-1.984906
H	0.129356	-3.616414	-1.805413
C	1.343740	-0.679014	-2.847967
H	2.372629	-0.857376	-2.539673
H	1.223891	-0.894138	-3.914677
H	1.088384	0.359202	-2.647550
C	0.821469	-2.961231	2.331869
H	1.837131	-3.144519	1.984906
H	0.755282	-3.152471	3.408220
H	0.129356	-3.616414	1.805413
C	1.343740	-0.679014	2.847967
H	1.223891	-0.894138	3.914677
H	2.372629	-0.857376	2.539673
H	1.088384	0.359202	2.647550
C	-3.204733	-1.994142	1.217935
H	-3.757331	-2.107104	2.144378
F	2.722593	-1.505807	0.000000

4

C	-1.867233	-1.739101	1.213982
C	-1.867233	-1.739101	-1.213982
C	-3.208963	-2.095313	-1.218075
H	-3.760629	-2.217276	-2.144319
C	-1.009267	-1.338934	2.378100
H	-1.130825	-0.266004	2.547892
H	-1.242761	-1.855666	3.314771
C	-1.009267	-1.338934	-2.378100

H	-1.242761	-1.855666	-3.314771
H	-1.130825	-0.266004	-2.547892
Pt	0.734009	-1.335435	0.000000
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N	0.452561	-1.548867	2.064363
C	-3.861439	-2.284000	0.000000
H	-4.906887	-2.566874	0.000000
C	-1.214146	-1.600107	0.000000
C	0.794635	-2.954495	-2.351705
H	1.827722	-3.139404	-2.065512
H	0.135651	-3.607312	-1.781937
C	1.265500	-0.672855	-2.919722
H	2.317440	-0.860981	-2.719117
H	1.048111	-0.872444	-3.974350
H	1.039919	0.365208	-2.685191
C	0.794635	-2.954495	2.351705
H	1.827722	-3.139404	2.065512
H	0.135651	-3.607312	1.781937
C	1.265500	-0.672855	2.919722
H	1.048111	-0.872444	3.974350
H	2.317440	-0.860981	2.719117
H	1.039919	0.365208	2.685191
C	-3.208963	-2.095313	1.218075
H	-3.760629	-2.217276	2.144319
H	0.667446	-3.154872	-3.421240
H	0.667446	-3.154872	3.421240
C	2.865699	-1.232556	0.000000
H	3.331383	-1.709512	0.872845
H	3.331383	-1.709512	-0.872845
H	3.212896	-0.192644	0.000000

5

C	-1.304244	2.311449	1.212752
C	-1.304240	2.311425	-1.212785
C	-1.428474	3.693771	-1.216909
H	-1.452061	4.256045	-2.144127
C	-1.039525	1.407642	2.376742
H	0.039890	1.363040	2.543018
H	-1.510357	1.722135	3.313399
C	-1.039523	1.407591	-2.376755
H	-1.510345	1.722071	-3.313421
H	0.039892	1.362972	-2.543023

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I	1.560319	-0.062967	-0.000005
I	4.338290	-0.012071	-0.000003
N	-1.477855	-0.002297	-2.071913
N	-1.477838	-0.002260	2.071930
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C	-1.282808	1.642331	-0.000009
C	-2.918963	-0.114968	-2.378895
H	-3.268325	-1.109045	-2.113117
H	-3.465071	0.635489	-1.810072
C	-0.726317	-0.927347	-2.937252
H	-1.096215	-1.936955	-2.786140
H	-0.858230	-0.638251	-3.984928
H	0.328376	-0.884699	-2.673757
C	-2.918940	-0.114950	2.378925
H	-3.268285	-1.109042	2.113176
H	-3.465069	0.635480	1.810087
C	-0.726275	-0.927276	2.937286
H	-0.858189	-0.638157	3.984956
H	-1.096153	-1.936894	2.786200
H	0.328416	-0.884612	2.673785
C	-1.428477	3.693796	1.216847
H	-1.452068	4.256089	2.144054
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H	-3.077668	0.056170	3.448919
C	-1.527528	-2.432822	0.000006
F	-0.372846	-3.146532	-0.000124
F	-2.229424	-2.940419	-1.076155
F	-2.229217	-2.940472	1.076274

6

C	-1.985812	-1.584380	1.216772
C	-1.985812	-1.584380	-1.216772
C	-3.351036	-1.833970	-1.217930
H	-3.909281	-1.914128	-2.144266
C	-1.103116	-1.260401	2.384824
H	-1.154848	-0.185086	2.573574
H	-1.371241	-1.776730	3.311593
C	-1.103116	-1.260401	-2.384824
H	-1.371241	-1.776730	-3.311593
H	-1.154848	-0.185086	-2.573574
Pt	0.616780	-1.375866	0.000000
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N	0.338341	-1.563261	2.062712
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H	-5.079835	-2.169415	0.000000
C	-1.327387	-1.495943	0.000000
C	0.604381	-2.986126	-2.358384
H	1.623776	-3.228354	-2.064941
H	-0.095345	-3.606913	-1.801688
C	1.222409	-0.731546	-2.896060
H	2.255881	-0.990387	-2.676369
H	1.007805	-0.908385	-3.954790
H	1.059841	0.316731	-2.655178
C	0.604381	-2.986126	2.358384
H	1.623776	-3.228354	2.064941
H	-0.095345	-3.606913	1.801688
C	1.222409	-0.731546	2.896060
H	1.007805	-0.908385	3.954790
H	2.255881	-0.990387	2.676369
H	1.059841	0.316731	2.655178
C	-3.351036	-1.833970	1.217930
H	-3.909281	-1.914128	2.144266
H	0.476577	-3.166609	-3.430798
H	0.476577	-3.166609	3.430798
C	2.658743	-1.481590	0.000000
N	3.806517	-1.645257	0.000000

7

C	-2.715817	-0.692361	1.210905
C	-2.715817	-0.692361	-1.210905
C	-4.103893	-0.626673	-1.199136
H	-4.646697	-0.574675	-2.136510
C	-1.960086	-0.585115	2.507887
H	-1.851461	0.471388	2.776288
H	-2.467215	-1.080816	3.338406
C	-1.960086	-0.585115	-2.507887
H	-2.467215	-1.080816	-3.338406
H	-1.851461	0.471388	-2.776288
Pt	-0.019357	-1.160434	0.000000
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I	0.582228	4.493851	0.000000
P	-0.265084	-1.237926	-2.261580
P	-0.265084	-1.237926	2.261580
C	-4.798204	-0.612482	0.000000

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C	-2.004579	-0.784347	0.000000
C	-0.262514	-2.931746	-2.916745
H	-0.467666	-2.935936	-3.988475
H	0.714596	-3.374376	-2.720993
H	-1.020699	-3.515146	-2.394782
C	0.853557	-0.308879	-3.340332
H	1.859358	-0.710149	-3.211526
H	0.550807	-0.390404	-4.385267
H	0.854323	0.736151	-3.030869
C	-0.262514	-2.931746	2.916745
H	0.714596	-3.374376	2.720993
H	-0.467666	-2.935936	3.988475
H	-1.020699	-3.515146	2.394782
C	0.853557	-0.308879	3.340332
H	0.550807	-0.390404	4.385267
H	1.859358	-0.710149	3.211526
H	0.854323	0.736151	3.030869
I	2.488571	-2.079415	0.000000
C	-4.103893	-0.626673	1.199136
H	-4.646697	-0.574675	2.136510

8

C	-2.589027	-0.977511	1.218522
C	-2.589027	-0.977511	-1.218522
C	-3.975476	-0.916305	-1.216446
H	-4.535814	-0.862199	-2.143377
C	-1.669323	-0.830532	2.394005
H	-1.559953	0.233202	2.621368
H	-2.024372	-1.332112	3.297309
C	-1.669323	-0.830532	-2.394005
H	-2.024372	-1.332112	-3.297309
H	-1.559953	0.233202	-2.621368
Pt	-0.016603	-1.280632	0.000000
I	0.144249	1.607007	0.000000
I	0.371648	4.380284	0.000000
N	-0.295486	-1.342431	-2.050372
N	-0.295486	-1.342431	2.050372
C	-4.654654	-0.905783	0.000000
H	-5.736650	-0.865016	0.000000
C	-1.931645	-1.050347	0.000000
C	-0.082671	-2.707709	-2.565464
H	-0.206803	-2.726208	-3.651290
H	0.919377	-3.034225	-2.294625

H	-0.813946	-3.372418	-2.108489
H	0.390698	-0.732638	-2.483886
C	-0.082671	-2.707709	2.565464
H	0.919377	-3.034225	2.294625
H	-0.206803	-2.726208	3.651290
H	-0.813946	-3.372418	2.108489
H	0.390698	-0.732638	2.483886
I	2.618931	-1.834027	0.000000
C	-3.975476	-0.916305	1.216446
H	-4.535814	-0.862199	2.143377

9

C	1.060517	2.603636	-1.218982
C	1.060469	2.603625	1.219053
C	0.974210	3.988690	1.215719
H	0.926644	4.549545	2.142750
C	1.014817	1.704265	-2.419755
H	-0.007764	1.652173	-2.800221
H	1.652359	2.049036	-3.236195
C	1.014728	1.704246	2.419818
H	1.652266	2.048999	3.236270
H	-0.007858	1.652175	2.800270
Pt	1.400168	0.034683	0.000030
I	-1.499506	-0.144747	-0.000033
I	-4.257686	-0.487337	-0.000093
N	1.410381	0.301083	2.035951
N	1.410489	0.301108	-2.035887
C	0.940406	4.667066	0.000042
H	0.876807	5.747896	0.000045
C	1.121772	1.943679	0.000034
H	2.348729	0.090829	2.360197
H	0.798186	-0.374046	2.482919
H	2.348864	0.090891	-2.360077
H	0.798344	-0.374033	-2.482905
I	2.167766	-2.534464	0.000034
C	0.974258	3.988701	-1.215640
H	0.926729	4.549564	-2.142668

10

C	0.962803	2.579278	-1.216944
C	0.962747	2.579275	1.216952
C	0.832315	3.960127	1.217125
H	0.750200	4.517759	2.143252

C	0.854815	1.650076	-2.389428
H	-0.199740	1.483359	-2.633194
H	1.373738	1.968643	-3.294034
C	0.854704	1.650073	2.389430
H	1.373601	1.968632	3.294054
H	-0.199861	1.483371	2.633160
Pt	1.340241	0.008117	0.000008
I	-1.609005	-0.195739	-0.000020
I	-4.367655	-0.341858	-0.000014
N	1.377694	0.298061	2.010132
N	1.377808	0.298073	-2.010110
C	0.789708	4.637011	0.000002
H	0.696973	5.715529	0.000001
C	1.068017	1.926626	0.000006
F	2.700557	0.227837	2.475552
H	0.920620	-0.434206	2.552527
F	2.700703	0.227881	-2.475447
H	0.920785	-0.434201	-2.552541
I	1.792318	-2.619945	-0.000001
C	0.832371	3.960129	-1.217120
H	0.750299	4.517763	-2.143251

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C	1.086190	2.259594	-1.218484
C	1.086157	2.259499	1.218690
C	1.193603	3.637790	1.223701
H	1.213525	4.206809	2.145326
C	0.842814	1.356587	-2.385790
H	-0.235169	1.298453	-2.556180
H	1.314062	1.686413	-3.316021
C	0.842748	1.356401	2.385919
H	1.313971	1.686155	3.316189
H	-0.235240	1.298254	2.556274
Pt	1.152674	-0.332117	0.000003
I	-1.753428	-0.125955	-0.000029
I	-4.526911	-0.122549	-0.000067
N	1.301278	-0.040937	2.074012
N	1.301335	-0.040776	-2.073980
C	1.265816	4.317317	0.000185
C	1.076868	1.594864	0.000077
C	2.741833	-0.148693	2.388246
H	2.893738	0.014685	3.460031
H	3.091618	-1.140668	2.109773
H	3.292144	0.603588	1.825746

C	0.559015	-0.992126	2.919561
H	0.931417	-1.995663	2.727377
H	0.700199	-0.732515	3.973399
H	-0.497659	-0.949388	2.664642
C	2.741899	-0.148507	-2.388181
H	3.091676	-1.140504	-2.109776
H	2.893834	0.014954	-3.459950
H	3.292195	0.603731	-1.825609
C	0.559096	-0.991899	-2.919623
H	0.700309	-0.732206	-3.973437
H	0.931493	-1.995450	-2.727507
H	-0.497585	-0.949181	-2.664730
I	1.683197	-2.976702	-0.000092
C	1.193637	3.637885	-1.223385
H	1.213584	4.206976	-2.144966
C	1.399029	5.736066	0.000242
N	1.511626	6.882849	0.000289

12

C	-0.271855	2.293115	1.207049
C	-0.271855	2.293115	-1.207049
C	0.131705	3.616700	-1.216531
H	0.328411	4.112611	-2.156938
C	-0.351429	1.364664	2.377992
H	0.640382	0.938641	2.549140
H	-0.681105	1.836809	3.308541
C	-0.351429	1.364664	-2.377992
H	-0.681105	1.836809	-3.308541
H	0.640382	0.938641	-2.549140
Pt	-1.230625	-0.129289	0.000000
I	1.536458	-0.900814	0.000000
I	4.162709	-1.870861	0.000000
N	-1.264063	0.207606	-2.073020
N	-1.264063	0.207606	2.073020
C	0.309087	4.309932	0.000000
C	-0.509524	1.662002	0.000000
C	-2.652478	0.604043	-2.385691
H	-2.739964	0.810619	-3.457608
H	-3.323611	-0.206080	-2.107010
H	-2.906231	1.499735	-1.821464
C	-0.895641	-0.938240	-2.920813
H	-1.589988	-1.753162	-2.728389
H	-0.940185	-0.644701	-3.974639
H	0.111611	-1.261831	-2.667505

C	-2.652478	0.604043	2.385691
H	-3.323611	-0.206080	2.107010
H	-2.739964	0.810619	3.457608
H	-2.906231	1.499735	1.821464
C	-0.895641	-0.938240	2.920813
H	-0.940185	-0.644701	3.974639
H	-1.589988	-1.753162	2.728389
H	0.111611	-1.261831	2.667505
I	-2.661318	-2.433548	0.000000
C	0.131705	3.616700	1.216531
H	0.328411	4.112611	2.156938
N	0.659996	5.643122	0.000000
C	1.072510	6.260669	-1.232841
H	1.296088	7.309141	-1.047256
H	1.965433	5.790129	-1.667523
H	0.273417	6.223112	-1.977695
C	1.072510	6.260669	1.232841
H	1.965433	5.790129	1.667523
H	1.296088	7.309141	1.047256
H	0.273417	6.223112	1.977695

13

C	-2.614075	-0.889872	1.216522
C	-2.614075	-0.889872	-1.216522
C	-4.000880	-0.819101	-1.213799
H	-4.556330	-0.771069	-2.143879
C	-1.702228	-0.785014	2.394332
H	-1.497300	0.272169	2.582833
H	-2.109617	-1.214857	3.315759
C	-1.702228	-0.785014	-2.394332
H	-2.109617	-1.214857	-3.315759
H	-1.497300	0.272169	-2.582833
I	0.068393	1.578813	0.000000
I	0.568630	4.299932	0.000000
N	-0.391044	-1.430636	-2.084586
N	-0.391044	-1.430636	2.084586
C	-4.681698	-0.797233	0.000000
H	-5.763389	-0.747678	0.000000
C	-1.954881	-0.956458	0.000000
C	-0.492459	-2.877609	-2.347456
H	-0.681473	-3.045223	-3.414118
H	0.439585	-3.358830	-2.056950
H	-1.314342	-3.295288	-1.767922
C	0.657474	-0.858343	-2.939355

H	1.597504	-1.364850	-2.731599
H	0.386790	-0.985865	-3.993599
H	0.768530	0.200450	-2.713602
C	-0.492459	-2.877609	2.347456
H	0.439585	-3.358830	2.056950
H	-0.681473	-3.045223	3.414118
H	-1.314342	-3.295288	1.767922
C	0.657474	-0.858343	2.939355
H	0.386790	-0.985865	3.993599
H	1.597504	-1.364850	2.731599
H	0.768530	0.200450	2.713602
I	2.484393	-2.235583	0.000000
C	-4.000880	-0.819101	1.213799
H	-4.556330	-0.771069	2.143879
Pd	-0.056918	-1.302235	0.000000

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C	-2.496571	-1.144207	1.208854
C	-2.496571	-1.144207	-1.208854
C	-3.883125	-1.190795	-1.213076
H	-4.437924	-1.197682	-2.144779
C	-1.581053	-1.005290	2.373730
H	-1.456488	0.055462	2.607051
H	-1.924545	-1.507583	3.284249
C	-1.581053	-1.005290	-2.373730
H	-1.924545	-1.507583	-3.284249
H	-1.456488	0.055462	-2.607051
I	-0.214819	1.463315	0.000000
I	0.457696	4.136518	0.000000
N	-0.241851	-1.533197	-1.985174
N	-0.241851	-1.533197	1.985174
C	-4.564897	-1.221436	0.000000
H	-5.647161	-1.262012	0.000000
C	-1.819688	-1.148658	0.000000
C	-0.239972	-2.994183	-2.193560
H	-0.398543	-3.215216	-3.254992
H	0.716501	-3.400122	-1.871087
H	-1.042512	-3.444809	-1.611160
C	0.771309	-0.923772	-2.859533
H	1.739203	-1.375522	-2.660714
H	0.492288	-1.080581	-3.907459
H	0.830231	0.143204	-2.652091
C	-0.239972	-2.994183	2.193560
H	0.716501	-3.400122	1.871087

H	-0.398543	-3.215216	3.254992
H	-1.042512	-3.444809	1.611160
C	0.771309	-0.923772	2.859533
H	0.492288	-1.080581	3.907459
H	1.739203	-1.375522	2.660714
H	0.830231	0.143204	2.652091
I	2.531848	-1.981615	0.000000
C	-3.883125	-1.190795	1.213076
H	-4.437924	-1.197682	2.144779
Ni	0.014167	-1.345486	0.000000

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C	-2.544319	-0.970896	1.164430
C	-2.544319	-0.970896	-1.164430
C	-3.922968	-0.887147	-1.201310
H	-4.441120	-0.829970	-2.149223
C	-1.610378	-0.855651	2.319740
H	-1.406315	0.211149	2.455682
H	-2.037045	-1.244723	3.250078
C	-1.610378	-0.855651	-2.319740
H	-2.037045	-1.244723	-3.250078
H	-1.406315	0.211149	-2.455682
I	0.254499	1.290316	0.000000
I	0.392045	4.228910	0.000000
N	-0.327121	-1.511341	-2.005371
N	-0.327121	-1.511341	2.005371
C	-4.616968	-0.860593	0.000000
H	-5.697795	-0.799844	0.000000
C	-0.461478	-2.961822	-2.218525
H	-0.711729	-3.169898	-3.265631
H	0.478651	-3.444446	-1.959502
H	-1.252165	-3.360270	-1.581300
C	0.702686	-0.985112	-2.913548
H	1.638044	-1.505550	-2.725138
H	0.395165	-1.133755	-3.955113
H	0.845591	0.075325	-2.714512
C	-0.461478	-2.961822	2.218525
H	0.478651	-3.444446	1.959502
H	-0.711729	-3.169898	3.265631
H	-1.252165	-3.360270	1.581300
C	0.702686	-0.985112	2.913548
H	0.395165	-1.133755	3.955113
H	1.638044	-1.505550	2.725138
H	0.845591	0.075325	2.714512

I	2.367984	-2.138436	0.000000
C	-3.922968	-0.887147	1.201310
H	-4.441120	-0.829970	2.149223
Co	-0.055252	-1.331682	0.000000
N	-1.897073	-1.053206	0.000000

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C	-2.601925	-0.880344	1.172653
C	-2.601925	-0.880344	-1.172653
C	-3.981718	-0.813035	-1.203735
H	-4.505065	-0.760687	-2.149204
C	-1.667366	-0.742415	2.333597
H	-1.453593	0.326274	2.432642
H	-2.113096	-1.090565	3.271028
C	-1.667366	-0.742415	-2.333597
H	-2.113096	-1.090565	-3.271028
H	-1.453593	0.326274	-2.432642
I	0.247409	1.427085	0.000000
I	0.450049	4.334524	0.000000
N	-0.370325	-1.418515	-2.086753
N	-0.370325	-1.418515	2.086753
C	-4.674464	-0.796059	0.000000
H	-5.755748	-0.748655	0.000000
C	-0.500735	-2.854739	-2.379835
H	-0.748105	-3.004470	-3.438064
H	0.441168	-3.347347	-2.146282
H	-1.289819	-3.286978	-1.764303
C	0.652733	-0.837665	-2.969000
H	1.593303	-1.355287	-2.794610
H	0.353836	-0.946317	-4.018150
H	0.780746	0.214628	-2.723201
C	-0.500735	-2.854739	2.379835
H	0.441168	-3.347347	2.146282
H	-0.748105	-3.004470	3.438064
H	-1.289819	-3.286978	1.764303
C	0.652733	-0.837665	2.969000
H	0.353836	-0.946317	4.018150
H	1.593303	-1.355287	2.794610
H	0.780746	0.214628	2.723201
I	2.436608	-2.167421	0.000000
C	-3.981718	-0.813035	1.203735
H	-4.505065	-0.760687	2.149204
N	-1.963562	-0.957187	0.000000
Rh	-0.051202	-1.297057	0.000000

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C	-2.596168	-0.740168	1.175361
C	-2.596168	-0.740168	-1.175361
C	-3.973512	-0.660727	-1.202995
H	-4.495199	-0.597555	-2.148814
C	-1.656594	-0.596190	2.331424
H	-1.430001	0.470814	2.416638
H	-2.097868	-0.932341	3.274034
C	-1.656594	-0.596190	-2.331424
H	-2.097868	-0.932341	-3.274034
H	-1.430001	0.470814	-2.416638
I	0.238075	1.560044	0.000000
I	0.491535	4.483451	0.000000
N	-0.359607	-1.287019	-2.086399
N	-0.359607	-1.287019	2.086399
C	-4.668873	-0.641206	0.000000
H	-5.749337	-0.584234	0.000000
C	-0.497649	-2.714646	-2.429819
H	-0.731842	-2.824037	-3.494994
H	0.437642	-3.221281	-2.200600
H	-1.297614	-3.157736	-1.837115
C	0.671167	-0.687841	-2.952782
H	1.607303	-1.216425	-2.788205
H	0.373325	-0.769694	-4.003773
H	0.802335	0.356806	-2.678594
C	-0.497649	-2.714646	2.429819
H	0.437642	-3.221281	2.200600
H	-0.731842	-2.824037	3.494994
H	-1.297614	-3.157736	1.837115
C	0.671167	-0.687841	2.952782
H	0.373325	-0.769694	4.003773
H	1.607303	-1.216425	2.788205
H	0.802335	0.356806	2.678594
I	2.416614	-2.116067	0.000000
C	-3.973512	-0.660727	1.202995
H	-4.495199	-0.597555	2.148814
N	-1.953648	-0.833701	0.000000
Ir	-0.051693	-1.185588	0.000000

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C	-1.951955	-1.911336	1.189271
C	-1.951955	-1.911336	-1.189271
C	-3.297829	-2.231376	-1.213160

H	-3.815852	-2.348461	-2.155273
I	0.168097	1.569392	0.000000
I	-0.456525	4.331020	0.000000
C	-3.956107	-2.386569	0.000000
H	-5.010832	-2.632179	0.000000
C	1.061917	-2.853222	-3.095961
H	0.629310	-2.955459	-4.091977
H	2.139703	-2.704622	-3.174896
H	0.872484	-3.756184	-2.517105
C	0.546698	-0.063568	-3.393218
H	1.612844	0.140211	-3.502360
H	0.116210	-0.323308	-4.360874
H	0.061983	0.823389	-2.987544
C	1.061917	-2.853222	3.095961
H	2.139703	-2.704622	3.174896
H	0.629310	-2.955459	4.091977
H	0.872484	-3.756184	2.517105
C	0.546698	-0.063568	3.393218
H	0.116210	-0.323308	4.360874
H	1.612844	0.140211	3.502360
H	0.061983	0.823389	2.987544
C	-3.297829	-2.231376	1.213160
H	-3.815852	-2.348461	2.155273
Ir	0.742414	-1.253503	0.000000
O	-1.285900	-1.742064	-2.379929
O	-1.285900	-1.742064	2.379929
P	0.332084	-1.432817	2.238547
P	0.332084	-1.432817	-2.238547
C	2.596155	-0.892003	0.000000
O	3.724883	-0.700512	0.000000
C	-1.239190	-1.745655	0.000000

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C	-2.528670	2.165621	0.941098
H	-2.581517	2.028454	-0.142310
H	-2.988390	3.128611	1.173643
C	-3.207069	1.024798	1.677933
H	-3.238020	1.212978	2.753763
H	-4.238171	0.885886	1.346657
C	3.207069	-1.024798	1.677933
H	3.238020	-1.212978	2.753763
H	4.238171	-0.885886	1.346657
C	2.528670	-2.165621	0.941098
H	2.581517	-2.028454	-0.142310

H	2.988390	-3.128611	1.173643
Pt	0.000000	0.000000	1.344093
I	0.000000	0.000000	-1.862620
I	0.000000	0.000000	-4.552344
P	-0.756243	2.204209	1.397443
P	-2.277448	-0.536449	1.408091
P	0.756243	-2.204209	1.397443
P	2.277448	0.536449	1.408091
C	2.804965	1.639348	2.748703
H	3.894599	1.636948	2.812501
H	2.477457	2.659324	2.548495
H	2.390148	1.309112	3.700499
C	3.011399	1.240857	-0.093338
H	2.495304	2.152271	-0.388215
H	4.061330	1.465914	0.102097
H	2.936997	0.529484	-0.914314
C	0.000000	3.445947	0.318930
H	-0.589335	4.363845	0.353724
H	1.011546	3.673982	0.653906
H	0.032279	3.075322	-0.705541
C	-0.720179	2.918474	3.067277
H	0.307634	3.032462	3.407603
H	-1.200086	3.898648	3.057552
H	-1.241883	2.269905	3.770224
C	-3.011399	-1.240857	-0.093338
H	-2.495304	-2.152271	-0.388215
H	-4.061330	-1.465914	0.102097
H	-2.936997	-0.529484	-0.914314
C	0.000000	-3.445947	0.318930
H	0.589335	-4.363845	0.353724
H	-1.011546	-3.673982	0.653906
H	-0.032279	-3.075322	-0.705541
C	-2.804965	-1.639348	2.748703
H	-3.894599	-1.636948	2.812501
H	-2.477457	-2.659324	2.548495
H	-2.390148	-1.309112	3.700499
C	0.720179	-2.918474	3.067277
H	-0.307634	-3.032462	3.407603
H	1.200086	-3.898648	3.057552
H	1.241883	-2.269905	3.770224

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C	-2.505444	2.183297	0.355472
H	-2.624444	2.019655	-0.718607

H	-2.942955	3.154727	0.594647
C	-3.144447	1.063619	1.158826
H	-3.044589	1.238157	2.233078
H	-4.207009	0.956425	0.931512
C	3.144447	-1.063619	1.158826
H	3.044589	-1.238157	2.233078
H	4.207009	-0.956425	0.931512
C	2.505444	-2.183297	0.355472
H	2.624444	-2.019655	-0.718607
H	2.942955	-3.154727	0.594647
I	0.000000	0.000000	3.719944
Pt	0.000000	0.000000	0.812121
I	0.000000	0.000000	-2.203571
I	0.000000	0.000000	-5.016646
P	-0.706479	2.228038	0.706247
P	-2.281796	-0.509336	0.788702
P	0.706479	-2.228038	0.706247
P	2.281796	0.509336	0.788702
C	2.884433	1.699832	2.014580
H	3.973250	1.650116	2.063568
H	2.598859	2.708690	1.715588
H	2.450519	1.471588	2.987506
C	3.057418	1.074337	-0.754396
H	2.572115	1.978131	-1.118208
H	4.111256	1.280905	-0.560002
H	2.964346	0.316986	-1.529877
C	0.000000	3.339124	-0.542296
H	-0.577431	4.264645	-0.566641
H	1.027975	3.583084	-0.273366
H	-0.014075	2.867711	-1.523261
C	-0.585378	3.200299	2.232813
H	0.450404	3.258384	2.562082
H	-0.967578	4.204911	2.043906
H	-1.150344	2.718738	3.028333
C	-3.057418	-1.074337	-0.754396
H	-2.572115	-1.978131	-1.118208
H	-4.111256	-1.280905	-0.560002
H	-2.964346	-0.316986	-1.529877
C	0.000000	-3.339124	-0.542296
H	0.577431	-4.264645	-0.566641
H	-1.027975	-3.583084	-0.273366
H	0.014075	-2.867711	-1.523261
C	-2.884433	-1.699832	2.014580
H	-3.973250	-1.650116	2.063568
H	-2.598859	-2.708690	1.715588

H	-2.450519	-1.471588	2.987506
C	0.585378	-3.200299	2.232813
H	-0.450404	-3.258384	2.562082
H	0.967578	-4.204911	2.043906
H	1.150344	-2.718738	3.028333