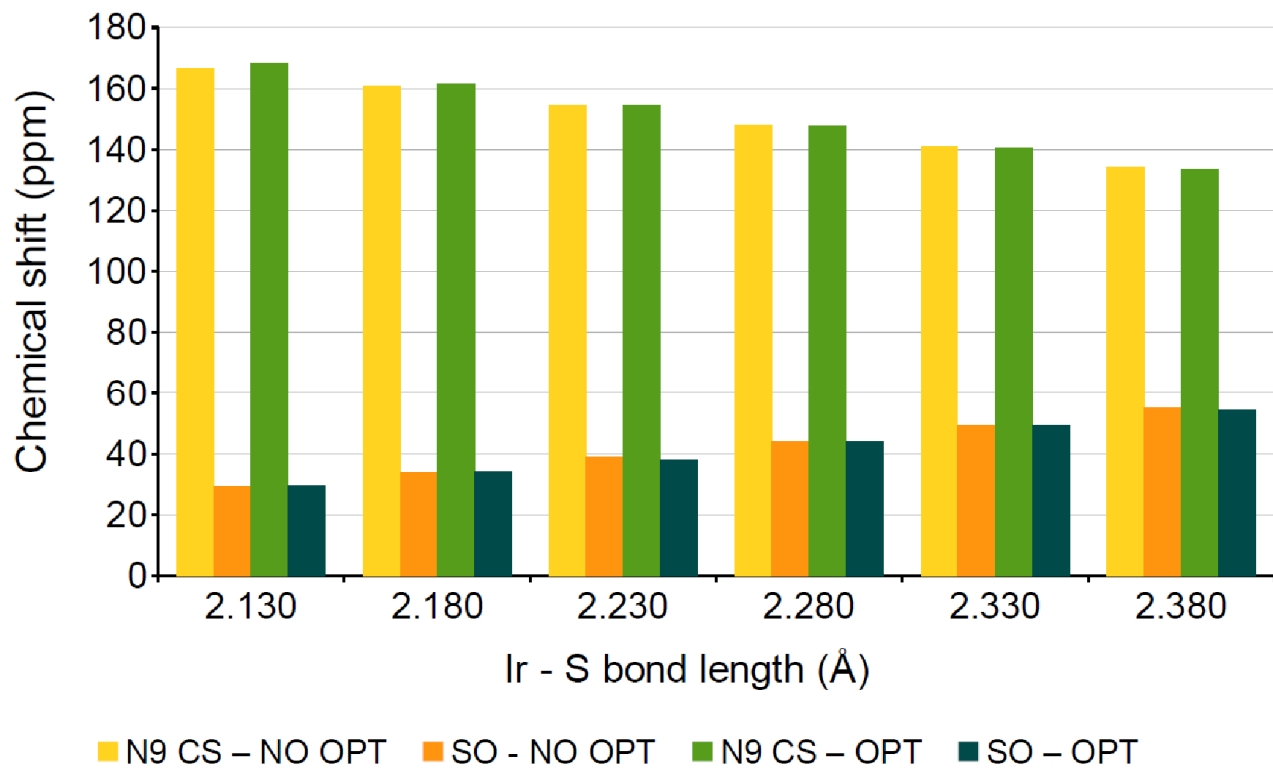


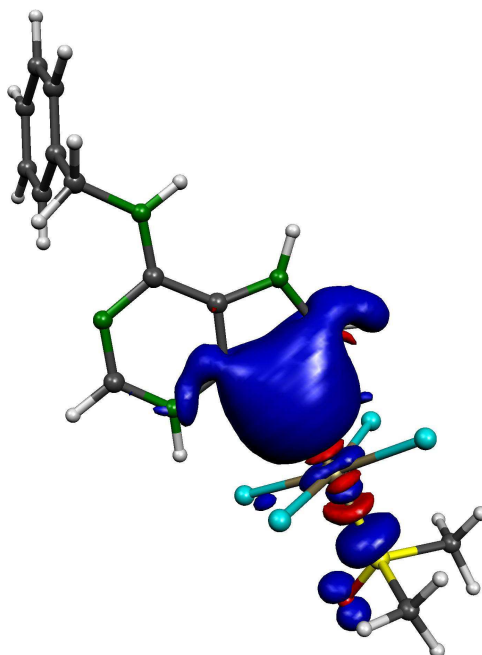
## SUPPORTING INFORMATION

A relativistic DFT methodology for calculating the  
structures and NMR chemical shifts of octahedral  
platinum and iridium complexes

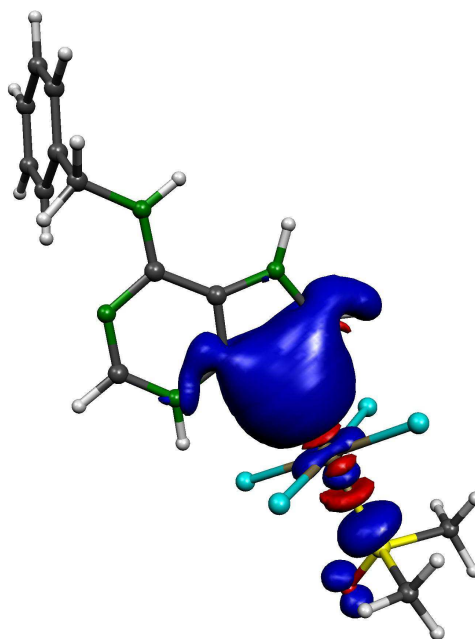
*Jan Vicha, Michael Patzschke, Radek Marek*



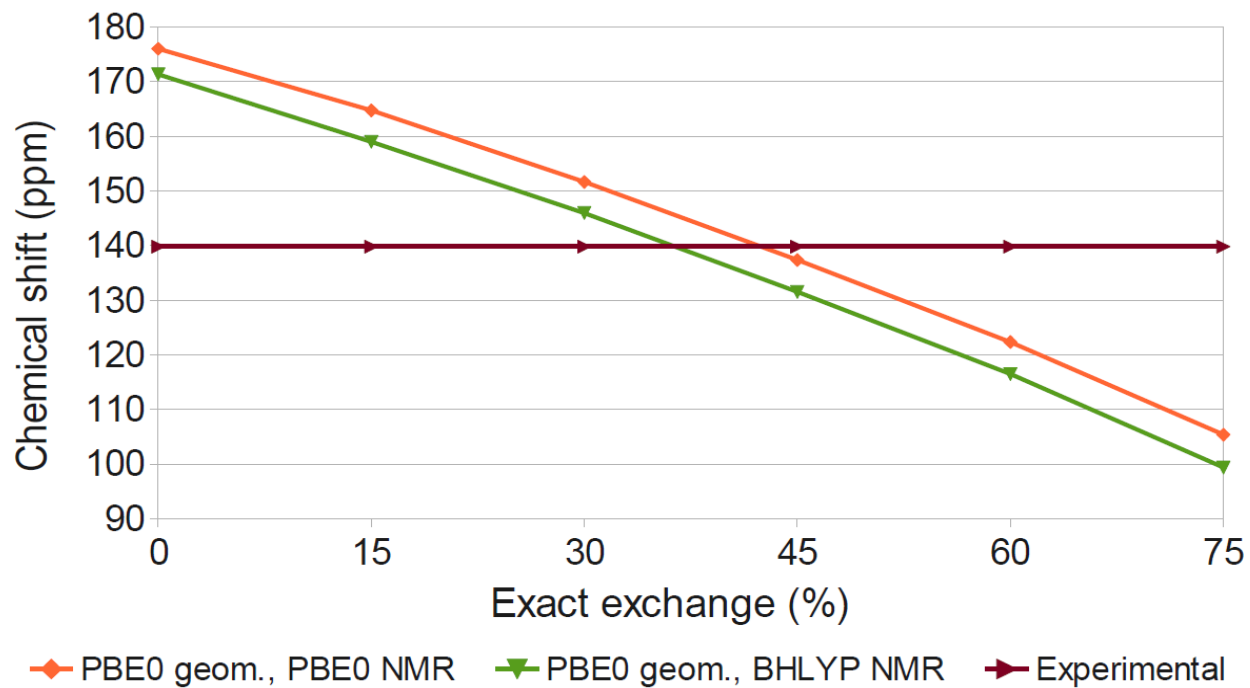
**Figure S1:** The  $^{15}\text{N}$  NMR chemical shift (CS) and spin-orbit (SO) contribution to the chemical shift for IrBAP calculated as a function of Ir-S distance using flexible and rigid geometries.



**Figure S2:** Visualization of the spin density induced by the FC perturbation on N9 atom for IrBAP with Ir-S bond length 2.13Å re-optimized using PBE0/TZVPP/COSMO.



**Figure S3:** Visualization of the spin density induced by the FC perturbation on N9 atom for IrBAP with Ir-S bond length 2.38Å re-optimized using PBE0/TZVPP/COSMO.



**Figure S4:** The  $^{15}\text{N}$  NMR chemical shift of the N9 atom of PtKIN calculated using the BHandHLYP and PBE0 functionals (TZP/COSMO) with various amounts of exact-exchange admixture. The PBE0 geometry, optimized with the COSMO solvent model, was used.

**Table S1:** Experimental NMR chemical shifts for PtKIN and IrBAP at 303K; different pH.

Atom	PtKIN		Atom	IrBAP	
	DMF	0.1M HCl		DMSO	0.1M HCl
H2	8.8	8.9	H2	8.8	8.8
H8	8.6	9.1	H8	8.9	9.0
H10	9.8	10.9	H10	9.8	10.6
H11	5.0	5.0	H11	4.9	4.9
H13	6.4	6.4	H13.17	7.4	7.4
H14	6.5	6.6	H14.16	7.4	7.4
H15	7.7	7.7	H15	7.3	7.3
			H18.19	3.5	3.4
C2	146.0	147.2	C2	146.4	146.9
C4	143.8	142.7	C4	144.7	144.5
C5	117.9	114.3	C5	111.8	111.0
C6	155.0	153.8	C6	152.3	152.6
C8	148.5	146.2	C8	148.1	147.1
C11	38.5	38.0	C11	44.3	44.3
C12	151.6	150.6	C12	136.4	136.4
C13	108.7	108.5	C13.17	127.6	127.6
C14	111.2	110.9	C14.16	128.4	128.5
C15	143.4	143.1	C15	127.5	127.5
			C18.19	40.6	40.8
N1	226.6	228.1	N1	227.2	227.6
N3	153.8	153.4	N3	154.5	154.2
N7	211.2	185.3	N7	-	162.7
N9	139.8	144.0	N9	150.3	150.9
N10	105.5	114.7	N10	114.2	118.7

**Table S2a:** Geometrical parameters and RMSDs for PtBAP cluster.

	Experimental	BLYP	B3LYP	BHLYP	BP86	TPSS	PBE	PBE0
Bond	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)
N1 C2	1.307	1.322	1.311	1.301	1.320	1.319	1.319	1.309
N1 C6	1.356	1.366	1.354	1.343	1.362	1.361	1.360	1.349
N3 C2	1.343	1.360	1.347	1.334	1.356	1.355	1.355	1.341
N3 C4	1.349	1.363	1.355	1.346	1.360	1.358	1.359	1.350
C4 C5	1.368	1.405	1.391	1.376	1.402	1.397	1.402	1.387
C5 C6	1.415	1.429	1.420	1.412	1.426	1.423	1.426	1.417
N7 C8	1.331	1.348	1.334	1.319	1.345	1.341	1.344	1.329
N7 C5	1.379	1.386	1.377	1.370	1.379	1.380	1.378	1.370
N9 C8	1.341	1.353	1.341	1.330	1.350	1.348	1.349	1.337
N9 C4	1.373	1.374	1.364	1.354	1.370	1.368	1.369	1.358
N10 C6	1.326	1.349	1.336	1.324	1.345	1.343	1.345	1.331
Pt1 N9	2.050	2.092	2.076	2.060	2.064	2.063	2.062	2.045
Pt1 Cl5	2.298	2.348	2.323	2.300	2.323	2.319	2.319	2.285
Pt1 Cl2	2.315	2.434	2.356	2.357	2.360	2.352	2.355	2.346
Pt1 Cl1	2.315	2.397	2.386	2.328	2.385	2.379	2.382	2.323
Pt1 Cl3	2.321	2.399	2.373	2.326	2.360	2.352	2.370	2.322
Pt1 Cl4	2.327	2.416	2.354	2.343	2.374	2.369	2.356	2.336
<b>RMSD</b>		0.050	0.027	0.014	0.029	0.025	0.027	0.011

**Table S2b:** Geometrical parameters and RMSDs for PtBAP cluster.

	BHLYP-D3	PBE-D2	PBE-D3	PBE0-D3	PBE0-TZVPP	PBE0-D3 TZVPP	BHLYP TZVPP
Bond	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)
N1 C2	1.302	1.321	1.320	1.309	1.305	1.305	1.297
N1 C6	1.345	1.362	1.361	1.350	1.347	1.348	1.340
N3 C2	1.334	1.355	1.356	1.342	1.336	1.337	1.329
N3 C4	1.346	1.358	1.359	1.350	1.345	1.345	1.341
C4 C5	1.377	1.401	1.403	1.388	1.379	1.380	1.367
C5 C6	1.412	1.425	1.426	1.417	1.409	1.409	1.404
N7 C8	1.319	1.343	1.344	1.329	1.325	1.325	1.314
N7 C5	1.372	1.378	1.380	1.371	1.369	1.370	1.368
N9 C8	1.331	1.349	1.350	1.338	1.333	1.334	1.326
N9 C4	1.356	1.368	1.370	1.359	1.356	1.357	1.352
N10 C6	1.324	1.344	1.345	1.331	1.327	1.326	1.319
Pt1 N9	2.057	2.060	2.061	2.045	2.051	2.049	2.064
Pt1 C15	2.306	2.324	2.322	2.299	2.290	2.294	2.296
Pt1 C12	2.363	2.389	2.387	2.350	2.341	2.346	2.354
Pt1 C11	2.336	2.365	2.361	2.328	2.315	2.321	2.321
Pt1 C13	2.334	2.365	2.362	2.327	2.317	2.323	2.323
Pt1 C14	2.347	2.374	2.372	2.339	2.334	2.336	2.343
<b>RMSD</b>	0.016	0.030	0.029	0.012	0.010	0.010	0.015

**Table S3a:** Geometrical parameters and RMSDs for IrADEC3 cluster.

	Experimental	BLYP	B3LYP	BHLYP	BP86	TPSS	PBE	PBE0
Bond	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)
N1 C2	1.301	1.322	1.311	1.299	1.320	1.318	1.319	1.307
N1 C6	1.346	1.371	1.359	1.347	1.366	1.365	1.365	1.353
N3 C2	1.352	1.367	1.352	1.338	1.361	1.360	1.360	1.345
N3 C4	1.361	1.370	1.360	1.351	1.364	1.363	1.363	1.354
C4 C5	1.362	1.406	1.393	1.379	1.403	1.399	1.403	1.389
C5 C6	1.396	1.429	1.421	1.412	1.427	1.424	1.427	1.418
N7 C8	1.332	1.350	1.337	1.333	1.348	1.344	1.347	1.333
N7 C5	1.386	1.383	1.375	1.369	1.379	1.379	1.377	1.370
N9 C8	1.324	1.350	1.337	1.325	1.347	1.344	1.346	1.333
N9 C4	1.375	1.374	1.363	1.351	1.368	1.366	1.367	1.356
N10 C6	1.308	1.348	1.335	1.322	1.344	1.342	1.350	1.329
Ir1 N9	2.069	2.102	2.090	2.084	2.080	2.079	2.081	2.071
Ir1 S1	2.231	2.299	2.298	2.305	2.267	2.271	2.261	2.261
Ir1 Cl2	2.344	2.449	2.422	2.401	2.375	2.377	2.374	2.355
Ir1 Cl1	2.358	2.413	2.391	2.372	2.410	2.409	2.405	2.383
Ir1 Cl3	2.358	2.456	2.425	2.402	2.419	2.412	2.416	2.387
Ir1 Cl4	2.351	2.417	2.391	2.414	2.385	2.380	2.382	2.357
<b>RMSD</b>		0.049	0.035	0.032	0.030	0.029	0.029	0.017



**Table S3b:** Geometrical parameters and RMSDs for IrADEC3 cluster.

	BHLYP-D3	PBE-D2	PBE-D3	PBE0-D3	PBE0-TZVPP	PBE0-D3 TZVPP	BHLYP TZVPP
Bond	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)	(Å)
N1 C2	1.300	1.318	1.318	1.307	1.304	1.304	1.296
N1 C6	1.348	1.366	1.366	1.354	1.350	1.351	1.344
N3 C2	1.339	1.359	1.359	1.345	1.340	1.340	1.333
N3 C4	1.351	1.363	1.363	1.354	1.350	1.350	1.347
C4 C5	1.379	1.403	1.404	1.390	1.380	1.381	1.369
C5 C6	1.412	1.427	1.427	1.418	1.408	1.408	1.402
N7 C8	1.325	1.348	1.349	1.335	1.328	1.330	1.319
N7 C5	1.372	1.379	1.379	1.372	1.368	1.370	1.367
N9 C8	1.327	1.347	1.348	1.334	1.328	1.330	1.321
N9 C4	1.352	1.365	1.368	1.356	1.354	1.355	1.350
N10 C6	1.321	1.342	1.343	1.329	1.326	1.325	1.318
Pt1 N9	2.082	2.088	2.080	2.071	2.091	2.089	2.100
Pt1 Cl5	2.309	2.258	2.262	2.264	2.246	2.248	2.292
Pt1 Cl2	2.378	2.379	2.375	2.358	2.352	2.355	2.371
Pt1 Cl1	2.400	2.404	2.406	2.383	2.378	2.378	2.398
Pt1 Cl3	2.406	2.419	2.419	2.390	2.378	2.382	2.396
Pt1 Cl4	2.377	2.387	2.385	2.361	2.353	2.358	2.370
<b>RMSD</b>	0.029	0.030	0.030	0.018	0.014	0.015	0.025

**Table S4a:** Geometrical parameters for PtKIN optimized using PBE0/def2-SV(P)-QZVPP *in vacuo*.

Bond	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP
N1 C2	1.311	1.311	1.309	1.309	1.309	1.309
N1 C6	1.347	1.347	1.346	1.346	1.345	1.345
N3 C2	1.335	1.335	1.330	1.330	1.329	1.329
N3 C4	1.348	1.347	1.343	1.343	1.342	1.342
C4 C5	1.391	1.391	1.381	1.381	1.380	1.380
C5 C6	1.418	1.417	1.408	1.408	1.407	1.407
N7 C8	1.350	1.349	1.345	1.345	1.345	1.345
N7 C5	1.384	1.382	1.380	1.380	1.378	1.378
N9 C8	1.319	1.320	1.316	1.316	1.315	1.315
N9 C4	1.347	1.347	1.346	1.346	1.346	1.346
N10 C6	1.338	1.337	1.333	1.333	1.330	1.330
Pt1 N9	2.103	2.081	2.075	2.072	2.066	2.065
Pt1 Cl5	2.295	2.279	2.265	2.263	2.260	2.262
Pt1 Cl2	2.352	2.328	2.321	2.319	2.316	2.317
Pt1 Cl1	2.344	2.337	2.311	2.309	2.306	2.307
Pt1 Cl3	2.374	2.381	2.340	2.338	2.336	2.335
Pt1 Cl4	2.397	2.358	2.360	2.358	2.355	2.354
RMSD	0.023	0.016	0.004	0.002	0.001	-

**Table S4b:** Geometrical parameters for IrBAP optimized using PBE0/def2-SV(P)-QZVPP *in vacuo*.

Bond	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP
N1 C2	1.313	1.314	1.312	1.312	1.312	1.312
N1 C6	1.347	1.347	1.345	1.345	1.345	1.345
N3 C2	1.333	1.333	1.328	1.328	1.327	1.327
N3 C4	1.348	1.347	1.342	1.342	1.342	1.342
C4 C5	1.391	1.391	1.382	1.382	1.380	1.380
C5 C6	1.417	1.417	1.407	1.407	1.406	1.406
N7 C8	1.353	1.353	1.349	1.349	1.348	1.348
N7 C5	1.382	1.381	1.378	1.378	1.377	1.377
N9 C8	1.320	1.321	1.316	1.316	1.315	1.315
N9 C4	1.348	1.348	1.348	1.347	1.347	1.347
N10 C6	1.340	1.339	1.333	1.333	1.333	1.333
Ir1 N9	2.079	2.069	2.085	2.082	2.078	2.078
Ir1 S1	2.278	2.262	2.234	2.232	2.225	2.225
Ir1 Cl2	2.308	2.374	2.356	2.358	2.353	2.350
Ir1 Cl1	2.387	2.368	2.359	2.355	2.350	2.353
Ir1 Cl3	2.399	2.396	2.374	2.372	2.374	2.366
Ir1 Cl4	2.409	2.386	2.381	2.378	2.366	2.374
RMSD	0.022	0.015	0.004	0.003	0.003	-

**Table S5a:** NMR shielding parameters for PtKIN calculated using ADF with PBE0/TZP.

<sup>13</sup> C	BLYP	PBE0	PBE0_D3	PBE0 TZVPP	PBE0 TZVPP D3	X-ray
2	32.1	36.4	36.4	37.4	37.1	37.0
4	36.5	41.8	41.5	43.0	42.6	41.0
5	66.5	70.5	70.3	72.4	72.3	73.1
6	25.4	29.9	29.8	30.7	30.8	30.2
8	33.5	38.8	38.6	39.9	39.6	37.8
<sup>15</sup> N						
1	-0.7	10.7	10.4	12.7	12.5	11.8
3	86.7	92.5	92.3	95.6	95.5	91.5
7	82.9	90.0	89.6	92.2	91.7	95.2
9	89.4	92.5	92.0	93.4	93.1	85.1
10	128.7	134.4	134.0	136.1	135.9	133.4

**Table S5b:** NMR shielding parameters for PtKIN calculated using ADF with PBE0/TZP.

<sup>13</sup> C	BLYP	PBE0	PBE0_D3	PBE0 TZVPP	PBE0 TZVPP D3	X-ray
2	33.8	38.9	39.1	39.9	40.0	39.3
4	33.4	38.4	38.0	39.8	39.5	37.3
5	65.8	69.8	69.7	71.4	71.4	73.8
6	25.8	31.0	31.1	31.6	31.6	36.4
8	32.3	37.6	37.4	38.5	38.4	35.4
<sup>15</sup> N						
1	0.3	11.1	10.3	12.3	11.6	14.5
3	82.6	88.3	87.9	92.1	91.4	87.4
7	86.1	93.3	92.8	95.3	94.9	98.4
9	91.0	91.1	90.7	88.9	88.7	85.9
10	124.7	130.5	130.3	132.6	132.4	131.7

**Table S6:** Calculated NMR chemical shifts (PBE0/TZP/COSMO) for PBE0/def2-TZVPP/COSMO optimized geometries.

IrBAP			PtKIN		
Atom	Experimental	Calculated	Atom	Experimental	Calculated
H2	8.8	8.2	H2	8.8	7.2
H8	9.0	9.0	H8	8.6	8.1
H10	10.6	6.1	H10	9.8	7.9
H11	4.9	4.8	H11	5.0	5.0
H13.17	7.4	7.4	H13	6.4	7.0
H14.16	7.4	7.2	H14	6.5	6.5
H15	7.3	7.2	H15	7.7	7.7
H18.19	3.4	2.9			
<b>RMSD</b>		<b>1.4</b>	<b>RMSD</b>		<b>1.2</b>
C2	146.9	142.9	C2	146.0	142.2
C4	144.5	143.9	C4	143.8	140.1
C5	111.0	111.0	C5	117.9	117.6
C6	152.6	149.6	C6	155.0	151.0
C8	147.1	144.8	C8	148.5	146.1
C11	44.3	39.1	C11	38.5	31.0
C12	136.4	138.3	C12	151.6	152.8
C13.17	127.6	128.3	C13	108.7	111.9
C14.16	128.5	128.9	C14	111.2	112.7
C15	127.5	127.8	C15	143.4	146.0
C18.19	40.8	35.8			
<b>RMSD</b>		<b>2.9</b>	<b>RMSD</b>		<b>3.7</b>
N1	227.6	233.5	N1	226.6	231.1
N3	154.2	159.0	N3	153.8	156.5
N7	162.7	162.7	N7	211.2	211.2
N9	150.9	163.9	N9	139.8	156.1
N10	118.7	122.7	N10	105.5	107.0
<b>RMSD</b>		<b>7.0</b>	<b>RMSD</b>		<b>7.7</b>

**Table S7:** Interatomic distances for BHLYP, PBE0, and MP2 optimized structures of PtKIN and IrBAP.

Bond	PtKIN			Bond	IrBAP		
	PBE0	BHLYP	MP2		PBE0	BHLYP	MP2
N1 C2	1,301	1,295	1,313	N1 C2	1,304	1,295	1,316
N1 C6	1,351	1,345	1,358	N1 C6	1,351	1,346	1,359
N3 C2	1,339	1,332	1,341	N3 C2	1,336	1,330	1,341
N3 C4	1,348	1,345	1,356	N3 C4	1,349	1,346	1,357
C4 C5	1,377	1,366	1,383	C4 C5	1,379	1,367	1,385
C5 C6	1,414	1,408	1,420	C5 C6	1,413	1,407	1,420
N7 C8	1,328	1,318	1,340	N7 C8	1,333	1,323	1,345
N7 C5	1,371	1,370	1,372	N7 C5	1,371	1,370	1,371
N9 C8	1,329	1,322	1,336	N9 C8	1,327	1,320	1,336
N9 C4	1,355	1,353	1,364	N9 C4	1,353	1,349	1,363
N10 C6	1,319	1,311	1,320	N10 C6	1,321	1,313	1,323
Pt1 N9	2,056	2,071	2,045	Ir1 N9	2,095	2,106	2,088
Pt1 Cl5	2,291	2,299	2,279	Ir1 S1	2,244	2,294	2,208
Pt1 Cl2	2,321	2,330	2,311	Ir1 Cl2	2,358	2,377	2,338
Pt1 Cl1	2,319	2,330	2,308	Ir1 Cl1	2,361	2,381	2,340
Pt1 Cl3	2,331	2,340	2,319	Ir1 Cl3	2,367	2,386	2,353
Pt1 Cl4	2,335	2,340	2,324	Ir1 Cl4	2,365	2,381	2,339
<b>RMSD vs. PBE0</b>	<b>-</b>	<b>0,009</b>	<b>0,008</b>		<b>-</b>	<b>0,016</b>	<b>0,015</b>

## Cartesian coordinates

PtBAP cluster PBE0/def2-TZVPP optimized geometry:

Pt	-0.171756	-1.879509	8.303174
Cl	-0.118553	0.298740	7.447791
Cl	-0.735232	-2.731003	6.253915
Cl	-2.441538	-1.682659	8.812275
Cl	-0.151766	-4.026487	9.173960
Cl	2.080897	-2.113288	7.825866
N	0.347882	-1.150002	10.148103
N	1.554689	-0.095336	11.648822
H	2.316986	0.455876	12.074293
N	-0.630091	-1.922584	14.000383
N	-1.108769	-2.315730	11.741820
H	-1.689766	-2.816701	11.069271
N	1.062726	-0.507119	14.681695
H	1.856833	0.072325	14.413310
C	1.357726	-0.305593	10.355636
H	1.967522	0.143794	9.589471
C	0.632530	-0.836941	12.336531
C	0.369268	-1.071045	13.701172
C	-1.325052	-2.484661	13.049563
H	-2.131576	-3.166551	13.301368
C	-0.116556	-1.484255	11.376973
C	0.922211	-0.896044	16.069319
H	1.924461	-0.922963	16.503455
H	0.534591	-1.914824	16.093703
C	0.024674	-0.039337	16.925386
C	-0.983416	0.752235	16.391403
H	-1.132001	0.821438	15.320193
C	-1.830402	1.460318	17.233195
H	-2.604967	2.076069	16.795964
C	-1.691169	1.369931	18.608949
H	-2.368722	1.906497	19.262972
C	-0.684706	0.580990	19.150217
H	-0.539324	0.523650	20.222411
C	0.168151	-0.115113	18.308960
H	0.951875	-0.720942	18.752622
O	-1.413949	-3.209122	17.290188
N	-3.261582	-1.883320	17.523388
C	-2.276635	-2.411744	16.828411
H	-2.195425	-2.175070	15.932804
C	-4.135884	-0.919196	16.926560
H	-3.820575	-0.692522	16.049356
H	-4.155340	-0.130838	17.472512
H	-5.021225	-1.286708	16.863172
C	-3.501876	-2.210904	18.901802
H	-2.791723	-2.765922	19.233053
H	-4.337338	-2.678419	18.977458
H	-3.540610	-1.400045	19.412994
O	-1.513598	-2.445078	21.299904
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C	-1.149391	-1.797558	22.273621

H	-0.628191	-1.040033	22.130487
C	-0.836961	-1.395878	24.604652
H	-0.222531	-1.975063	25.060634
H	-1.519040	-1.106702	25.216036
H	-0.365623	-0.630854	24.265221
C	-2.239442	-3.302606	23.780612
H	-2.790242	-3.510112	23.022004
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Pt	-3.608303	-6.375062	12.124881
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H	-2.228919	-5.566011	9.254605
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C	-4.449494	-7.477742	8.110355
C	-4.216932	-7.246068	6.732593
C	-2.517240	-5.821020	7.356859
H	-1.827365	-5.255168	7.095334
C	-3.698644	-6.821888	9.046652
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H	-5.683634	-7.461908	3.952529
H	-4.513227	-6.493542	4.322631
C	-3.855376	-8.253600	3.539895
C	-2.882556	-9.067793	4.086461
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C	-2.025878	-9.796983	3.275712
H	-1.381548	-10.348667	3.660128
C	-2.122655	-9.706980	1.911854
H	-1.549141	-10.200329	1.372037
C	-3.069109	-8.885287	1.345455
H	-3.125931	-8.812785	0.419177
C	-3.934406	-8.171098	2.145571
H	-4.578999	-7.626914	1.754408
O	3.395144	1.721722	9.371565
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C	3.030937	2.369242	8.397849
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H	2.247168	3.535946	6.406246
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H	4.671788	0.656688	7.649465
H	4.676040	1.023366	6.124068



H	3.532189	0.126671	6.712963
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H	5.702121	3.474278	14.622111
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H	6.902773	2.880092	13.808294
C	5.383422	1.955896	11.769665
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Pt	-3.608303	1.958538	12.124881
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N	-2.710149	2.354242	8.675732
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C	-5.148038	0.319177	10.117086
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C	-2.517240	2.512580	7.356859
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C	-3.855376	0.080003	3.539895
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C	-2.025878	-1.463380	3.275712
H	-1.381548	-2.015064	3.660128
C	-2.122655	-1.373377	1.911854
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H	-4.578999	0.706689	1.754408
O	8.033117	-0.937530	7.094721
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H	7.262663	-1.991730	5.708981
C	5.322201	-3.247604	6.702739
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H	4.436860	-2.880092	6.639352
C	5.956208	-1.955896	8.677982
H	6.666364	-1.400878	9.009233
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O	2.274671	-2.445078	0.852258
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H	2.269230	-1.106702	4.768390
H	3.422647	-0.630854	3.817574
C	1.548827	-3.302606	3.332965
H	0.998027	-3.510112	2.574358
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Pt	2.061513	-6.125338	22.348704
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H	0.166715	-4.092631	16.198624
C	0.521778	-4.485977	20.340910
H	0.033238	-4.091798	21.026314
C	1.220321	-5.022661	18.334175
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H	3.842450	-7.245235	17.319154
C	1.971171	-5.678515	19.270473
C	0.863170	-5.082663	14.586941
H	-0.013819	-5.038495	14.176352
H	1.156588	-6.006859	14.546454
C	1.814439	-4.246803	13.763719
C	2.787260	-3.432610	14.310284
H	2.866964	-3.371775	15.235540
C	3.643937	-2.703420	13.499535
H	4.288268	-2.151736	13.883951
C	3.547160	-2.793423	12.135678
H	4.120674	-2.300074	11.595860
C	2.600707	-3.615116	11.569278
H	2.543884	-3.687618	10.643000
C	1.735409	-4.329305	12.369394
H	1.090816	-4.873489	11.978231
Pt	2.061513	2.208262	22.348704
Cl	2.034472	4.348139	23.232001
Cl	2.629246	1.323709	24.392610

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Cl	2.038655	0.067335	21.436699
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N	0.734983	3.630950	15.989240
H	0.166715	4.240969	16.198624
C	0.521778	3.847623	20.340910
H	0.033238	4.241802	21.026314
C	1.220321	3.310939	18.334175
C	1.452883	3.079265	16.956413
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H	3.842450	1.088368	17.319154
C	1.971171	2.655085	19.270473
C	0.863170	3.250937	14.586941
H	-0.013819	3.295105	14.176352
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C	1.814439	4.086797	13.763719
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H	2.866964	4.961825	15.235540
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H	4.288268	6.181864	13.883951
C	3.547160	5.540177	12.135678
H	4.120674	6.033526	11.595860
C	2.600707	4.718484	11.569278
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H	-2.195425	6.158530	15.932804
C	-4.135884	7.414407	16.926560
H	-3.820575	7.641081	16.049356
H	-4.155340	8.202765	17.472512
H	-5.021225	7.046895	16.863172
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H	-6.057499	1.106702	15.679254
H	-7.210919	0.630854	16.630069
C	-5.337097	3.302606	17.114678
H	-4.786297	3.510112	17.873285
H	-4.782045	3.143434	16.347891

H	-5.925896	4.040129	16.936783
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N	-4.321976	1.892561	23.377384
C	-5.299905	2.411744	24.066879
H	-5.381115	2.175070	24.962485
C	-3.440655	0.919196	23.968730
H	-3.755964	0.692522	24.845934
H	-3.421199	0.130838	23.422778
H	-2.555315	1.286708	24.032118
C	-4.074663	2.210904	21.993488
H	-4.784816	2.765922	21.662236
H	-3.239201	2.678419	21.917832
H	-4.035929	1.400045	21.482297
O	-2.363298	3.229270	3.129102
N	-0.533707	1.892561	2.929738
C	-1.511635	2.411744	3.619232
H	-1.592845	2.175070	4.514839
C	0.347614	0.919196	3.521084
H	0.032306	0.692522	4.398287
H	0.367070	0.130838	2.975132
H	1.232955	1.286708	3.584471
C	-0.286393	2.210904	1.545842
H	-0.996546	2.765922	1.214590
H	0.549068	2.678419	1.470185
H	-0.247660	1.400045	1.034651
Pt	-0.179967	-10.292141	8.322765
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Cl	-2.427239	-10.078075	8.863442
Cl	-0.157110	-12.433068	9.234771
Cl	2.069811	-10.510256	7.824088
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N	1.569042	-8.432773	11.626122
H	2.163768	-7.910256	11.959828
N	-0.572753	-10.276165	14.041398
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H	-1.559350	-11.101192	11.193041
N	1.146562	-8.869453	14.682227
H	1.714831	-8.259434	14.472843
C	1.359768	-8.652780	10.330560
H	1.848308	-8.258601	9.645155
C	0.661225	-9.189464	12.337291
C	0.428663	-9.421138	13.715053
C	-1.271029	-10.846183	13.090787
H	-1.960904	-11.412035	13.352312
C	-0.089625	-9.845318	11.400994
C	1.018375	-9.249466	16.084526
H	1.895365	-9.205298	16.495114
H	0.724957	-10.173662	16.125012
C	0.067106	-8.413606	16.907748
C	-0.905714	-7.599413	16.361182
H	-0.985418	-7.538578	15.435927
C	-1.762392	-6.870223	17.171931
H	-2.406722	-6.318536	16.787516
C	-1.665615	-6.960226	18.535789

H	-2.239128	-6.466875	19.075607
C	-0.719161	-7.781919	19.102189
H	-0.662338	-7.854421	20.028470
C	0.146137	-8.496108	18.302072
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IrC3P cluster PBE0/def2-TZVPP optimized geometry:

C	4.225839	7.491203	6.399716
H	4.395713	8.563954	6.433590
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C	2.153181	3.851136	5.125386
H	1.552623	3.052448	4.737089
C	6.928756	5.003454	8.138043
H	6.809917	5.462837	9.123550
H	7.303429	5.768151	7.453401
C	7.907587	3.851196	8.228189
H	7.520629	3.086842	8.911295
H	7.989705	3.400639	7.233506
C	9.263262	4.333201	8.715463
H	9.654893	5.102822	8.045326
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H	9.188129	4.771110	9.713021
C	-2.534874	7.002309	2.917314
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H	-2.869151	6.055831	3.332762
H	-3.244823	7.369827	2.180010
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H	-1.893984	4.790564	1.271795
H	-0.567097	5.378630	0.235031
Cl	0.061048	7.640493	5.070728
Cl	2.245870	7.135763	2.594501
Cl	1.063124	4.063754	2.147206
Cl	-1.120078	4.469933	4.571353
Ir	0.507474	5.869172	3.547719
N	5.013879	6.676293	7.044671
N	3.166602	7.111206	5.672251
H	2.550407	7.782832	5.220920
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H	5.513078	3.542044	7.505607
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H	3.558320	2.736983	6.218260
N	1.937856	5.139981	4.886882
O	-0.605376	8.063995	1.530798
S	-0.977121	6.758861	2.116849
C	-0.241010	0.887128	2.000012
H	-0.451033	1.787302	1.899070
C	1.104132	-0.757973	2.940993
C	0.353921	-1.685543	2.284017
C	-0.732163	-1.307209	1.491882
C	1.938509	-2.636597	3.452544
H	2.480325	-3.295420	3.823804

C	-2.774387	-1.796434	0.222414
H	-2.625687	-1.660756	-0.725411
H	-3.108610	-0.966709	0.597095
C	-3.811407	-2.909258	0.427719
H	-3.530305	-3.711587	-0.039350
H	-3.887376	-3.119299	1.372121
C	-5.127933	-2.457866	-0.095809
H	-5.314244	-1.573348	0.225835
H	-5.815189	-3.057982	0.205305
H	-5.105900	-2.452648	-1.055609
C	6.495279	0.834944	5.348192
H	6.272163	1.553779	4.752808
H	6.800897	0.080885	4.840063
H	7.189920	1.120651	5.946998
C	5.751694	-0.726662	7.461125
H	6.399750	-0.262225	7.994918
H	6.176623	-1.457238	7.006032
H	5.053006	-1.064554	8.027424
Cl	3.843483	1.181968	3.414734
Cl	1.769430	0.695221	5.969240
Cl	3.048200	-2.315665	6.462314
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Ir	3.509070	-0.546236	4.973819
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N	-1.510157	-2.157808	0.874257
H	-1.265816	-2.982316	0.848594
N	0.921886	-2.900126	2.633035
H	0.665277	-3.677667	2.371271
N	2.100323	-1.343738	3.685223
O	4.659083	1.586394	7.006032
S	5.065371	0.377551	6.280277
C	-3.844715	7.410131	6.554362
H	-3.634692	8.310305	6.655303
C	-5.189857	5.765027	5.613378
C	-4.439646	4.837457	6.270353
C	-3.353562	5.215791	7.062491
C	-6.024234	3.886403	5.101826
H	-6.566053	3.227580	4.730567
C	-1.311338	4.726566	8.331960
H	-1.460038	4.862244	9.279784
H	-0.977115	5.556291	7.957278
C	-0.274318	3.613742	8.126655
H	-0.555420	2.811413	8.593723
H	-0.198349	3.403701	7.182252
C	1.042208	4.065134	8.650182
H	1.228520	4.949652	8.328538
H	1.729464	3.465018	8.349068
H	1.020175	4.070352	9.609983
C	-10.581005	7.357947	3.206178
H	-10.357891	8.076782	3.801562
H	-10.886622	6.603888	3.714308
H	-11.275645	7.643654	2.607372
C	-9.837421	5.796338	1.093249

H	-10.485478	6.260775	0.559456
H	-10.262351	5.065762	1.548341
H	-9.138734	5.458446	0.526949
Cl	-7.929211	7.704971	5.139637
Cl	-5.855155	7.218224	2.585131
Cl	-7.133928	4.207335	2.092057
Cl	-9.214848	4.615675	4.589078
Ir	-7.594798	5.976764	3.580551
N	-3.107581	6.534744	7.173698
N	-4.897294	7.085286	5.770778
H	-5.366379	7.693229	5.384121
N	-2.575567	4.365192	7.680117
H	-2.819909	3.540684	7.705780
N	-5.007611	3.622874	5.921335
H	-4.751002	2.845333	6.183099
N	-6.186047	5.179262	4.869148
O	-8.744810	8.109397	1.548341
S	-9.151099	6.900554	2.274094
C	12.499288	7.410131	6.554362
H	12.709311	8.310305	6.655303
C	11.154146	5.765027	5.613378
C	11.904357	4.837457	6.270353
C	12.990441	5.215791	7.062491
C	10.319769	3.886403	5.101826
H	9.777953	3.227580	4.730567
C	15.032665	4.726566	8.331960
H	14.883965	4.862244	9.279784
H	15.366888	5.556291	7.957278
C	16.069685	3.613742	8.126655
H	15.788583	2.811413	8.593723
H	16.145654	3.403701	7.182252
C	17.386211	4.065134	8.650182
H	17.572523	4.949652	8.328538
H	18.073467	3.465018	8.349068
H	17.364178	4.070352	9.609983
C	5.762998	7.357947	3.206178
H	5.986112	8.076782	3.801562
H	5.457381	6.603888	3.714308
H	5.068358	7.643654	2.607372
C	6.506583	5.796338	1.093249
H	5.858525	6.260775	0.559456
H	6.081652	5.065762	1.548341
H	7.205272	5.458446	0.526949
Cl	8.414795	7.704971	5.139637
Cl	10.488848	7.218224	2.585131
Cl	9.210078	4.207335	2.092057
Cl	7.129158	4.615675	4.589078
Ir	8.749208	5.976764	3.580551
N	13.236422	6.534744	7.173698
N	11.446709	7.085286	5.770778
H	10.977624	7.693229	5.384121
N	13.768436	4.365192	7.680117
H	13.524094	3.540684	7.705780
N	11.336392	3.622874	5.921335
H	11.593001	2.845333	6.183099

N	10.157956	5.179262	4.869148
O	7.599196	8.109397	1.548341
S	7.192907	6.900554	2.274094
C	-0.241010	13.933131	2.000012
H	-0.451033	14.833305	1.899070
C	1.104132	12.288030	2.940993
C	0.353921	11.360460	2.284017
C	-0.732163	11.738794	1.491882
C	1.938509	10.409406	3.452544
H	2.480325	9.750583	3.823804
C	-2.774387	11.249569	0.222414
H	-2.625687	11.385247	-0.725411
H	-3.108610	12.079294	0.597095
C	-3.811407	10.136745	0.427719
H	-3.530305	9.334416	-0.039350
H	-3.887376	9.926704	1.372121
C	-5.127933	10.588137	-0.095809
H	-5.314244	11.472655	0.225835
H	-5.815189	9.988021	0.205305
H	-5.105900	10.593355	-1.055609
C	6.495279	13.880947	5.348192
H	6.272163	14.599782	4.752808
H	6.800897	13.126888	4.840063
H	7.189920	14.166654	5.946998
C	5.751694	12.319341	7.461125
H	6.399750	12.783778	7.994918
H	6.176623	11.588765	7.006032
H	5.053006	11.981449	8.027424
Cl	3.843483	14.227971	3.414734
Cl	1.769430	13.741224	5.969240
Cl	3.048200	10.730338	6.462314
Cl	5.129120	11.138678	3.965293
Ir	3.509070	12.499767	4.973819
N	-0.978144	13.057744	1.380675
N	0.811569	13.608286	2.783592
H	1.280654	14.216229	3.170250
N	-1.510157	10.888195	0.874257
H	-1.265816	10.063687	0.848594
N	0.921886	10.145877	2.633035
H	0.665277	9.368336	2.371271
N	2.100323	11.702265	3.685223
O	4.659083	14.632397	7.006032
S	5.065371	13.423554	6.280277
C	-4.327285	5.635872	-6.554362
H	-4.537308	4.735698	-6.655303
C	-2.982143	7.280976	-5.613378
C	-3.732354	8.208546	-6.270353
C	-4.818438	7.830212	-7.062491
C	-2.147766	9.159600	-5.101826
H	-1.605950	9.818423	-4.730567
C	-6.860665	8.319437	-8.331960
H	-6.711965	8.183759	-9.279784
H	-7.194888	7.489712	-7.957278
C	-7.897685	9.432261	-8.126655
H	-7.616583	10.234590	-8.593723



H	-7.973654	9.642302	-7.182252
C	-9.214211	8.980869	-8.650182
H	-9.400523	8.096351	-8.328538
H	-9.901467	9.580985	-8.349068
H	-9.192178	8.975651	-9.609983
C	2.409002	5.688056	-3.206178
H	2.185888	4.969221	-3.801562
H	2.714619	6.442115	-3.714308
H	3.103642	5.402349	-2.607372
C	1.665418	7.249665	-1.093249
H	2.313475	6.785228	-0.559456
H	2.090348	7.980241	-1.548341
H	0.966731	7.587557	-0.526949
Cl	-0.242792	5.341032	-5.139637
Cl	-2.316845	5.827779	-2.585131
Cl	-1.038075	8.838668	-2.092057
Cl	1.042845	8.430328	-4.589078
Ir	-0.577205	7.069239	-3.580551
N	-5.064419	6.511262	-7.173698
N	-3.274706	5.960717	-5.770778
H	-2.805621	5.352774	-5.384121
N	-5.596433	8.680811	-7.680117
H	-5.352091	9.505319	-7.705780
N	-3.164389	9.423129	-5.921335
H	-3.420998	10.200670	-6.183099
N	-1.985953	7.866741	-4.869148
O	0.572807	4.936606	-1.548341
S	0.979096	6.145449	-2.274094
C	3.845266	5.635872	10.554385
H	3.635242	4.735698	10.453444
C	5.190407	7.280976	11.495366
C	4.440196	8.208546	10.838390
C	3.354112	7.830212	10.046256
C	6.024785	9.159600	12.006917
H	6.566603	9.818423	12.378177
C	1.311888	8.319437	8.776787
H	1.460588	8.183759	7.828963
H	0.977666	7.489712	9.151468
C	0.274868	9.432261	8.982092
H	0.555970	10.234590	8.515023
H	0.198899	9.642302	9.926494
C	-1.041658	8.980869	8.458564
H	-1.227969	8.096351	8.780209
H	-1.728913	9.580985	8.759678
H	-1.019624	8.975651	7.498764
C	10.581556	5.688056	13.902566
H	10.358441	4.969221	13.307182
H	10.887172	6.442115	13.394436
H	11.276195	5.402349	14.501372
C	9.837972	7.249665	16.015495
H	10.486029	6.785228	16.549288
H	10.262901	7.980241	15.560403
H	9.139284	7.587557	16.581795
Cl	7.929761	5.341032	11.969107
Cl	5.855705	5.827779	14.523613

Cl	7.134479	8.838668	15.016687
Cl	9.215398	8.430328	12.519666
Ir	7.595348	7.069239	13.528192
N	3.108131	6.511262	9.935049
N	4.897844	5.960717	11.337966
H	5.366930	5.352774	11.724623
N	2.576118	8.680811	9.428630
H	2.820460	9.505319	9.402967
N	5.008161	9.423129	11.187409
H	4.751552	10.200670	10.925645
N	6.186598	7.866741	12.239596
O	8.745361	4.936606	15.560403
S	9.151649	6.145449	14.834650

PtKIN PBE0/def2-TZVPP/COSMO optimized geometry:

C	6.623473	4.583760	9.038898
O	6.025791	5.519085	8.264819
C	5.041410	4.894922	7.570113
C	5.007231	3.578785	7.893682
C	6.039820	3.376083	8.858019
C	4.227298	5.725741	6.652699
N	4.991937	6.220643	5.514216
C	5.409381	7.463743	5.368937
N	5.119994	8.379592	6.318633
C	5.527949	9.609350	6.202022
N	6.242001	10.084004	5.173048
C	6.558780	9.221517	4.186946
C	6.157589	7.905956	4.253326
N	6.645872	7.326780	3.110389
C	7.293553	8.258459	2.420287
N	7.260139	9.430562	3.046711
H	5.288645	10.320880	6.981576
H	6.590952	11.039349	5.137997
H	5.226549	5.549807	4.799896
H	7.777740	8.084974	1.474535
H	3.403364	5.124843	6.270718
H	3.811624	6.589854	7.167757
H	4.326378	2.843556	7.494911
H	6.309873	2.454268	9.347634
H	7.437103	4.928383	9.655412
H	6.537112	6.371613	2.804458
Pt	8.079682	11.172099	2.323301
Cl	8.989529	13.104263	1.495289
Cl	6.059143	12.259341	2.732780
Cl	7.342053	10.589277	0.203799
Cl	10.065937	10.031730	1.946486
Cl	8.805156	11.743166	4.468247

PtKIN B3LYP/def2-TZVPP/COSMO optimized geometry:

C	6.648599	4.623107	8.994618
O	6.028418	5.540126	8.225206
C	5.044974	4.903293	7.554216
C	5.029965	3.600398	7.885278
C	6.081387	3.416960	8.834387
C	4.209969	5.714909	6.640948
N	4.963874	6.229554	5.504725
C	5.386621	7.464166	5.374451
N	5.106068	8.372142	6.325497
C	5.517751	9.592925	6.216091
N	6.232288	10.066821	5.196060
C	6.546393	9.210792	4.207148
C	6.135493	7.909552	4.267343
N	6.612156	7.330041	3.120310
C	7.260526	8.254248	2.440635
N	7.244817	9.418383	3.067862
H	5.283372	10.294582	6.992774
H	6.569834	11.014767	5.176700
H	5.195095	5.572243	4.788318
H	7.734321	8.079522	1.500243
H	3.409469	5.100323	6.257647
H	3.775944	6.557083	7.156268
H	4.358028	2.859550	7.506408
H	6.367901	2.509356	9.321452
H	7.461660	4.975911	9.590857
H	6.493077	6.386001	2.810343
Pt	8.103550	11.156801	2.333604
Cl	9.049905	13.077366	1.498932
Cl	6.075749	12.264894	2.695295
Cl	7.397959	10.558195	0.196796
Cl	10.093162	9.988362	2.006357
Cl	8.804717	11.743991	4.490757

PtKIN MP2/def2-TZVPP/COSMO optimized geometry:

C	6.644729	4.553519	8.965689
O	6.030397	5.516568	8.213476
C	4.995339	4.905695	7.560920
C	4.943637	3.582509	7.887955
C	6.019253	3.353576	8.809527
C	4.174874	5.757395	6.655816
N	4.963882	6.242896	5.519527
C	5.428183	7.473077	5.402840
N	5.139448	8.394609	6.357580
C	5.568170	9.629268	6.230672
N	6.286270	10.098000	5.199651
C	6.614304	9.222722	4.217485
C	6.213449	7.901961	4.300024
N	6.714228	7.298564	3.174115
C	7.373821	8.225934	2.466810
N	7.329552	9.415743	3.072303

H	5.338462	10.345590	7.005634
H	6.631739	11.052937	5.175575
H	5.201415	5.570772	4.805117
H	7.865112	8.028379	1.531496
H	3.349515	5.166410	6.265535
H	3.775828	6.624476	7.172134
H	4.229300	2.867352	7.516485
H	6.291797	2.427818	9.286784
H	7.493916	4.878803	9.539975
H	6.623865	6.331744	2.893759
Pt	8.040099	11.169795	2.298169
Cl	8.809446	13.130497	1.427258
Cl	5.959209	12.123704	2.675039
Cl	7.332113	10.496369	0.207097
Cl	10.088188	10.162023	1.935937
Cl	8.753502	11.837659	4.407141

IrBAP PBE0/def2-TZVPP/COSMO optimized geometry:

C	2.828044	2.979006	5.166452
C	3.781976	1.966139	5.093085
C	5.109361	2.265029	5.376236
C	5.482347	3.556185	5.728471
C	4.527552	4.559863	5.796686
C	3.197904	4.268342	5.514769
C	3.380486	0.563697	4.719383
N	2.956506	0.454488	3.331386
C	1.711002	0.288210	2.922826
C	1.352834	0.166021	1.561924
C	0.028409	-0.009300	1.221317
N	-0.921462	-0.053681	2.177993
C	-0.524312	0.071352	3.447819
N	0.711965	0.229252	3.830942
N	2.023880	0.172072	0.366781
C	1.125567	0.007979	-0.604562
N	-0.105086	-0.111385	-0.121439
Ir	-1.811859	-0.478796	-1.279274
S	-3.604864	-0.899202	-2.561104
Cl	-0.500327	-1.924330	-2.607340
Cl	-3.019449	0.979224	0.137785
Cl	-1.162018	1.356002	-2.609571
Cl	-2.319872	-2.260832	0.193893
H	1.371867	-0.030935	-1.651683
H	-1.305026	0.040781	4.196269
H	3.677691	0.521387	2.631248
H	2.554922	0.217860	5.337783
H	6.520222	3.776038	5.948807
H	4.815981	5.567562	6.071143
H	2.447110	5.047508	5.571906
H	1.787960	2.754407	4.956632
H	4.219758	-0.117543	4.861655
H	5.857258	1.481163	5.325029
H	-1.902426	-0.108490	1.900684
O	-4.871642	-0.236599	-2.226427

C	-3.915569	-2.642985	-2.655082
C	-3.249902	-0.559190	-4.265417
H	-4.109931	-0.895443	-4.843192
H	-3.104904	0.514082	-4.356189
H	-2.340259	-1.087496	-4.545282
H	-4.715181	-2.786828	-3.380744
H	-2.998076	-3.145191	-2.956515
H	-4.215767	-2.970547	-1.663170
H	3.016180	0.264393	0.214186

IrBAP BHLYP/def2-TZVPP/COSMO optimized geometry:

C	2.822841	2.965312	5.229915
C	3.786610	1.976448	5.096548
C	5.113374	2.296169	5.321150
C	5.476854	3.584125	5.672673
C	4.512526	4.563400	5.799778
C	3.182525	4.250882	5.577566
C	3.396379	0.574187	4.719157
N	2.954537	0.468491	3.335145
C	1.716144	0.290989	2.936655
C	1.354180	0.168999	1.582503
C	0.043272	-0.023422	1.244176
N	-0.899409	-0.086594	2.202657
C	-0.502781	0.040340	3.465464
N	0.723773	0.217882	3.842599
N	2.027423	0.183483	0.389241
C	1.136301	0.008602	-0.572757
N	-0.086651	-0.124778	-0.095107
Ir	-1.793209	-0.478853	-1.277471
S	-3.614450	-0.885293	-2.611033
Cl	-0.491715	-1.979263	-2.590302
Cl	-3.004318	1.029547	0.111448
Cl	-1.105089	1.343382	-2.639876
Cl	-2.366615	-2.252799	0.211546
H	1.383774	-0.024297	-1.610385
H	-1.273324	-0.007427	4.210024
H	3.663605	0.539493	2.634809
H	2.594424	0.215334	5.343417
H	6.510822	3.818688	5.846068
H	4.792107	5.564003	6.073060
H	2.427205	5.007919	5.680467
H	1.787177	2.726833	5.067020
H	4.239323	-0.091336	4.839611
H	5.867609	1.535848	5.225371
H	-1.869577	-0.186507	1.949985
O	-4.848747	-0.171416	-2.306321
C	-3.988121	-2.614405	-2.661573
C	-3.225782	-0.591740	-4.312705
H	-4.083723	-0.905303	-4.890122
H	-3.046623	0.465067	-4.424413
H	-2.341947	-1.152217	-4.575371
H	-4.775858	-2.746272	-3.389548
H	-3.098079	-3.160204	-2.934687

H	-4.317154	-2.902547	-1.676553
H	3.009238	0.298516	0.236262

IrBAP MP2 /def2-TZVPP/COSMO optimized geometry:

C	3.046218	3.301458	5.225044
C	3.772372	2.106834	5.165628
C	5.153683	2.135947	5.366533
C	5.804299	3.344513	5.625650
C	5.075049	4.531153	5.685243
C	3.692698	4.508269	5.483786
C	3.065398	0.807028	4.881579
N	2.659335	0.748828	3.470858
C	1.479012	0.343478	3.030705
C	1.142367	0.293342	1.652084
C	-0.112799	-0.145560	1.263531
N	-1.018574	-0.529768	2.198501
C	-0.647379	-0.458482	3.484674
N	0.524722	-0.044618	3.917044
N	1.796429	0.586959	0.483712
C	0.952980	0.329952	-0.531869
N	-0.227400	-0.116364	-0.094480
Ir	-1.864044	-0.545679	-1.317844
S	-3.564055	-0.978539	-2.659052
Cl	-0.433727	-1.842981	-2.639245
Cl	-3.147581	0.777061	0.122402
Cl	-1.308980	1.368554	-2.540738
Cl	-2.321694	-2.416338	0.034671
H	1.206201	0.476605	-1.565748
H	-1.385423	-0.774581	4.206479
H	3.359981	0.991179	2.786319
H	2.165568	0.707464	5.480755
H	6.874884	3.357194	5.783138
H	5.577296	5.467683	5.888523
H	3.122197	5.426256	5.533863
H	1.972988	3.284205	5.073109
H	3.718837	-0.039782	5.089956
H	5.721390	1.214160	5.325093
H	-1.926146	-0.887995	1.912601
O	-4.863405	-0.335029	-2.389504
C	-3.859611	-2.728219	-2.781428
C	-3.147033	-0.630560	-4.352418
H	-3.993060	-0.965409	-4.949048
H	-3.009163	0.442269	-4.433651
H	-2.231048	-1.155000	-4.609519
H	-4.567597	-2.866877	-3.594717
H	-2.917050	-3.236576	-2.971100
H	-4.284617	-3.044317	-1.834339
H	2.735333	0.941550	0.369311