Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Computational Study of the Photophysical Properties and Electronic Structure of Iridium(III) Photosensitizers Complexes with Electron-Withdrawing Groups

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1. Supplemental Figures

1.1 Comparison of Structures with RMSD Value

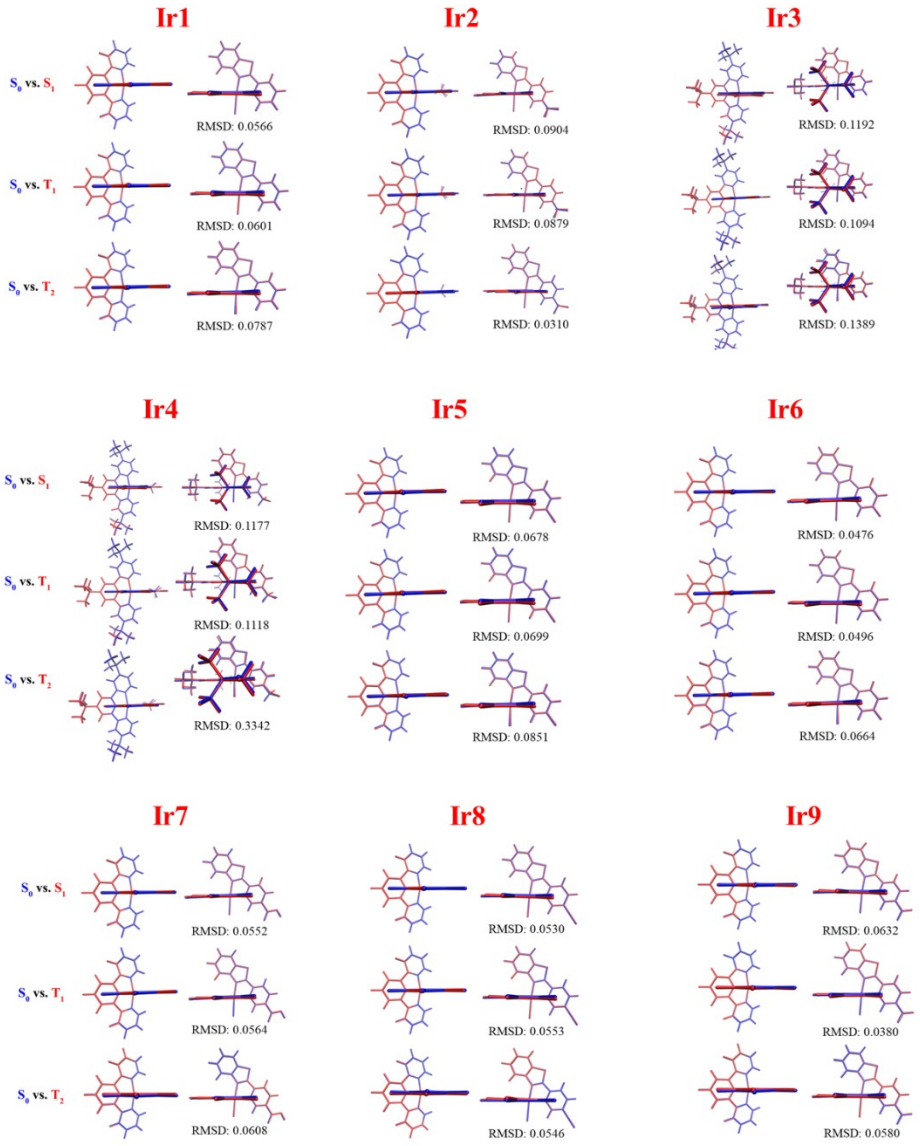


Figure S1. Comparison of Ir1-Ir9 structures of ground state (blue) and excited states (red) with RMSD of total structure.

1.2 Isosurfaces of Fragment or Complex Orbitals

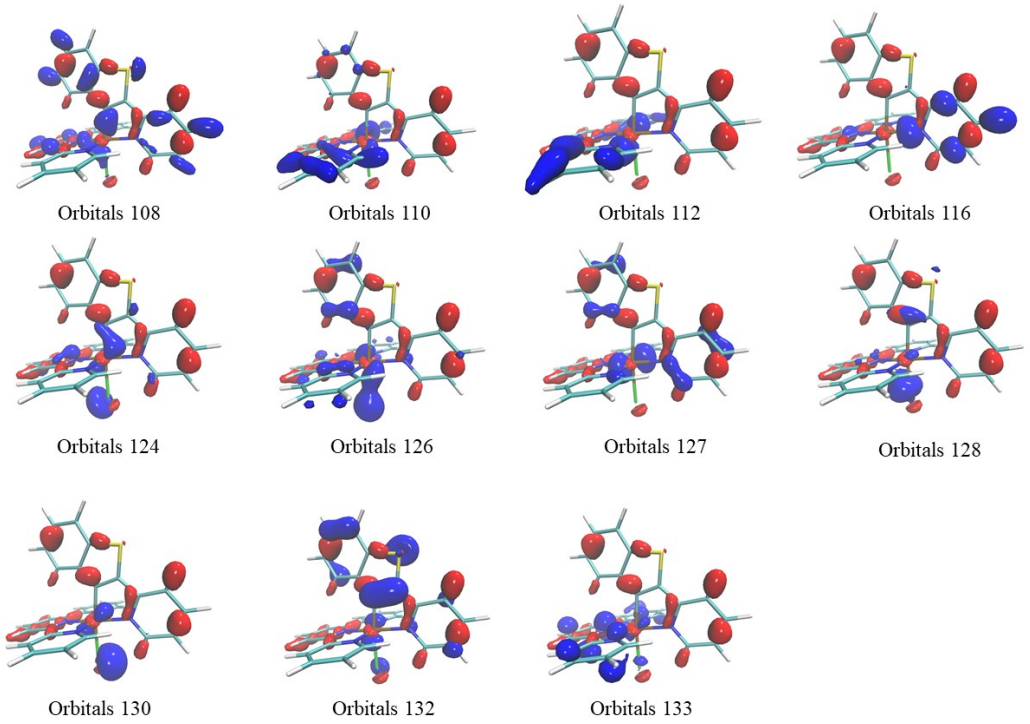


Figure S2. Complex orbitals of **Ir1**

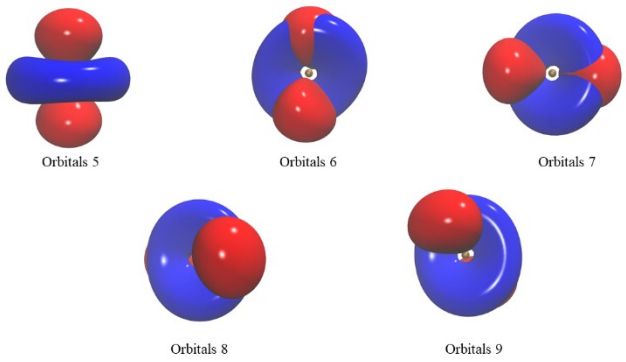


Figure S3. Fragment orbitals of F1 in **Ir1**

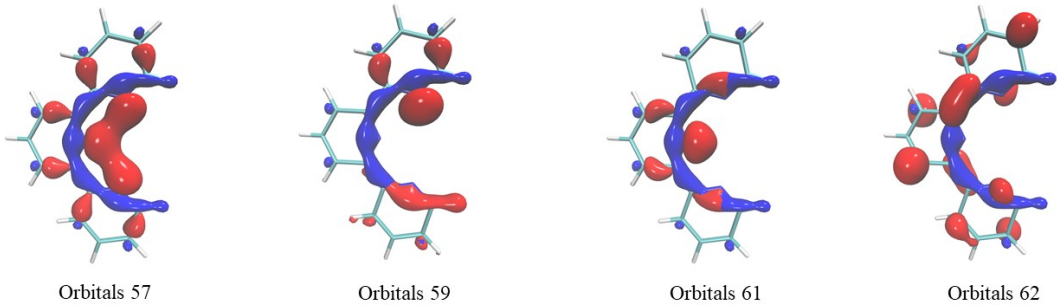
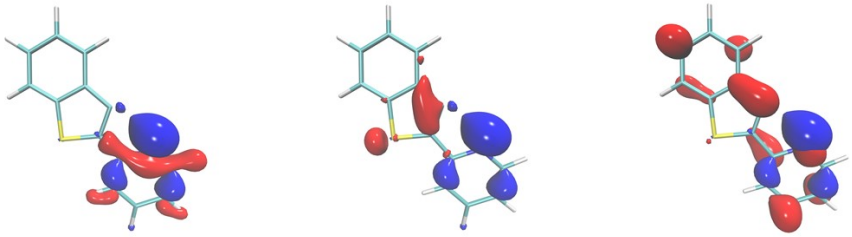


Figure S4. Fragment orbitals of F2 in **Ir1**



Orbitals 52 Orbitals 55 Orbitals 56

Figure S5. Fragment orbitals of F3 in **Ir1**

1.3 Density of States of Ir1

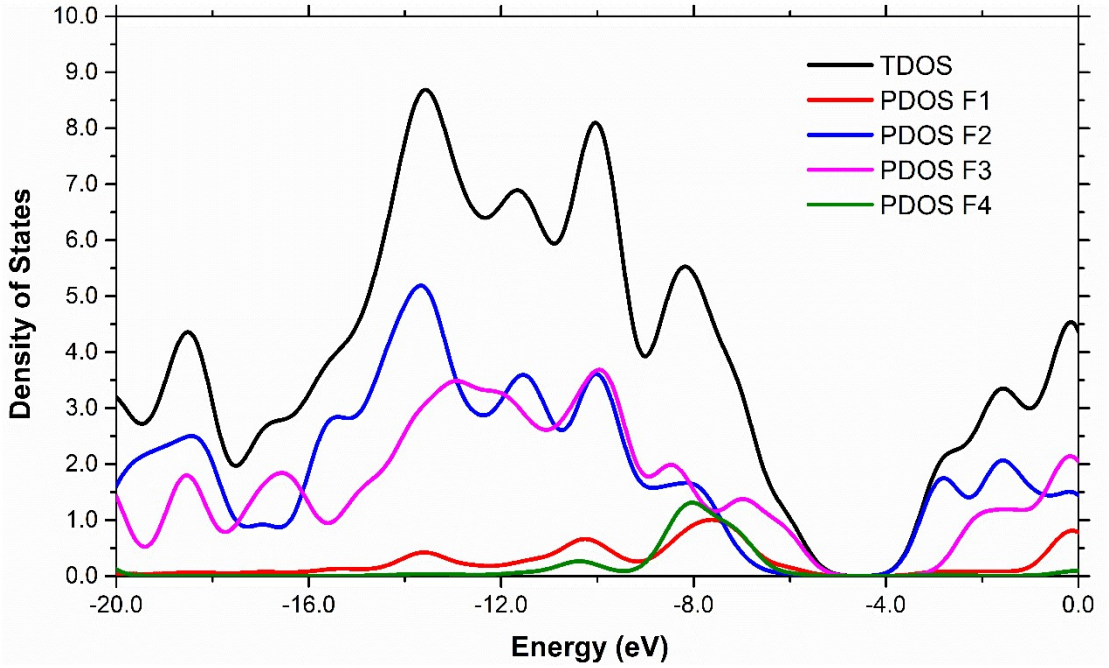
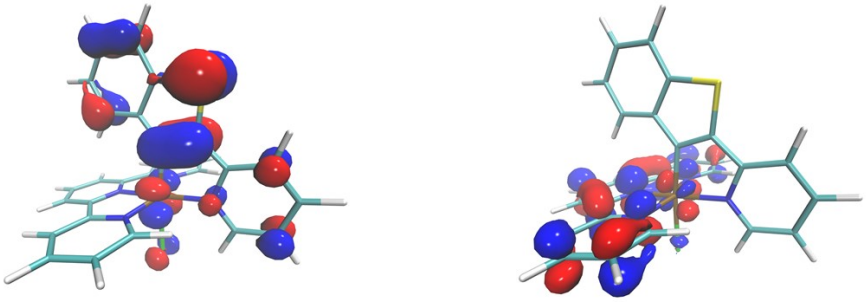


Figure S6. Total Density of States (TDOS) and Partial Density of States (PDOS) of Ir1. F1 stands for Ir^{3+}, F2 stands for tpy ligand, F3 stands for btp ligand and F4 stands for Cl^-.

1.4 Isosurfaces of Molecular Orbitals



HOMO **LUMO**

Figure S7. Molecular orbitals of **Ir1**: HOMO and LUMO

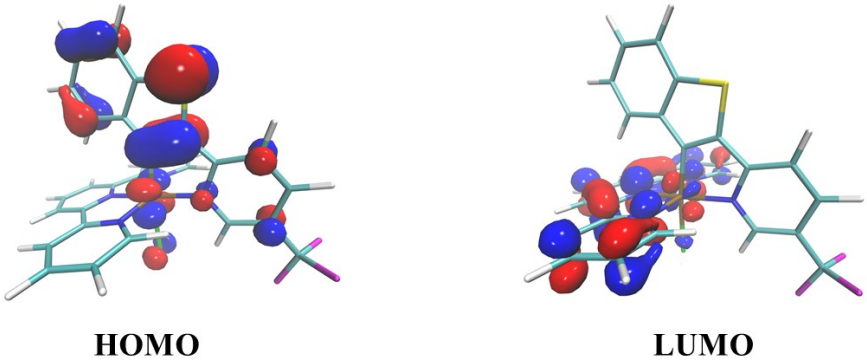


Figure S8. Molecular orbitals of **Ir2**: HOMO and LUMO

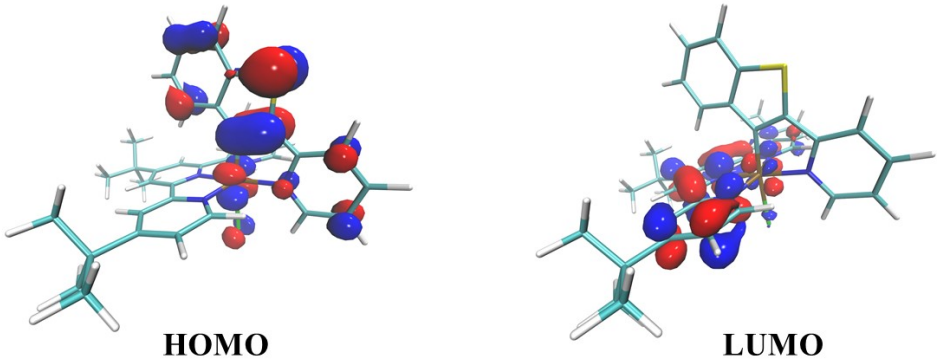


Figure S9. Molecular orbitals of **Ir3**: HOMO and LUMO

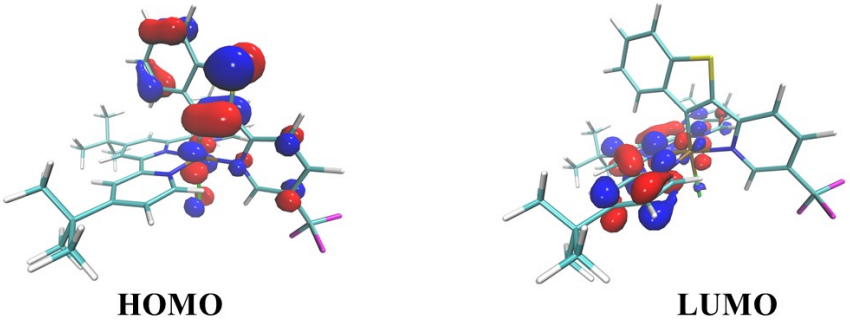


Figure S10. Molecular orbitals of **Ir4**: HOMO and LUMO

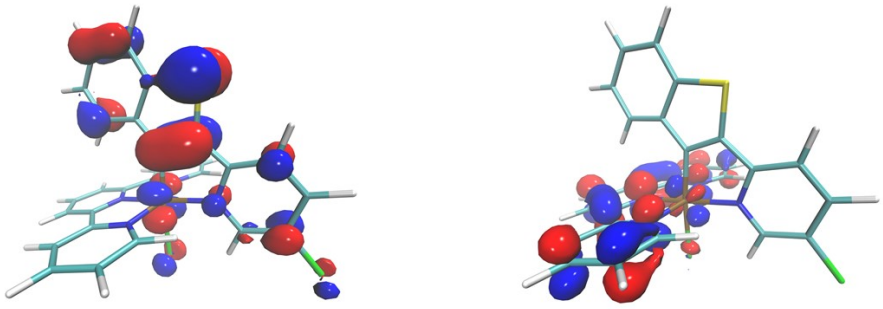


Figure S11. Molecular orbitals of **Ir5**: HOMO and LUMO

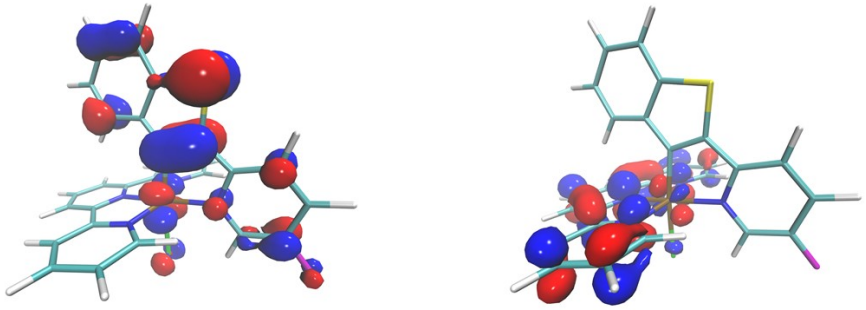


Figure S12. Molecular orbitals of **Ir6**: HOMO and LUMO

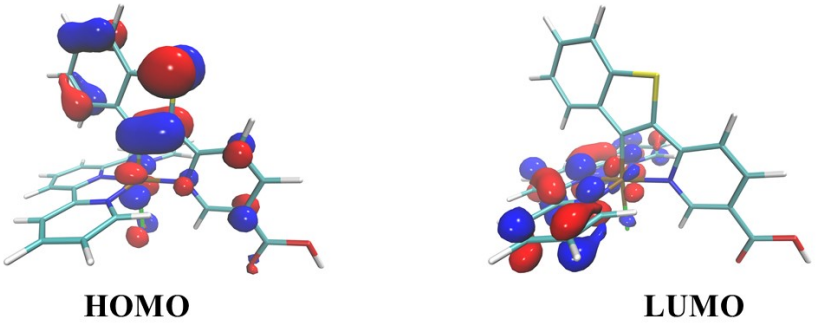


Figure S13. Molecular orbitals of **Ir7**: HOMO and LUMO

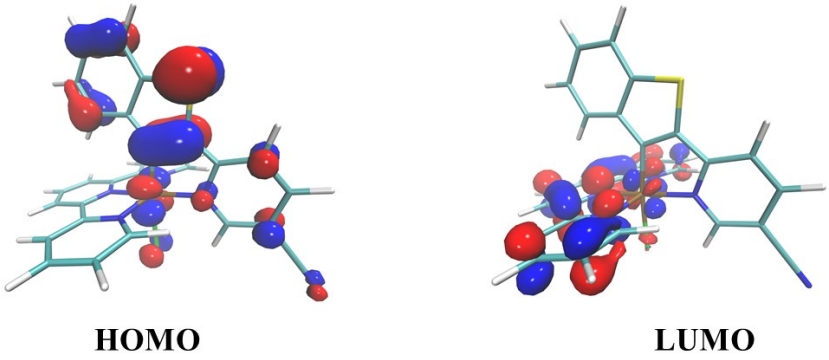


Figure S14. Molecular orbitals of **Ir8**: HOMO and LUMO

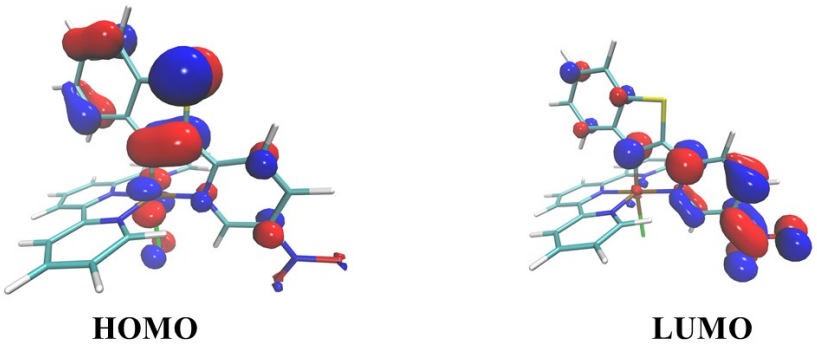


Figure S15. Molecular orbitals of **Ir9**: HOMO and LUMO

1.5 Natural Transition Orbital (NTO) Couples

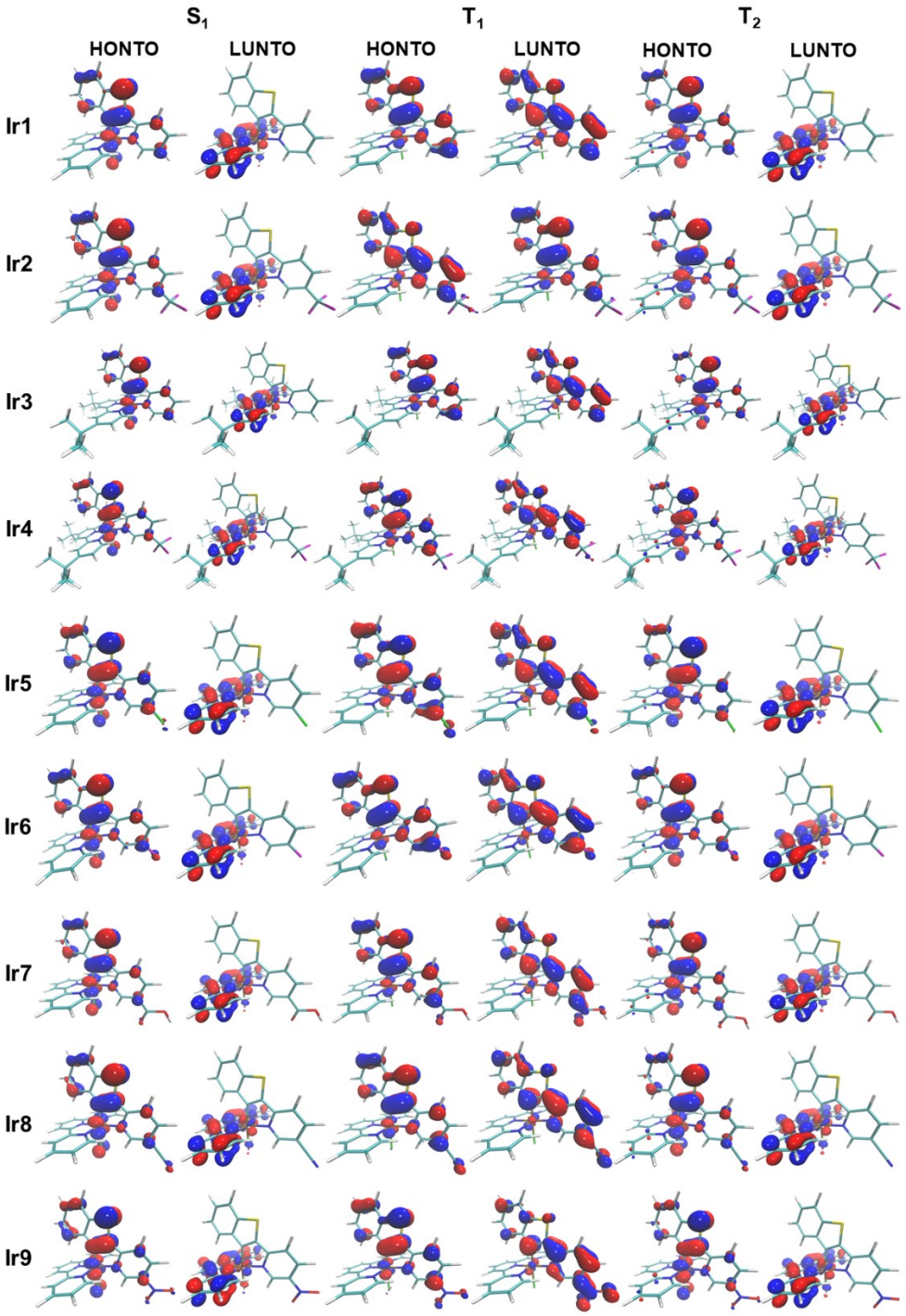


Figure S16. The ground state structure-based natural transition orbital couples related to excitation features of the S1, T1 and T2 states in this work.

1.6 UV-Vis Absorption Spectra.

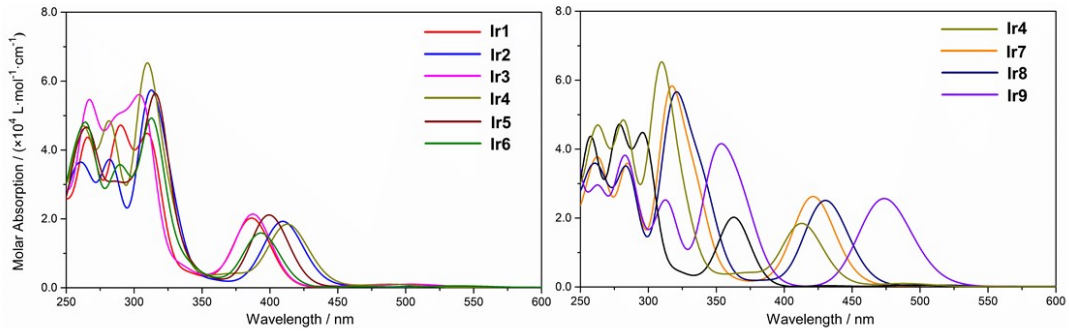


Figure S17. UV-Vis spectra of Ir1-Ir9 calculated by TD-DFT method combined with IEFPCM model in acetonitrile. The damping constant of the Lorentzian linewidth function in our work is taken to be 0.25 eV.

2. Calculation Result

2.1 Key Geometrical Parameters

Table S1. Calculated bond lengths and dihedral angles of **Ir1**~**Ir9** in their S_0, S_1, T_1 and T_2 optimized structure. (in angstrom and degree)

Mol.	**Ir1**				**Ir2**				**Ir3**			
States	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**
***L*$_1$**	2.0161	1.9520	1.9493	2.0214	2.0141	1.9513	1.9489	1.9966	2.0144	1.9520	1.9506	2.0179
***L*$_2$**	2.0921	2.1003	2.1043	2.1459	2.0912	2.1001	2.1044	2.0881	2.0917	2.0999	2.1038	2.1413
***L*$_3$**	1.4408	1.4421	1.4411	1.4406	1.4354	1.4420	1.4411	1.3974	1.4408	1.4421	1.4413	1.4408
***D*$_1$**	0.0000	0.0000	0.1487	0.0229	0.0124	0.1473	0.0838	0.1422	0.1338	1.9250	0.1862	4.0197
***D*$_2$**	0.0000	0.0000	0.0197	0.0069	0.0310	0.1678	0.1297	0.0515	0.0193	0.0639	0.1211	0.8534
***D*$_3$**	0.0000	0.0000	0.0131	0.0010	0.0283	0.0409	0.0264	0.1361	0.0027	0.5780	0.2980	0.2381
Mol.	**Ir4**				**Ir5**				**Ir6**			
States	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**
***L*$_1$**	2.0122	1.9514	1.9505	1.9826	2.0158	1.9527	1.9499	2.0216	2.0175	1.9529	1.9500	2.0215
***L*$_2$**	2.0903	2.0996	2.1032	2.1142	2.0918	2.1008	2.1051	2.1479	2.0915	2.0993	2.1037	2.1472
***L*$_3$**	1.4356	1.4419	1.4412	1.4396	1.4387	1.4391	1.4382	1.4384	1.4409	1.4399	1.4391	1.4408
***D*$_1$**	0.2606	1.7008	0.0552	0.8002	0.4012	0.0399	0.3299	0.0016	0.0153	0.0114	0.0185	0.0015
***D*$_2$**	0.1539	0.0101	0.2598	0.1034	0.0403	0.0248	0.2281	0.0020	0.0156	0.0014	0.0146	0.0011
***D*$_3$**	0.0074	0.4529	0.0677	0.0520	0.1890	0.0072	0.0291	0.0009	0.0013	0.0104	0.0034	0.0005
Mol.	**Ir7**				**Ir8**				**Ir9**			
States	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**	**S_0**	**S_1**	**T_1**	**T_2**
***L*$_1$**	2.0140	1.9515	1.9493	1.9561	2.0130	1.9513	1.9491	1.9561	2.0112	1.9510	1.9846	1.9571
***L*$_2$**	2.0915	2.1005	2.1046	2.1005	2.0927	2.1021	2.1065	2.1024	2.0906	2.1002	2.0885	2.1000
***L*$_3$**	1.4342	1.4407	1.4398	1.4409	1.4318	1.4398	1.4389	1.4401	1.4297	1.4401	1.4088	1.4400
***D*$_1$**	0.0131	0.0192	0.1117	1.7061	0.0064	0.0076	0.1017	1.8034	0.2082	0.0143	0.0087	1.7472
***D*$_2$**	0.0007	0.0068	0.0774	0.5605	0.0080	0.0093	0.1408	0.4808	0.0969	0.0062	0.0017	0.5928
***D*$_3$**	0.0060	0.0013	0.0039	0.1221	0.0027	0.0111	0.0031	0.1010	0.0719	0.0003	0.0026	0.0013

2.2 Geometric Structures in Cartesian

Structure of Ir1, S_0 state

C	-0.46678200	-1.98841700	3.66376700
C	-0.53008000	-1.57976500	2.33598500
C	-0.74314800	0.65448700	2.98942800
C	-0.68498900	0.30568900	4.33455700
C	-0.54697400	-1.03538600	4.67615100
H	-0.35225600	-3.04504800	3.90491800
H	-0.84955200	1.69223100	2.66963100
H	-0.74727900	1.08557500	5.09430000
H	-0.49822500	-1.34231100	5.72240400

C	-0.44203800	-2.50062600	1.18770300
C	-0.32583000	-3.88938300	1.21317900
C	-0.26139200	-4.57472900	0.00000000
H	-0.28911500	-4.43136400	2.15789100
C	-0.44203800	-2.50062600	-1.18770300
C	-0.32583000	-3.88938300	-1.21317900
H	-0.16783500	-5.66181400	0.00000000
H	-0.28911500	-4.43136400	-2.15789100
C	-0.53008000	-1.57976500	-2.33598500
C	-0.46678200	-1.98841700	-3.66376700
C	-0.74314800	0.65448700	-2.98942800
C	-0.54697400	-1.03538600	-4.67615100
H	-0.35225600	-3.04504800	-3.90491800
C	-0.68498900	0.30568900	-4.33455700
H	-0.84955200	1.69223100	-2.66963100
H	-0.49822500	-1.34231100	-5.72240400
H	-0.74727900	1.08557500	-5.09430000
N	-0.67370000	-0.26048500	2.01980800
N	-0.47445500	-1.87245400	0.00000000
N	-0.67370000	-0.26048500	-2.01980800
Ir	-0.73215300	0.06616800	0.00000000
Cl	-3.14582400	-0.41235700	0.00000000
C	1.19407100	0.66153700	0.00000000
C	2.47897900	0.00897400	0.00000000
C	1.34213800	2.03321300	0.00000000
C	3.55340900	0.94256400	0.00000000
C	2.79748600	-1.36422000	0.00000000
S	2.99611100	2.59092800	0.00000000
C	0.16613600	2.86554200	0.00000000
C	4.89061300	0.53254000	0.00000000
C	4.12183300	-1.77216800	0.00000000
H	2.00309100	-2.10924800	0.00000000
C	0.13063200	4.26424100	0.00000000
N	-0.98901800	2.14241200	0.00000000
C	5.16459800	-0.82882000	0.00000000
H	5.69974700	1.26610600	0.00000000
H	4.35832000	-2.83857000	0.00000000
C	-1.09689400	4.91171600	0.00000000
H	1.06571600	4.82688500	0.00000000
C	-2.17343200	2.77103200	0.00000000
H	6.20311400	-1.16819000	0.00000000
C	-2.27054600	4.15508200	0.00000000
H	-1.14060000	6.00293000	0.00000000
H	-3.04907000	2.11705000	0.00000000

H	-3.25417000	4.62582200	0.00000000

Structure of Ir1, S_1 state

C	-1.98243000	-0.45302200	-3.68390400
C	-1.58896000	-0.51619500	-2.33797700
C	0.65512800	-0.80406300	-3.00636700
C	0.31292400	-0.75259600	-4.34325800
C	-1.03902800	-0.57233900	-4.68674600
H	-3.03540100	-0.30841000	-3.92735000
H	1.69020900	-0.93944800	-2.68761400
H	1.08820600	-0.85194700	-5.10324000
H	-1.34316300	-0.52519100	-5.73400500
C	-2.48928300	-0.40199100	-1.20858700
C	-3.87232700	-0.25622200	-1.21876300
C	-4.55867500	-0.17204500	-0.00000100
H	-4.41919700	-0.21505800	-2.16120100
C	-2.48928300	-0.40199000	1.20858600
C	-3.87232700	-0.25622200	1.21876200
H	-5.64325300	-0.05754000	-0.00000100
H	-4.41919700	-0.21505700	2.16120000
C	-1.58896000	-0.51619400	2.33797600
C	-1.98242900	-0.45302000	3.68390300
C	0.65512800	-0.80406300	3.00636600
C	-1.03902800	-0.57233700	4.68674500
H	-3.03540000	-0.30840800	3.92734900
C	0.31292400	-0.75259500	4.34325700
H	1.69020900	-0.93944800	2.68761300
H	-1.34316300	-0.52518900	5.73400400
H	1.08820600	-0.85194600	5.10323900
N	-0.25632600	-0.69397600	-2.02629200
N	-1.85551100	-0.42960000	-0.00000100
N	-0.25632600	-0.69397600	2.02629100
Ir	0.08135900	-0.70781000	-0.00000100
Cl	-0.39237200	-3.11598500	0.00000000
C	0.62473800	1.16702300	-0.00000100
C	-0.03102200	2.45103300	0.00000000
C	2.03749200	1.34627700	0.00000000
C	0.89163500	3.52756200	0.00000100
C	-1.40343700	2.75593200	0.00000100
S	2.55584600	2.97123000	0.00000000
C	2.88321400	0.17821400	0.00000000
C	0.49172500	4.85637600	0.00000200
C	-1.81619100	4.08535800	0.00000200
H	-2.13875700	1.95423100	0.00000100

C	4.27914100	0.16480600	0.00000100
N	2.16415000	-0.97806500	0.00000000
C	-0.88101800	5.12446700	0.00000200
H	1.22046600	5.66877500	0.00000200
H	-2.88289700	4.31689800	0.00000200
C	4.93882600	-1.05938400	0.00000000
H	4.83427300	1.10426300	0.00000100
C	2.79832300	-2.15227700	0.00000000
H	-1.22114400	6.16218200	0.00000300
C	4.18952600	-2.23349000	0.00000000
H	6.02973400	-1.09497900	0.00000100
H	2.15354800	-3.03504700	-0.00000100
H	4.66803300	-3.21347100	0.00000000

Structure of Ir1, T_1 state

C	-1.97746500	-0.45332000	-3.68159500
C	-1.58976500	-0.50840000	-2.33032600
C	0.66031600	-0.80242300	-2.99456300
C	0.32172700	-0.76053200	-4.33110100
C	-1.03224700	-0.58054100	-4.67873400
H	-3.02959100	-0.30916000	-3.92943700
H	1.69457000	-0.93599900	-2.67203500
H	1.09826900	-0.86575300	-5.08902000
H	-1.33329600	-0.54009200	-5.72733500
C	-2.48835600	-0.39096400	-1.20847600
C	-3.87598900	-0.24825100	-1.21486800
C	-4.56368600	-0.17062000	-0.00150800
H	-4.42179100	-0.20691200	-2.15831500
C	-2.49689700	-0.39989200	1.21036900
C	-3.87673800	-0.26054500	1.22259800
H	-5.64877200	-0.05946100	-0.00260000
H	-4.42469700	-0.22980900	2.16474400
C	-1.59577600	-0.52397400	2.34372100
C	-1.99377900	-0.48062900	3.68696000
C	0.64577600	-0.81564700	3.01121900
C	-1.05096800	-0.61260800	4.69078400
H	-3.04769600	-0.34286000	3.92977500
C	0.29971600	-0.78465600	4.34838700
H	1.68148800	-0.94418800	2.69196000
H	-1.35759200	-0.58167100	5.73800800
H	1.07347100	-0.89303000	5.10885500
N	-0.25394300	-0.68499100	-2.01595000
N	-1.85625800	-0.41482800	0.00621700
N	-0.26556700	-0.69235800	2.03262100

Ir	0.07967600	-0.69035500	0.00508200
Cl	-0.39000200	-3.10122700	0.00671600
C	0.62977200	1.17970300	0.00822900
C	-0.02579400	2.46383100	0.00816100
C	2.04314800	1.35603200	0.00953600
C	0.89864900	3.53911200	0.01042000
C	-1.39839900	2.76824100	0.00525900
S	2.56402500	2.98287500	0.01159100
C	2.88649100	0.18751700	0.00779000
C	0.49792000	4.86848900	0.01067100
C	-1.81047200	4.09652300	0.00551500
H	-2.13281100	1.96500700	0.00229700
C	4.28283100	0.17133800	0.00820500
N	2.16557400	-0.96807900	0.00529800
C	-0.87367800	5.13594900	0.00836500
H	1.22661800	5.68104700	0.01237500
H	-2.87704600	4.32920600	0.00325700
C	4.93984600	-1.05440000	0.00617800
H	4.83975700	1.10975300	0.01002100
C	2.79709900	-2.14343500	0.00355400
H	-1.21406500	6.17378200	0.00847300
C	4.18839300	-2.22724600	0.00390800
H	6.03074600	-1.09219900	0.00635400
H	2.15073600	-3.02510200	0.00174500
H	4.66497200	-3.20822000	0.00224300

Structure of Ir1, T_2 state

C	-1.98628800	-0.45950800	-3.70011300
C	-1.59799400	-0.52195800	-2.35273200
C	0.64426600	-0.82522500	-2.99262000
C	0.31077100	-0.77162400	-4.34012100
C	-1.03019600	-0.58690000	-4.69439400
H	-3.03588000	-0.30834700	-3.95257700
H	1.67556900	-0.96610000	-2.66445400
H	1.09335900	-0.87381900	-5.09218900
H	-1.32416400	-0.54008800	-5.74458600
C	-2.49687300	-0.39248800	-1.22957400
C	-3.87380200	-0.22158500	-1.22866900
C	-4.56030800	-0.12473800	0.00281500
H	-4.42536100	-0.16719200	-2.16732800
C	-2.49525100	-0.38685400	1.23382500
C	-3.87207100	-0.21603500	1.23391100
H	-5.64212200	0.01089900	0.00324800
H	-4.42246600	-0.15740800	2.17300700

C	-1.59480900	-0.51102200	2.35652500
C	-1.98130500	-0.44233600	3.70402200
C	0.64824300	-0.81122200	2.99482200
C	-1.02391900	-0.56525800	4.69763200
H	-3.03054200	-0.28994600	3.95722300
C	0.31661600	-0.75159300	4.34242500
H	1.67908800	-0.95341400	2.66576000
H	-1.31651000	-0.51365600	5.74798200
H	1.10016600	-0.85034000	5.09395000
N	-0.27443600	-0.71193300	-2.03104100
N	-1.84324200	-0.44264700	0.00197600
N	-0.27185200	-0.70231800	2.03397300
Ir	0.02984900	-0.75225900	0.00127200
Cl	-0.25599000	-3.16117500	0.00739600
C	0.65123000	1.17125900	-0.00340200
C	-0.02895100	2.44171300	-0.00526900
C	2.01665900	1.33216200	-0.00490700
C	0.89412900	3.52548700	-0.00811600
C	-1.40470200	2.74482800	-0.00469800
S	2.54870300	2.99056200	-0.00851000
C	2.86480600	0.16775200	-0.00326900
C	0.46973700	4.85810900	-0.01026600
C	-1.82544200	4.06457900	-0.00681300
H	-2.14092800	1.94310900	-0.00266600
C	4.26261100	0.16525800	-0.00439600
N	2.16167900	-0.99757200	-0.00027000
C	-0.89376700	5.11763900	-0.00957100
H	1.19562000	5.67396700	-0.01243300
H	-2.89436300	4.28864800	-0.00633700
C	4.93780100	-1.04702900	-0.00244400
H	4.80286900	1.11330200	-0.00680900
C	2.81942000	-2.16668800	0.00156900
H	-1.24431200	6.15230500	-0.01117900
C	4.20504500	-2.23433000	0.00058200
H	6.02956000	-1.06741000	-0.00326900
H	2.19445000	-3.06164300	0.00390100
H	4.69406300	-3.20888900	0.00220300

Structure of Ir2, S_0 state

C	1.96580600	-1.44891400	3.66391400
C	1.59413000	-1.27014300	2.33576200
C	-0.39239000	-0.22483800	2.98796000
C	-0.07336700	-0.37403000	4.33340100
C	1.12215100	-0.99664300	4.67557200

H	2.91013800	-1.93586000	3.90708100
H	-1.31796700	0.25598100	2.66819000
H	-0.76212000	-0.00207600	5.09266900
H	1.40218400	-1.12940000	5.72206300
C	2.41466000	-1.69740600	1.18775400
C	3.63982600	-2.36121400	1.21410500
C	4.25135000	-2.67990700	0.00174600
H	4.11148500	-2.62921800	2.15901300
C	2.41977400	-1.69212000	-1.18782100
C	3.64501100	-2.35589800	-1.21181100
H	5.21230000	-3.19671300	0.00266700
H	4.12065100	-2.61988200	-2.15584800
C	1.60419500	-1.25978200	-2.33747700
C	1.98155700	-1.43278300	-3.66479800
C	-0.37965200	-0.21187800	-2.99363300
C	1.14210000	-0.97636700	-4.67808800
H	2.92701200	-1.91851100	-3.90603400
C	-0.05495700	-0.35539000	-4.33833600
H	-1.30663200	0.26751200	-2.67578100
H	1.42654900	-1.10467900	-5.72394200
H	-0.74057500	0.01962800	-5.09893000
N	0.41418700	-0.66328900	2.01891600
N	1.87435700	-1.37679300	-0.00049600
N	0.42287700	-0.65433500	-2.02305100
Ir	0.11497800	-0.52334900	-0.00239500
Cl	-0.82848400	-2.79210300	-0.00970900
C	0.67780700	1.41046200	0.00319700
C	1.92867400	2.12361100	0.00774500
C	-0.38656700	2.29320300	0.00242900
C	1.74123700	3.53470800	0.01020800
C	3.24977400	1.63107100	0.00986000
S	0.05987000	3.98069500	0.00707200
C	-1.72352600	1.77076700	-0.00210800
C	2.82089300	4.42403700	0.01459300
C	4.31982100	2.51059600	0.01418200
H	3.43250100	0.55755000	0.00807700
C	-2.91449400	2.51126700	-0.00608700
N	-1.75761900	0.40757600	-0.00456000
C	4.10693800	3.90092200	0.01652800
H	2.65546700	5.50350800	0.01639100
H	5.33995000	2.12043700	0.01575800
C	-4.12662300	1.84657700	-0.01159900
H	-2.87277700	3.60128000	-0.00668100
C	-2.92958400	-0.23697400	-0.00926100

H	4.96282000	4.57995300	0.01988700
C	-4.13582000	0.44597400	-0.01219900
H	-5.06262700	2.40921400	-0.01851900
H	-2.87006700	-1.32840000	-0.01281900
C	-5.43694200	-0.30231600	-0.00067800
F	-6.09505700	-0.11693000	1.14965900
F	-6.24513100	0.11772900	-0.97980200
F	-5.26010000	-1.61518300	-0.15462600

Structure of Ir2, S_1 state

C	1.96521700	-1.41654300	3.68728700
C	1.60590800	-1.25547200	2.33969500
C	-0.43230100	-0.26739800	3.00081300
C	-0.12223300	-0.41035800	4.33861600
C	1.10709800	-0.99886200	4.68656700
H	2.92433500	-1.87218300	3.93527300
H	-1.37215400	0.18458900	2.67944600
H	-0.82831000	-0.06910400	5.09587200
H	1.38401400	-1.12472700	5.73485300
C	2.42379800	-1.65508100	1.21359800
C	3.66074700	-2.29111000	1.22749800
C	4.28394700	-2.59970500	0.01156800
H	4.13846000	-2.55416800	2.17158500
C	2.43064700	-1.65993100	-1.20411000
C	3.66691400	-2.29605400	-1.20961100
H	5.25364400	-3.09872700	0.01513900
H	4.14926800	-2.56340900	-2.15007700
C	1.61826800	-1.26489000	-2.33692500
C	1.98534600	-1.43124900	-3.68133900
C	-0.41724900	-0.28254500	-3.01273900
C	1.13189600	-1.01895700	-4.68723100
H	2.94645600	-1.88654400	-3.92211000
C	-0.09984600	-0.43115600	-4.34837000
H	-1.35965400	0.16905800	-2.69834700
H	1.41462300	-1.14887200	-5.73346500
H	-0.80250900	-0.09452000	-5.11086800
N	0.39431300	-0.67451400	2.02371900
N	1.88166900	-1.33323200	0.00227900
N	0.40509200	-0.68379200	-2.02971100
Ir	0.11068600	-0.50306100	-0.00389400
Cl	-0.82529600	-2.76830700	-0.00179800
C	0.68487500	1.36181900	-0.00596700
C	1.93761100	2.07566100	-0.00154600
C	-0.39725900	2.28761400	-0.01369200

C	1.75643700	3.48171500	-0.00662200
C	3.25195600	1.57800500	0.00683500
S	0.06103100	3.92903200	-0.01636900
C	-1.74523600	1.77540300	-0.01674000
C	2.81925300	4.37441800	-0.00374400
C	4.32609100	2.46408300	0.00979400
H	3.42782800	0.50444100	0.01109700
C	-2.92189700	2.52777000	-0.02853300
N	-1.77814600	0.41480200	-0.01059200
C	4.11408000	3.84566000	0.00455900
H	2.65434700	5.45322100	-0.00766800
H	5.34495800	2.07265700	0.01632400
C	-4.14173700	1.86675300	-0.02883000
H	-2.87666300	3.61763900	-0.03979600
C	-2.94747400	-0.22360400	-0.01046800
H	4.96765900	4.52668300	0.00698900
C	-4.15331600	0.47197300	-0.01603600
H	-5.07567300	2.43135100	-0.04488600
H	-2.89408000	-1.31600100	-0.01078900
C	-5.45470000	-0.28506500	0.02836600
F	-5.92710100	-0.35249900	1.27591500
F	-6.38424000	0.31409700	-0.71647700
F	-5.31037800	-1.53360300	-0.41433800

Structure of Ir2, T_1 state

C	1.94886000	-1.47110300	3.67994600
C	1.60318700	-1.28439400	2.33248400
C	-0.44273300	-0.30975700	2.99121600
C	-0.14646700	-0.47915000	4.32882600
C	1.07913600	-1.07338300	4.67765200
H	2.90554400	-1.93106200	3.92916400
H	-1.37905000	0.14820500	2.66801900
H	-0.86034200	-0.15292200	5.08551100
H	1.34489800	-1.21958100	5.72629600
C	2.43170600	-1.66403800	1.20639600
C	3.66602100	-2.30202300	1.21978100
C	4.29792100	-2.59554300	0.00214200
H	4.13578800	-2.58064700	2.16351900
C	2.45009900	-1.63917400	-1.21298500
C	3.68661600	-2.27754300	-1.21696800
H	5.26701500	-3.09604500	0.00496700
H	4.17187000	-2.53712000	-2.15839300
C	1.64018700	-1.23935800	-2.34195200
C	2.00639200	-1.39816700	-3.68897000

C	-0.40012900	-0.25774400	-3.01439100
C	1.15105500	-0.98430500	-4.69123900
H	2.96851600	-1.84991300	-3.93254000
C	-0.08334200	-0.40073700	-4.34978500
H	-1.34324100	0.19041400	-2.69711100
H	1.43325100	-1.10915000	-5.73836600
H	-0.78695400	-0.06303600	-5.11099700
N	0.39584800	-0.69797800	2.01575000
N	1.89721100	-1.31932700	-0.00324400
N	0.42470900	-0.66124900	-2.03284500
Ir	0.12555500	-0.49416500	-0.00999400
Cl	-0.80575100	-2.76370700	-0.03551300
C	0.68346900	1.37306800	0.01199600
C	1.93279800	2.09228400	0.03035600
C	-0.40494400	2.29169800	0.01006900
C	1.74324800	3.49747100	0.04083900
C	3.24913800	1.59960300	0.03837300
S	0.04467800	3.93793100	0.02843600
C	-1.74898200	1.77194900	-0.00533700
C	2.80308700	4.39456100	0.05874100
C	4.31812100	2.48951200	0.05627900
H	3.42777600	0.52598300	0.03044600
C	-2.93058000	2.51739800	-0.01355200
N	-1.77419900	0.41094200	-0.01568600
C	4.09884100	3.87131700	0.06640300
H	2.63363400	5.47272300	0.06668800
H	5.33918700	2.10352100	0.06244200
C	-4.14613600	1.84860700	-0.02743800
H	-2.89197400	3.60759400	-0.01158600
C	-2.93920400	-0.23482200	-0.02857000
H	4.94972600	4.55586900	0.08044800
C	-4.14939700	0.45355700	-0.03146500
H	-5.08350200	2.40771700	-0.04101300
H	-2.87924800	-1.32682100	-0.04153100
C	-5.44667500	-0.31119900	-0.00274100
F	-5.93148300	-0.38568300	1.23966700
F	-6.37208500	0.28550300	-0.75476100
F	-5.29092500	-1.55728300	-0.44847300

Structure of Ir2, T_2 state

C	1.94299600	-1.55679300	3.63172300
C	1.58110200	-1.33275200	2.30751700
C	-0.42069200	-0.32858500	2.98058300
C	-0.11193300	-0.52443400	4.32236500

C	1.08701600	-1.14804500	4.65166700
H	2.88837800	-2.04606800	3.86581300
H	-1.34762900	0.15524500	2.66842300
H	-0.81041000	-0.18734000	5.08905400
H	1.35955300	-1.31669400	5.69493800
C	2.41308600	-1.71967800	1.15188200
C	3.64483400	-2.37196100	1.16642700
C	4.26517400	-2.65022600	-0.05147200
H	4.11537600	-2.66131600	2.10559600
C	2.43196700	-1.64467800	-1.22318100
C	3.66350700	-2.29678300	-1.25947800
H	5.23115500	-3.15753000	-0.05968700
H	4.14806300	-2.52853300	-2.20744100
C	1.61856400	-1.18378600	-2.36522100
C	2.00286600	-1.32049600	-3.69495700
C	-0.37439500	-0.14127700	-3.00475400
C	1.16212500	-0.84871900	-4.70025200
H	2.95366100	-1.79114200	-3.94461400
C	-0.04373200	-0.25026400	-4.35114300
H	-1.30741600	0.32023800	-2.67726800
H	1.45209900	-0.94915400	-5.74766600
H	-0.73112600	0.13377100	-5.10560200
N	0.39953600	-0.72223500	2.00415300
N	1.87682400	-1.37296000	-0.03030600
N	0.43102900	-0.59541900	-2.04246800
Ir	0.11680000	-0.51989400	-0.01676300
Cl	-0.83380000	-2.78760500	-0.09594100
C	0.72315900	1.38143700	0.04253900
C	1.94253900	2.09324700	0.06877200
C	-0.42763200	2.31201400	0.06115500
C	1.76271200	3.51294100	0.10560500
C	3.28112800	1.62083300	0.06411800
S	0.04031300	3.96212200	0.10741500
C	-1.72586300	1.79543500	0.04065000
C	2.80732000	4.40558200	0.13512700
C	4.34971500	2.52087900	0.09404600
H	3.48199600	0.55108300	0.03716700
C	-2.94360300	2.53011300	0.05591200
N	-1.75623300	0.40294600	0.00054400
C	4.13202600	3.89600000	0.12916000
H	2.62959900	5.48285100	0.16258100
H	5.37124300	2.13395100	0.08979000
C	-4.14300500	1.86509600	0.03281500
H	-2.90780500	3.62046000	0.08555500

C	-2.92309300	-0.23147900	-0.02119200
H	4.97395600	4.59054100	0.15218600
C	-4.13975600	0.44920800	-0.00614800
H	-5.08431800	2.41768700	0.04251700
H	-2.87016900	-1.32316000	-0.05292500
C	-5.43284200	-0.30171700	-0.01904600
F	-6.13404600	-0.09324700	1.10457600
F	-6.21661200	0.09094900	-1.03270500
F	-5.25157000	-1.61889200	-0.13743800

Structure of Ir3, S_0 state

C	3.65873900	1.19741800	-0.41143000
C	2.33383200	0.79618400	-0.47518400
C	2.98373100	-1.42392500	-0.70930200
C	4.32824000	-1.07414700	-0.65035000
C	4.70227800	0.26332400	-0.49992800
H	3.87876200	2.25771600	-0.28756100
H	2.67282600	-2.46364400	-0.82466000
H	5.06714700	-1.87063800	-0.72354500
C	1.18863900	1.72226400	-0.37188100
C	1.21897500	3.10103700	-0.20983400
C	0.01947900	3.82779500	-0.11051700
H	2.17884900	3.61367000	-0.15371200
C	-1.17489200	1.73942600	-0.36830200
C	-1.18752100	3.12304000	-0.20467800
H	-2.14052200	3.64429700	-0.14530800
C	-2.33471800	0.83201000	-0.46846300
C	-3.65317600	1.25402100	-0.40329200
C	-3.01940300	-1.37797300	-0.69964400
C	-4.71130600	0.33612600	-0.48934600
H	-3.85624700	2.31790800	-0.28080500
C	-4.35828600	-1.00711800	-0.63867500
H	-2.72516900	-2.42254800	-0.81480700
H	-5.10956200	-1.79214500	-0.70984000
N	2.00823700	-0.52006700	-0.63043600
N	0.00014400	1.09766500	-0.42378000
N	-2.02983000	-0.48953900	-0.62328300
Ir	-0.01341900	-0.83917300	-0.68376300
Cl	-0.01472100	-0.37959100	-3.10390600
C	-0.01238000	-1.41118500	1.24767700
C	-0.00238400	-0.74445000	2.52618700
C	-0.02228100	-2.78126700	1.41158200
C	-0.00606700	-1.66618300	3.61099500
C	0.01052500	0.63210700	2.83135400

S	-0.02104000	-3.32071500	3.07212500
C	-0.03149600	-3.62701200	0.24511500
C	0.00211400	-1.24206000	4.94386200
C	0.01901600	1.05405200	4.15131500
H	0.01417100	1.37046100	2.03106300
C	-0.04171600	-5.02617700	0.22601700
N	-0.02906900	-2.91756500	-0.91848100
C	0.01464600	0.12200100	5.20407100
H	-0.00106100	-1.96728100	5.76051300
H	0.02932200	2.12322100	4.37549500
C	-0.04956000	-5.68813700	-0.99372700
H	-0.04328800	-5.57765800	1.16775300
C	-0.03666400	-3.56014300	-2.09505700
H	0.02133600	0.47201000	6.23903900
C	-0.04704700	-4.94531100	-2.17624400
H	-0.05757000	-6.77978200	-1.02459800
H	-0.03403800	-2.91602400	-2.97807800
H	-0.05297700	-5.42765000	-3.15425200
C	0.07196200	5.33863000	0.09955700
C	-6.15360300	0.82311500	-0.41375400
C	6.15206600	0.72768500	-0.42485700
C	-6.36632000	1.52170400	0.93936400
H	-6.18312500	0.82879300	1.77476700
H	-5.70440000	2.39155400	1.06468300
H	-7.40458600	1.88000300	1.01215100
C	-6.39940000	1.81876200	-1.55916900
H	-7.43843700	2.17990100	-1.51929600
H	-5.73963600	2.69668900	-1.49384200
H	-6.23925300	1.34211000	-2.53829600
C	-7.15074200	-0.32963900	-0.53808900
H	-7.05055100	-0.85597300	-1.49966800
H	-7.03407500	-1.06223100	0.27505500
H	-8.17540500	0.06620600	-0.48222600
C	-1.32549800	5.95366800	0.18829400
H	-1.23639000	7.03893300	0.34192200
H	-1.90322700	5.79762800	-0.73555000
H	-1.90019400	5.54691600	1.03439200
C	0.82137500	5.62218000	1.41216100
H	0.30997200	5.15400400	2.26737500
H	1.85653300	5.25034200	1.38736300
H	0.86207300	6.70785300	1.58866700
C	0.82127100	5.97815900	-1.08061600
H	0.87081700	7.06872200	-0.94038800
H	1.85334100	5.60723300	-1.16734500

H	0.30450200	5.77745500	-2.03149000
C	6.37723500	1.41809400	0.93048000
H	5.72930000	2.29788400	1.05954500
H	6.18392900	0.72526400	1.76367000
H	7.42113200	1.75963900	1.00341500
C	7.13097200	-0.44000000	-0.55449900
H	7.02064200	-0.96192700	-1.51737000
H	8.16176300	-0.06028900	-0.49954900
H	7.00456800	-1.17305200	0.25676600
C	6.41205800	1.72347000	-1.56700800
H	7.45669200	2.06810200	-1.52710700
H	6.24336000	1.25290300	-2.54764100
H	5.76633500	2.61150000	-1.49779700

Structure of Ir3, S_1 state

C	3.72102300	1.13073300	-0.39614900
C	2.38606700	0.75040800	-0.46011600
C	3.01951000	-1.48794700	-0.65906800
C	4.36296100	-1.15487800	-0.60283500
C	4.75090300	0.18659300	-0.46766200
H	3.95136500	2.19090700	-0.29006100
H	2.69824400	-2.52594400	-0.76265200
H	5.09381300	-1.95938500	-0.66655000
C	1.25417300	1.68748400	-0.39152200
C	1.30359800	3.05597300	-0.23743200
C	0.08842300	3.80284100	-0.16059500
H	2.26682200	3.55957000	-0.16701200
C	-1.14742500	1.72177500	-0.44214500
C	-1.11580400	3.12082500	-0.27779200
H	-2.06037100	3.66065300	-0.23476500
C	-2.28069900	0.85540800	-0.55376900
C	-3.62680700	1.27313000	-0.51921300
C	-3.01077800	-1.37347400	-0.80267100
C	-4.67553900	0.37595000	-0.62905200
H	-3.82539100	2.33920800	-0.40020100
C	-4.33691700	-0.99577700	-0.77798300
H	-2.72784500	-2.42261800	-0.91160600
H	-5.09578700	-1.76934200	-0.87458300
N	2.04978100	-0.56982600	-0.59243400
N	0.05627100	1.06880700	-0.46122700
N	-2.00094400	-0.49966900	-0.69946000
Ir	0.00900400	-0.87739100	-0.64740200
Cl	0.08624700	-0.54304900	-3.07503700
C	-0.08733400	-1.30866600	1.25387400

C	-0.15466300	-0.57873800	2.49691300
C	-0.13546000	-2.70723300	1.51213400
C	-0.24484100	-1.43799500	3.62138000
C	-0.13970100	0.80861500	2.72648700
S	-0.25367400	-3.13100400	3.16044700
C	-0.09771000	-3.62005200	0.39628800
C	-0.31791900	-0.96337600	4.92392000
C	-0.21238100	1.29571600	4.02831200
H	-0.07255600	1.50118800	1.89066700
C	-0.12480900	-5.01413600	0.46512900
N	-0.03022600	-2.97144400	-0.79867600
C	-0.30095400	0.42156500	5.11579200
H	-0.38632100	-1.64525400	5.77341600
H	-0.20014900	2.37403800	4.19865200
C	-0.08101100	-5.74570200	-0.71662300
H	-0.17947800	-5.51106700	1.43514000
C	0.01176300	-3.67457800	-1.93214300
H	-0.35763600	0.81999600	6.13095100
C	-0.01203200	-5.06775500	-1.93151400
H	-0.10098600	-6.83664400	-0.68814700
H	0.06350800	-3.08359500	-2.85028900
H	0.02287800	-5.60376700	-2.88063400
C	0.16637100	5.31206800	0.05829900
C	-6.12162900	0.87055300	-0.58387600
C	6.20705200	0.63390600	-0.39577700
C	-6.37002300	1.56894000	0.76264500
H	-6.20416100	0.87585000	1.60197400
H	-5.70787000	2.43646200	0.90243000
H	-7.40965600	1.92886800	0.81605900
C	-6.34867700	1.86686100	-1.73182400
H	-7.38797100	2.23125100	-1.71624800
H	-5.68637000	2.74177700	-1.65244700
H	-6.16735000	1.39068800	-2.70784100
C	-7.12314200	-0.27719800	-0.72971000
H	-7.00511600	-0.80384800	-1.68912200
H	-7.02462800	-1.01253200	0.08349800
H	-8.14805500	0.12166900	-0.69388200
C	-1.21884600	5.95855500	0.10567400
H	-1.11426300	7.04218400	0.26447000
H	-1.77090500	5.81268300	-0.83555000
H	-1.82849400	5.56028200	0.93128500
C	0.87677900	5.57909100	1.39583900
H	0.32191800	5.12437800	2.23154400
H	1.89977700	5.17377600	1.40775600

H	0.94588900	6.66289800	1.57863900
C	0.96510900	5.95049500	-1.08935700
H	1.03735400	7.03898200	-0.93897600
H	1.99039900	5.55586100	-1.15059600
H	0.47321900	5.77003600	-2.05766400
C	6.44070400	1.33647000	0.95180600
H	5.80211300	2.22455100	1.07026800
H	6.23848400	0.65519100	1.79249000
H	7.48850500	1.66686900	1.02265900
C	7.17248600	-0.54671500	-0.51116300
H	7.05697200	-1.07805100	-1.46828200
H	8.20795800	-0.17925500	-0.45886200
H	7.03596800	-1.26959100	0.30759800
C	6.48327000	1.61388900	-1.54773500
H	7.53260100	1.94483000	-1.51077600
H	6.30888600	1.13537400	-2.52359400
H	5.84922700	2.51101600	-1.48872500

Structure of Ir3, T_1 state

C	3.68994100	1.14108000	-0.46528900
C	2.35462200	0.75874200	-0.49963100
C	2.98637200	-1.47736000	-0.72967500
C	4.33041400	-1.14236900	-0.70421200
C	4.71890200	0.19835600	-0.56745200
H	3.92148300	2.20074000	-0.35753200
H	2.66325500	-2.51471800	-0.83376100
H	5.06099200	-1.94485000	-0.79192800
C	1.22309700	1.69389100	-0.40089200
C	1.27386300	3.06185200	-0.24584900
C	0.05814100	3.80710400	-0.13895100
H	2.23767500	3.56700300	-0.19745400
C	-1.18005700	1.72391500	-0.40402800
C	-1.14600600	3.12455400	-0.23346900
H	-2.09059400	3.66250000	-0.16884200
C	-2.31027700	0.85684400	-0.50655900
C	-3.65888400	1.26980000	-0.46606300
C	-3.03686000	-1.37763700	-0.75650200
C	-4.70428300	0.37033200	-0.57502400
H	-3.85993000	2.33546000	-0.34622900
C	-4.36203300	-1.00239500	-0.72692800
H	-2.75125900	-2.42583300	-0.86751500
H	-5.11992500	-1.77747500	-0.82113000
N	2.01862300	-0.56062400	-0.63098800
N	0.02486800	1.07210700	-0.44394500

N	-2.02719600	-0.49976400	-0.65532800
Ir	-0.02568100	-0.87271400	-0.63429000
Cl	0.02235800	-0.53477300	-3.06385100
C	-0.03803900	-1.31717700	1.26490500
C	-0.02290000	-0.59204900	2.51273400
C	-0.06504400	-2.71644700	1.51608700
C	-0.03422100	-1.45833200	3.63576400
C	-0.00258500	0.79462600	2.74704000
S	-0.06847800	-3.15025400	3.16933600
C	-0.08876900	-3.62336800	0.39616000
C	-0.02230700	-0.98863300	4.94323300
C	0.01013700	1.27483900	4.05185100
H	0.00014300	1.49108300	1.91100800
C	-0.12326000	-5.01794900	0.45917100
N	-0.07482100	-2.96956600	-0.79812300
C	0.00117100	0.39400300	5.13946100
H	-0.03149400	-1.67473800	5.79214900
H	0.02635800	2.35245900	4.22702800
C	-0.14207400	-5.74314200	-0.72726800
H	-0.13516200	-5.51960000	1.42824600
C	-0.09110000	-3.66646900	-1.93586100
H	0.01110500	0.78820000	6.15799800
C	-0.12505200	-5.05957400	-1.94098900
H	-0.16960000	-6.83410600	-0.70332200
H	-0.07634100	-3.07123600	-2.85263300
H	-0.13854600	-5.59075300	-2.89341600
C	0.13953300	5.31550600	0.08407400
C	-6.15204600	0.85983600	-0.52829800
C	6.17550500	0.64728400	-0.52525500
C	-6.40169300	1.55782900	0.81823800
H	-6.23309100	0.86558300	1.65769500
H	-5.74236300	2.42759400	0.95717700
H	-7.44255300	1.91422600	0.87202800
C	-6.38336300	1.85530400	-1.67628700
H	-7.42408300	2.21567500	-1.66001500
H	-5.72427900	2.73263900	-1.59716600
H	-6.20087100	1.37978500	-2.65239400
C	-7.15002500	-0.29116700	-0.67318800
H	-7.03137600	-0.81747300	-1.63270200
H	-7.04865800	-1.02611600	0.13999800
H	-8.17611300	0.10462000	-0.63649500
C	-1.24486500	5.95964800	0.16995000
H	-1.13783900	7.04266300	0.33149300
H	-1.82056200	5.81779700	-0.75761200

H	-1.83265000	5.55611700	1.00876200
C	0.88432600	5.57886600	1.40355700
H	0.35238100	5.12035200	2.25196800
H	1.90808500	5.17563100	1.38732500
H	0.95617400	6.66219800	1.58824000
C	0.90747800	5.95925100	-1.08159700
H	0.98370200	7.04708400	-0.92817600
H	1.93075300	5.56495900	-1.17187900
H	0.38995800	5.78313800	-2.03725900
C	6.43651200	1.34526500	0.81974500
H	5.80014800	2.23252000	0.95495300
H	6.25274900	0.66077900	1.66203800
H	7.48533800	1.67612700	0.86940200
C	7.13980100	-0.53151700	-0.66536000
H	7.00515300	-1.05938200	-1.62186900
H	8.17553700	-0.16258300	-0.63338500
H	7.02146400	-1.25753900	0.15345400
C	6.42470300	1.63186700	-1.67948600
H	7.47401400	1.96438800	-1.66378600
H	6.23020800	1.15648300	-2.65304600
H	5.79059600	2.52765500	-1.60346000

Structure of Ir3, T_2 state

C	3.70225400	1.10760900	-0.52549100
C	2.35939200	0.74451400	-0.55352100
C	2.94904900	-1.50598200	-0.73160000
C	4.30110100	-1.19197800	-0.70976000
C	4.71316800	0.14385700	-0.60480000
H	3.95173000	2.16505400	-0.43741600
H	2.60723800	-2.53950900	-0.81075100
H	5.01736300	-2.00925400	-0.77480500
C	1.24227000	1.68304000	-0.45810800
C	1.28014400	3.04895500	-0.31243200
C	0.05284100	3.80709700	-0.17657000
H	2.24165800	3.56013600	-0.28440700
C	-1.20545200	1.73179000	-0.40325000
C	-1.16184100	3.12348900	-0.23657400
H	-2.10169000	3.66544600	-0.14704900
C	-2.34173400	0.86670200	-0.48496400
C	-3.68104800	1.29262300	-0.42140100
C	-3.06068300	-1.35244900	-0.70081100
C	-4.73600800	0.38642100	-0.50054700
H	-3.87634100	2.35920800	-0.30726600
C	-4.39711000	-0.97177500	-0.64368100

H	-2.78136000	-2.40215200	-0.81027600
H	-5.15422700	-1.75041300	-0.71325800
N	2.00083700	-0.57123000	-0.66068200
N	0.02320300	1.04964700	-0.48094000
N	-2.06076700	-0.47868700	-0.63115700
Ir	-0.03638500	-0.83754700	-0.67230900
Cl	-0.02004900	-0.69870300	-3.10127500
C	-0.01211100	-1.32104000	1.28660700
C	0.10675700	-0.56437700	2.50773300
C	-0.08957800	-2.67220800	1.54164200
C	0.09932800	-1.41222600	3.65110400
C	0.20164400	0.82580800	2.71748900
S	-0.03223900	-3.09480700	3.22924000
C	-0.16705900	-3.59520600	0.43806900
C	0.18231500	-0.90328700	4.95070400
C	0.28546200	1.33114500	4.00502600
H	0.20903300	1.50919800	1.87109400
C	-0.25822700	-4.98716800	0.53084700
N	-0.14721400	-2.97361600	-0.77251400
C	0.27801200	0.47211300	5.11742900
H	0.16914600	-1.57249200	5.81365000
H	0.35924500	2.41073600	4.15447000
C	-0.33563600	-5.73983000	-0.63259000
H	-0.26841300	-5.46221300	1.51316800
C	-0.22543600	-3.70483900	-1.89346900
H	0.34579500	0.88807100	6.12527400
C	-0.31918900	-5.08916800	-1.86668600
H	-0.40791800	-6.82804600	-0.57865500
H	-0.20691800	-3.14007300	-2.82772700
H	-0.37507700	-5.64125400	-2.80534900
C	0.15147200	5.30874200	0.04781300
C	-6.17860600	0.88109800	-0.42881700
C	6.17798600	0.56680600	-0.56717000
C	-6.39232500	1.59104200	0.91783100
H	-6.21037100	0.90455500	1.75896200
H	-5.72726700	2.45946200	1.03604500
H	-7.42983600	1.95269000	0.98876100
C	-6.42380500	1.86803600	-1.58148300
H	-7.46219900	2.23232300	-1.54641500
H	-5.76103800	2.74414900	-1.52258300
H	-6.26340400	1.38337900	-2.55678400
C	-7.18184000	-0.26790900	-0.54395000
H	-7.08480600	-0.80209300	-1.50152500
H	-7.06751100	-0.99551700	0.27403500

H	-8.20496800	0.13267200	-0.49012200
C	-1.22563200	5.96289400	0.16641400
H	-1.10563900	7.04452700	0.32624700
H	-1.82321800	5.82715900	-0.74804900
H	-1.79642600	5.56399800	1.01894500
C	0.92945200	5.55783600	1.35241300
H	0.41305200	5.10033400	2.21065700
H	1.95077600	5.15006900	1.31256100
H	1.01193300	6.64014200	1.53740600
C	0.90062200	5.94764300	-1.13399600
H	0.99117000	7.03327900	-0.97454600
H	1.91819500	5.54562400	-1.25040100
H	0.35869100	5.78303400	-2.07785200
C	6.44943400	1.27618500	0.76977200
H	5.82932600	2.17667100	0.89278900
H	6.25130700	0.60560100	1.61991200
H	7.50413700	1.58802200	0.81751200
C	7.12030800	-0.63139100	-0.69128400
H	6.97455500	-1.17046400	-1.63989700
H	8.16255600	-0.28083100	-0.66577100
H	6.99032200	-1.34314200	0.13818200
C	6.44691200	1.53214200	-1.73298200
H	7.50274700	1.84332400	-1.72080600
H	6.24308700	1.04924900	-2.70092700
H	5.83181000	2.44199500	-1.66803800

Structure of Ir4, S_0 state

C	2.88203600	-2.71780500	-0.59380400
C	1.96879600	-1.67713600	-0.53839900
C	0.23605000	-3.17632900	-0.14286400
C	1.11113000	-4.25587100	-0.18902500
C	2.47317500	-4.04894800	-0.41992600
H	3.93147200	-2.48416000	-0.77254100
H	-0.83047400	-3.31933500	0.03834400
H	0.70056500	-5.25319900	-0.03925700
C	2.33186800	-0.25520700	-0.69828500
C	3.59129800	0.28188400	-0.92925000
C	3.75739500	1.67371500	-1.03789900
H	4.44986400	-0.38294600	-1.01842900
C	1.37261400	1.90546000	-0.69960900
C	2.61904600	2.48320600	-0.93161100
H	2.69741800	3.56435200	-1.02202500
C	0.07547200	2.59154200	-0.53986200
C	-0.08382200	3.96705500	-0.59635400

C	-2.19815500	2.31284400	-0.13901100
C	-1.34504100	4.55698200	-0.42018000
H	0.79264100	4.58900200	-0.77774200
C	-2.41159100	3.68609100	-0.18545800
H	-3.01953400	1.61829900	0.04440300
H	-3.42616400	4.05097700	-0.03322600
N	0.64449600	-1.92015700	-0.31594200
N	1.28229100	0.57436800	-0.57226200
N	-0.99331600	1.77274000	-0.31491100
Ir	-0.48186800	-0.20999800	-0.27090000
Cl	-0.72213600	-0.31621600	-2.71645300
C	-0.48203100	-0.21045000	1.74124600
C	0.43458100	0.19187900	2.77765900
C	-1.64369300	-0.72208000	2.29047700
C	-0.09249400	-0.04073400	4.07952200
C	1.72291900	0.75708000	2.67793000
S	-1.68437800	-0.74090100	4.03589400
C	-2.68332500	-1.18263800	1.41420600
C	0.62734800	0.27444100	5.23682800
C	2.43714700	1.06908300	3.82305200
H	2.16245700	0.95045600	1.70076400
C	-3.91825100	-1.73027700	1.79138500
N	-2.36314200	-1.04407800	0.09580700
C	1.89241400	0.82925000	5.09732600
H	0.20403700	0.08799600	6.22613900
H	3.43441100	1.50601800	3.73460700
C	-4.81048000	-2.12995600	0.81383300
H	-4.16113000	-1.83793800	2.84938300
C	-3.22525300	-1.42979100	-0.85079200
H	2.46967900	1.08158000	5.98993600
C	-4.45901100	-1.97693200	-0.53320400
H	-5.77393800	-2.56301800	1.09114700
H	-2.89084400	-1.28781000	-1.88184700
C	5.15448100	2.24901500	-1.25331700
C	-1.49541600	6.07221100	-0.48561300
C	3.49611800	-5.17681900	-0.48524100
C	-0.61667000	6.70182700	0.60778200
H	-0.92338100	6.35847100	1.60757600
H	0.44808900	6.45932800	0.47402200
H	-0.71484900	7.79772100	0.57639200
C	-1.03134500	6.55417100	-1.86997700
H	-1.13411900	7.64818100	-1.93449900
H	0.02327500	6.30722600	-2.06297700
H	-1.64013000	6.10474100	-2.66927300

C	-2.94461200	6.50983000	-0.26937300
H	-3.61573900	6.09880000	-1.03896300
H	-3.32070500	6.20755100	0.71996200
H	-3.00746800	7.60641100	-0.32655000
C	5.13468400	3.77393600	-1.36838200
H	6.15972800	4.14041100	-1.52422200
H	4.52906600	4.11368100	-2.22248200
H	4.75027500	4.25054000	-0.45366400
C	6.02994800	1.85394500	-0.05209200
H	5.61364000	2.25106300	0.88654600
H	6.12407900	0.76259600	0.05026700
H	7.04278300	2.26543200	-0.17997500
C	5.74291700	1.66254200	-2.54667400
H	6.75194600	2.07007700	-2.71135900
H	5.83116100	0.56676400	-2.50488700
H	5.12142100	1.92332300	-3.41684500
C	4.55739500	-4.94382800	0.60266300
H	5.09230500	-3.99255600	0.46324000
H	4.10152600	-4.93687700	1.60451900
H	5.30358000	-5.75237900	0.57098300
C	2.84996100	-6.54464500	-0.26168100
H	2.09430900	-6.77118100	-1.02931100
H	3.62173500	-7.32638000	-0.31618900
H	2.37465100	-6.61649200	0.72854100
C	4.15865200	-5.16020600	-1.87274000
H	4.90180900	-5.96961400	-1.93779000
H	3.41356300	-5.31398600	-2.66817100
H	4.68059300	-4.21228200	-2.07147900
C	-5.41501900	-2.38029600	-1.61752700
F	-6.46421300	-1.55133300	-1.67762900
F	-4.83613500	-2.37912100	-2.81936900
F	-5.90332900	-3.60613400	-1.40097600

Structure of Ir4, S_1 state

C	2.25872600	-3.30387500	-0.54911000
C	1.58761300	-2.08759600	-0.50928000
C	-0.42909100	-3.19864300	-0.12001600
C	0.19766200	-4.43318900	-0.15387100
C	1.58121800	-4.51494100	-0.37317800
H	3.33475700	-3.29476100	-0.72367500
H	-1.50388500	-3.11594900	0.05025100
H	-0.41322500	-5.32233300	-0.00691200
C	2.23457000	-0.77882100	-0.68319000
C	3.57296700	-0.52219200	-0.88685600

C	4.02520300	0.82740100	-1.00301100
H	4.27985400	-1.34833700	-0.95058200
C	1.71937600	1.56783100	-0.73651900
C	3.08479600	1.84776200	-0.93870400
H	3.39342200	2.88733200	-1.03530500
C	0.62310600	2.47997500	-0.61990100
C	0.72595800	3.88384400	-0.69234700
C	-1.70191800	2.69769900	-0.28963700
C	-0.38029000	4.70702900	-0.56750400
H	1.71599400	4.31383500	-0.85023000
C	-1.63478700	4.07292900	-0.36198500
H	-2.65546600	2.19107000	-0.12772600
H	-2.55706200	4.64062400	-0.25798900
N	0.23618400	-2.05156500	-0.29283600
N	1.36718600	0.25248400	-0.58869200
N	-0.62735800	1.90693800	-0.41232100
Ir	-0.52169200	-0.13083000	-0.26274600
Cl	-0.81525700	-0.27760700	-2.68931700
C	-0.46732900	-0.02279500	1.68491800
C	0.52074100	0.26627200	2.69628300
C	-1.72938500	-0.25952500	2.29818600
C	-0.02416500	0.23373500	4.00495400
C	1.88891400	0.55896500	2.55858700
S	-1.73627100	-0.14372500	3.99913900
C	-2.86387700	-0.55145400	1.45742000
C	0.73589400	0.47885400	5.14075500
C	2.66095900	0.80599800	3.69051500
H	2.34560000	0.59381600	1.57219100
C	-4.16729000	-0.81841800	1.88311900
N	-2.54071500	-0.54684100	0.13573900
C	2.09290900	0.76757600	4.96724100
H	0.29296300	0.44809800	6.13774100
H	3.72273700	1.03261800	3.57578400
C	-5.14371300	-1.07969400	0.93325800
H	-4.40700600	-0.82198800	2.94727100
C	-3.47612300	-0.79656600	-0.77982600
H	2.71233200	0.96451300	5.84471400
C	-4.79263500	-1.06487400	-0.41701300
H	-6.16838600	-1.29737200	1.24003100
H	-3.14089900	-0.77789300	-1.82057300
C	5.51905200	1.08971400	-1.17996300
C	-0.22485800	6.22575000	-0.64970700
C	2.34441800	-5.83422600	-0.42245800
C	0.72783600	6.69334400	0.46215800

H	0.33314700	6.42930700	1.45555700
H	1.72681600	6.24314300	0.36254000
H	0.84834400	7.78739900	0.42132200
C	0.36087900	6.59660100	-2.02141700
H	0.47596400	7.68914200	-2.10035500
H	1.35076600	6.14341700	-2.18032200
H	-0.30090000	6.26231700	-2.83536900
C	-1.56365500	6.94701300	-0.47967200
H	-2.28160500	6.66827100	-1.26613600
H	-2.02161100	6.73469100	0.49857500
H	-1.40695600	8.03425600	-0.54383400
C	5.82974300	2.58213900	-1.30334000
H	6.91351700	2.72352000	-1.42907800
H	5.33273300	3.03267500	-2.17623000
H	5.52545300	3.13968100	-0.40416600
C	6.26446100	0.53407800	0.04507100
H	5.92206400	1.02653500	0.96878400
H	6.11414200	-0.54966700	0.16277000
H	7.34658200	0.71093100	-0.05757300
C	6.01145700	0.38065700	-2.45169700
H	7.09029900	0.55492300	-2.58703400
H	5.85506800	-0.70752800	-2.40645100
H	5.48801500	0.76267200	-3.34173800
C	3.40791100	-5.83068700	0.68800200
H	4.13118800	-5.01083800	0.56478900
H	2.94211900	-5.72958600	1.68025400
H	3.96990200	-6.77711700	0.66799100
C	1.42039100	-7.03559400	-0.21714000
H	0.64808200	-7.09656600	-0.99914500
H	2.01043400	-7.96288900	-0.26129100
H	0.92203000	-7.00660600	0.76388600
C	3.02539600	-5.96188000	-1.79492800
H	3.58150000	-6.91054700	-1.84742200
H	2.28185100	-5.95495200	-2.60654800
H	3.74009100	-5.14613500	-1.97938200
C	-5.83361800	-1.30224000	-1.47903100
F	-6.57293500	-0.20784300	-1.67862800
F	-5.28015900	-1.63239300	-2.64521800
F	-6.66516700	-2.28262500	-1.12326500

Structure of Ir4, T_1 state

C	3.30145700	-2.23152500	-0.60660900
C	2.23389900	-1.34463300	-0.53993100
C	0.76447800	-3.12030300	-0.16291500

C	1.79756100	-4.04094200	-0.22286000
C	3.11273800	-3.60905000	-0.44987700
H	4.29824500	-1.82856500	-0.78671900
H	-0.26525300	-3.43601000	0.01334800
H	1.55467200	-5.09382100	-0.08962000
C	2.35734400	0.11275500	-0.69257900
C	3.50660500	0.84177400	-0.90481000
C	3.43425800	2.26650200	-0.99969900
H	4.46412100	0.32993300	-0.99134500
C	1.01981100	2.11003200	-0.70287500
C	2.18915600	2.87220300	-0.90957000
H	2.09562600	3.95397900	-0.99204200
C	-0.33211500	2.55227800	-0.57584500
C	-0.75767100	3.89571000	-0.63823600
C	-2.57654600	1.89172200	-0.24237400
C	-2.08866800	4.24971000	-0.50926100
H	0.00302500	4.66209200	-0.79319000
C	-3.02084900	3.19362200	-0.30671100
H	-3.27408600	1.06711700	-0.08162800
H	-4.08723800	3.38046300	-0.19761200
N	0.96621600	-1.80776800	-0.31662000
N	1.17496600	0.75500300	-0.56849800
N	-1.28368700	1.55440700	-0.37132100
Ir	-0.44161700	-0.29414000	-0.24666400
Cl	-0.66439900	-0.52057900	-2.67681900
C	-0.40489000	-0.24216500	1.70278100
C	0.44442100	0.32724000	2.72090800
C	-1.48969400	-0.93498300	2.30659300
C	-0.02635200	0.04644600	4.02898800
C	1.61852400	1.08970700	2.58949800
S	-1.49947600	-0.90581800	4.01451300
C	-2.45881200	-1.58157500	1.45819200
C	0.62672900	0.49235500	5.17149700
C	2.28031200	1.53987100	3.72665300
H	2.00795800	1.32955800	1.60217500
C	-3.57711200	-2.30806600	1.87447500
N	-2.17511700	-1.42181300	0.13631600
C	1.79130100	1.24490900	5.00438400
H	0.24511900	0.26411000	6.16834400
H	3.19186800	2.13102900	3.61826500
C	-4.40910900	-2.86885600	0.91585500
H	-3.78703000	-2.43049000	2.93794300
C	-2.96889400	-1.96147900	-0.78659900
H	2.32360600	1.60682600	5.88672700

C	-4.10131400	-2.69057000	-0.43282300
H	-5.28665400	-3.44542800	1.21365100
H	-2.67119700	-1.79701500	-1.82623900
C	4.72776800	3.05651200	-1.18475200
C	-2.50746400	5.71834600	-0.58067600
C	4.30248000	-4.55895800	-0.53303200
C	-1.80676400	6.49344500	0.54683100
H	-2.08490600	6.09084400	1.53316600
H	-0.71119800	6.44645100	0.45691300
H	-2.10046600	7.55455400	0.51483500
C	-2.08792700	6.29566700	-1.94197600
H	-2.38743600	7.35330000	-2.01179000
H	-0.99894500	6.24619500	-2.09072000
H	-2.56935800	5.74820500	-2.76701800
C	-4.01992900	5.88999400	-0.42365500
H	-4.57564800	5.37059600	-1.21931900
H	-4.37591900	5.51625700	0.54860400
H	-4.27700600	6.95828600	-0.48242600
C	4.47295300	4.56098900	-1.28669600
H	5.42944400	5.08823900	-1.41921100
H	3.83449500	4.81027000	-2.14816900
H	3.99913300	4.95897400	-0.37621400
C	5.64074500	2.79502400	0.02493600
H	5.15610500	3.11959900	0.95914000
H	5.89486700	1.72922800	0.12723700
H	6.58374000	3.35326200	-0.08464200
C	5.42726100	2.59069000	-2.47180500
H	6.36586000	3.14886400	-2.61361300
H	5.68026700	1.52032800	-2.44230000
H	4.78832100	2.76517200	-3.35125200
C	5.32805600	-4.16577000	0.54278400
H	5.70143600	-3.14027000	0.40420900
H	4.89069600	-4.23767300	1.55037600
H	6.19374900	-4.84411700	0.49572200
C	3.88756300	-6.01409400	-0.31033200
H	3.17143500	-6.35776400	-1.07228100
H	4.77469600	-6.66115300	-0.37492500
H	3.43879200	-6.16459700	0.68351200
C	4.93581300	-4.43072100	-1.92835200
H	5.79847000	-5.10991100	-2.00867500
H	4.21412900	-4.69817200	-2.71529600
H	5.29467400	-3.40977000	-2.12647000
C	-4.99821700	-3.23977500	-1.51073900
F	-5.97879600	-2.38114100	-1.80387900

F	-4.32226300	-3.47334200	-2.63578000
F	-5.57020600	-4.38110400	-1.12661600

Structure of Ir4, T_2 state

C	-2.72503800	2.88079600	-0.65548300
C	-1.86944100	1.77669200	-0.59173200
C	-0.05103800	3.20949400	-0.22615600
C	-0.86308900	4.33048900	-0.28508300
C	-2.24671400	4.18215600	-0.50490900
H	-3.78658900	2.70060600	-0.82655400
H	1.02307300	3.30128600	-0.05356000
H	-0.40148400	5.30758700	-0.15694300
C	-2.29974000	0.39823300	-0.73282000
C	-3.59975700	-0.09320500	-0.92245700
C	-3.82532400	-1.48767700	-0.99445000
H	-4.43031700	0.60645400	-0.99521500
C	-1.43553300	-1.84585900	-0.71631800
C	-2.73298800	-2.36265000	-0.90356700
H	-2.87054800	-3.43909600	-0.96115800
C	-0.19484500	-2.57847200	-0.56878400
C	-0.08985700	-3.97287600	-0.62580100
C	2.11290700	-2.42079000	-0.20424200
C	1.13863500	-4.61681000	-0.47164800
H	-0.99789900	-4.55180700	-0.79487900
C	2.26254300	-3.79961000	-0.25585700
H	2.97205100	-1.76846900	-0.03582400
H	3.26029000	-4.21393100	-0.12539200
N	-0.52355200	1.97063900	-0.37462700
N	-1.28338900	-0.49673700	-0.62460800
N	0.93359700	-1.82047900	-0.35526200
Ir	0.49852900	0.19178000	-0.29746800
Cl	0.90680900	0.32779200	-2.68406800
C	0.40930500	0.17028700	1.68297200
C	-0.57780300	-0.18851000	2.66912900
C	1.58405900	0.61864500	2.30628000
C	-0.09892500	0.00381100	3.99309200
C	-1.88666500	-0.68212600	2.50672500
S	1.53512700	0.61797200	4.02455000
C	2.69164700	1.03595900	1.48679700
C	-0.87336500	-0.27737900	5.11527200
C	-2.66490100	-0.96483600	3.62336900
H	-2.29777500	-0.84508400	1.51355300
C	3.92594400	1.51143200	1.94051200
N	2.42739600	0.92930700	0.15565400

C	-2.16517800	-0.76469200	4.91605400
H	-0.48276500	-0.12214000	6.12271400
H	-3.67848000	-1.34715700	3.48619300
C	4.89133000	1.87316300	1.01497900
H	4.11770300	1.59642400	3.01085200
C	3.35609300	1.27599400	-0.73759300
H	-2.79038200	-0.99160000	5.78223700
C	4.60191000	1.75065200	-0.34550000
H	5.85983300	2.25324300	1.34559200
H	3.07458400	1.16944400	-1.78810700
C	-5.25828500	-1.99484400	-1.14191400
C	1.21742000	-6.13947900	-0.53814300
C	-3.20850500	5.36489300	-0.58010900
C	0.33496100	-6.72950100	0.57394700
H	0.67799100	-6.39934700	1.56653200
H	-0.71957100	-6.43667500	0.46214400
H	0.38166300	-7.82912300	0.54342700
C	0.70379300	-6.60419100	-1.91061500
H	0.75658000	-7.70197600	-1.97620000
H	-0.34231600	-6.30961600	-2.08139500
H	1.31446800	-6.18255300	-2.72369800
C	2.64856500	-6.64606600	-0.35151000
H	3.32223400	-6.26806000	-1.13566900
H	3.05984300	-6.36000000	0.62860100
H	2.65839400	-7.74468200	-0.40716500
C	-5.32564000	-3.52017400	-1.23655500
H	-6.37386200	-3.83515800	-1.34722800
H	-4.77038300	-3.90051500	-2.10757200
H	-4.92850700	-4.00505500	-0.33177500
C	-6.06236000	-1.54397100	0.08972200
H	-5.62171900	-1.94744100	1.01499000
H	-6.09742800	-0.44815400	0.17999100
H	-7.09904000	-1.90821500	0.01597300
C	-5.87963400	-1.39834500	-2.41509300
H	-6.91462100	-1.75650900	-2.52918900
H	-5.90942500	-0.29919000	-2.38696900
H	-5.31199900	-1.70132400	-3.30842700
C	-4.27364100	5.20982300	0.51761300
H	-4.85956400	4.28662400	0.39635800
H	-3.81095600	5.19198200	1.51638800
H	-4.97508900	6.05770600	0.48002900
C	-2.48879200	6.69990700	-0.38095100
H	-1.72774800	6.87468500	-1.15674200
H	-3.21762800	7.52177600	-0.44067100

H	-2.00149000	6.75933600	0.60427400
C	-3.88327400	5.36873900	-1.96156000
H	-4.58005400	6.21819600	-2.03470600
H	-3.13688500	5.46768800	-2.76466400
H	-4.45833300	4.44833700	-2.14193600
C	5.63508500	2.09572800	-1.38380200
F	6.33070800	3.17690900	-1.02735500
F	5.07840300	2.33566700	-2.57101400
F	6.50956400	1.09812400	-1.54471900

Structure of Ir5, S_0 state

C	-1.77563800	1.54468800	3.59636600
C	-1.39473200	1.32480900	2.27708700
C	0.65881400	0.44989600	2.97124300
C	0.33287400	0.64591900	4.30898300
C	-0.90174100	1.20240300	4.62541300
H	-2.75050700	1.97813100	3.81947900
H	1.61364600	0.01520400	2.67148100
H	1.04667000	0.36064600	5.08250000
H	-1.18882100	1.36835500	5.66524700
C	-2.24263700	1.63880800	1.11239000
C	-3.50683900	2.22540900	1.10929700
C	-4.13767600	2.44281000	-0.11551800
H	-3.99351000	2.51256100	2.04089800
C	-2.25016900	1.50798500	-1.25999500
C	-3.51407400	2.09338900	-1.31318400
H	-5.12818800	2.89986700	-0.13729700
H	-4.00599600	2.27834100	-2.26764100
C	-1.41073300	1.06583200	-2.38887900
C	-1.80339300	1.13358300	-3.72145500
C	0.63707600	0.11638800	-2.99717800
C	-0.93818900	0.67634900	-4.71245200
H	-2.78097900	1.53770900	-3.98397300
C	0.29946800	0.15914500	-4.34561600
H	1.59453100	-0.28204600	-2.65840700
H	-1.23449600	0.72264200	-5.76185500
H	1.00643500	-0.21298400	-5.08788300
N	-0.17722300	0.78295100	1.98528800
N	-1.68431200	1.29170000	-0.06000600
N	-0.19029700	0.56007700	-2.04823800
Ir	0.12793500	0.55964800	-0.02591600
Cl	0.91452100	2.88568700	-0.15142500
C	-0.30501000	-1.40636600	0.07780700
C	-1.50552900	-2.20228200	0.11513000

C	0.81598600	-2.21184100	0.11279900
C	-1.22237500	-3.59587800	0.17773500
C	-2.85773300	-1.80361700	0.10037200
S	0.48635400	-3.92373200	0.18989200
C	2.11780300	-1.60026900	0.07869800
C	-2.23759100	-4.55678100	0.22270000
C	-3.86480900	-2.75426400	0.14458200
H	-3.11559700	-0.74651100	0.05493700
C	3.35618400	-2.25299100	0.10783000
N	2.06019400	-0.24077800	0.00907000
C	-3.55725100	-4.12510200	0.20524500
H	-1.99740800	-5.62108900	0.27002400
H	-4.90933700	-2.43506900	0.13253700
C	4.52532900	-1.51125800	0.06602400
H	3.39303100	-3.34203600	0.16324200
C	3.18251500	0.48601100	-0.03168500
H	-4.36401800	-4.86104600	0.23917200
C	4.43336400	-0.11854800	-0.00499700
H	5.50142300	-1.99868600	0.08807800
H	3.05427500	1.57029700	-0.08568300
Cl	5.84829600	0.86369800	-0.06050800

Structure of Ir5, S_1 state

C	-1.79470400	1.33269400	3.68351200
C	-1.42215200	1.19171200	2.33762000
C	0.68284300	0.36293000	3.00568200
C	0.36136800	0.49034100	4.34262300
C	-0.90906000	0.98597000	4.68625700
H	-2.78563600	1.71664300	3.92772700
H	1.65473900	-0.01866400	2.68795300
H	1.09044100	0.20810800	5.10241100
H	-1.19614700	1.09644600	5.73354400
C	-2.26565300	1.52576700	1.20800300
C	-3.54683200	2.06609700	1.21802100
C	-4.18920500	2.32266700	-0.00072800
H	-4.04531600	2.29450300	2.16039500
C	-2.26701000	1.52240000	-1.20972000
C	-3.54850100	2.06277400	-1.21922600
H	-5.19427400	2.74599700	-0.00065900
H	-4.04822200	2.28858000	-2.16159000
C	-1.42512900	1.18527800	-2.33908000
C	-1.79913900	1.32228700	-3.68519600
C	0.67937200	0.35464500	-3.00741600
C	-0.91467600	0.97282600	-4.68783600

H	-2.79042000	1.70536700	-3.92939400
C	0.35640500	0.47824700	-4.34427600
H	1.65165800	-0.02598100	-2.68970000
H	-1.20297200	1.08024700	-5.73511100
H	1.08462500	0.19400900	-5.10412300
N	-0.17118400	0.69996900	2.02564600
N	-1.69726200	1.24335500	-0.00065500
N	-0.17349800	0.69441100	-2.02725700
Ir	0.12746500	0.54114300	-0.00090000
Cl	0.90304800	2.86844200	-0.00471500
C	-0.31597400	-1.36057400	0.00181600
C	-1.51501600	-2.16015300	0.00290600
C	0.82932900	-2.20898200	0.00296400
C	-1.23650700	-3.55057800	0.00497500
C	-2.86169800	-1.75522600	0.00220000
S	0.48675600	-3.88040100	0.00542800
C	2.13530100	-1.60438300	0.00174300
C	-2.23504600	-4.51408000	0.00637000
C	-3.87157800	-2.71304400	0.00356500
H	-3.11193300	-0.69658700	0.00053400
C	3.36441000	-2.26926000	0.00269300
N	2.07609200	-0.24381000	-0.00059300
C	-3.56356900	-4.07672700	0.00563600
H	-1.99627900	-5.57894900	0.00795800
H	-4.91530300	-2.39357900	0.00298600
C	4.53845900	-1.53068100	0.00120400
H	3.39825800	-3.35976400	0.00458300
C	3.19378100	0.47743200	-0.00206300
H	-4.36750100	-4.81580600	0.00668700
C	4.44868300	-0.13817700	-0.00124500
H	5.51238400	-2.02202300	0.00191400
H	3.07134700	1.56423900	-0.00388300
Cl	5.85563600	0.84008300	-0.00327400

Structure of Ir5, T_1 state

C	-1.78580900	-1.37804100	-3.67468700
C	-1.42012700	-1.21538800	-2.33093200
C	0.68842700	-0.39942200	-2.99842900
C	0.37468900	-0.54932700	-4.33527500
C	-0.89251300	-1.04839400	-4.67788400
H	-2.77559600	-1.76507100	-3.91835000
H	1.65825400	-0.01318700	-2.68006400
H	1.10843000	-0.28007600	-5.09542300
H	-1.17326200	-1.17576900	-5.72507000
C	-2.27090600	-1.53410500	-1.19822800

C	-3.54792100	-2.07612500	-1.20879300
C	-4.19587500	-2.32095200	0.01442200
H	-4.04128400	-2.31775600	-2.15058600
C	-2.27401700	-1.50769200	1.22119700
C	-3.55818000	-2.05008800	1.22826500
H	-5.20056400	-2.74557300	0.01583100
H	-4.05895200	-2.26971500	2.17190200
C	-1.43334600	-1.16869100	2.34384700
C	-1.80205300	-1.30186900	3.69450700
C	0.67759300	-0.33817700	3.00740800
C	-0.91415900	-0.95292800	4.69181000
H	-2.79320200	-1.68289300	3.94285600
C	0.35901700	-0.46006200	4.34411800
H	1.64918800	0.04119600	2.68579400
H	-1.19908100	-1.05839000	5.74036800
H	1.08956200	-0.17602200	5.10184400
N	-0.17382800	-0.71959200	-2.01976200
N	-1.70426800	-1.23319100	0.00653800
N	-0.17921700	-0.67847400	2.02906700
Ir	0.11980600	-0.53314500	0.00676200
Cl	0.89495400	-2.86285300	0.02613100
C	-0.31137500	1.36833900	-0.01307900
C	-1.50857700	2.17073500	-0.01960500
C	0.83782600	2.21193700	-0.02398200
C	-1.22483000	3.56020000	-0.03623100
C	-2.85604900	1.76837500	-0.01076700
S	0.50018500	3.88661000	-0.04293900
C	2.14080700	1.60307100	-0.01584400
C	-2.22209300	4.52603100	-0.04481300
C	-3.86264300	2.72780400	-0.01926000
H	-3.10713200	0.70948500	0.00333100
C	3.37292100	2.26319700	-0.02419200
N	2.07676200	0.24247600	0.00260700
C	-3.55031300	4.09173200	-0.03624100
H	-1.98104700	5.59039700	-0.05745200
H	-4.90752100	2.41182000	-0.01228200
C	4.54386700	1.51953700	-0.01317700
H	3.41118000	3.35348500	-0.03908900
C	3.19124500	-0.48327300	0.01318200
H	-4.35285600	4.83257300	-0.04256600
C	4.44876600	0.12742400	0.00586900
H	5.51982300	2.00692700	-0.01914600
H	3.06454800	-1.56954700	0.02733600
Cl	5.85205200	-0.85638600	0.02026400

Structure of Ir5, T_2 state

C	1.79142400	-1.32629400	3.70170000
C	1.42149700	-1.19329200	2.35419700
C	-0.67972800	-0.35385900	2.99324200
C	-0.36266800	-0.46898200	4.34101900
C	0.89674200	-0.96474600	4.69562700
H	2.78003300	-1.70948200	3.95500400
H	-1.64779400	0.02849700	2.66512800
H	-1.09469700	-0.17317500	5.09274400
H	1.17673900	-1.06531400	5.74583900
C	2.26536900	-1.52813300	1.23110200
C	3.54762600	-2.05912500	1.23012100
C	4.19167700	-2.31660400	-0.00115900
H	4.05478300	-2.28152100	2.16896100
C	2.26539600	-1.52679900	-1.23258800
C	3.54767700	-2.05780600	-1.23213500
H	5.19935000	-2.73288700	-0.00136500
H	4.05484300	-2.27919600	-2.17120900
C	1.42156800	-1.19077800	-2.35531500
C	1.79154700	-1.32230900	-3.70296500
C	-0.67967000	-0.35072400	-2.99353500
C	0.89689000	-0.95972800	-4.69652700
H	2.78018800	-1.70517200	-3.95664000
C	-0.36255900	-0.46439100	-4.34142900
H	-1.64775400	0.03126800	-2.66504700
H	1.17692900	-1.05914900	-5.74683700
H	-1.09457100	-0.16779500	-5.09285900
N	0.17631300	-0.70658900	2.03213500
N	1.67039900	-1.25337500	-0.00058200
N	0.17633800	-0.70446000	-2.03277800
Ir	-0.10772900	-0.59244300	-0.00026800
Cl	-1.06219100	-2.82268600	-0.00145000
C	0.30804300	1.38592600	0.00071600
C	1.52816300	2.15186700	0.00107700
C	-0.79828100	2.20451400	0.00107300
C	1.26414800	3.55091900	0.00176400
C	2.87342700	1.73297600	0.00084500
S	-0.43765600	3.90809900	0.00192600
C	-2.11043700	1.61519700	0.00075100
C	2.29317200	4.49781200	0.00221300
C	3.89298400	2.67050000	0.00129400
H	3.11598800	0.67188100	0.00031700
C	-3.32907600	2.30248500	0.00103900

N	-2.08139900	0.25504300	0.00012200
C	3.60591900	4.04699400	0.00197600
H	2.06694800	5.56613000	0.00273100
H	4.93235100	2.33515900	0.00111300
C	-4.51765500	1.59195900	0.00068000
H	-3.33541800	3.39341000	0.00154900
C	-3.22439100	-0.43992900	-0.00022700
H	4.42329500	4.77175900	0.00231800
C	-4.46014600	0.19644100	0.00003900
H	-5.48064600	2.10521600	0.00089300
H	-3.13595300	-1.52818500	-0.00072800
Cl	-5.89607500	-0.75330300	-0.00042900

Structure of Ir6, S_0 state

C	1.81441500	-1.08548200	3.67522700
C	1.41219700	-1.00917300	2.34608500
C	-0.75033000	-0.39949500	2.99132500
C	-0.40607800	-0.45911200	4.33749100
C	0.89472100	-0.80855900	4.68378000
H	2.84103300	-1.35652100	3.92119200
H	-1.75701300	-0.13013500	2.66803100
H	-1.15758300	-0.23150800	5.09423300
H	1.19737000	-0.86401500	5.73093000
C	2.30337500	-1.26957200	1.20055800
C	3.64200800	-1.65650300	1.23055200
C	4.30605600	-1.85319900	0.01986600
H	4.16109500	-1.80479300	2.17711700
C	2.30491300	-1.29349500	-1.17525500
C	3.64369100	-1.68064500	-1.19543000
H	5.35518800	-2.15287400	0.02350700
H	4.16446300	-1.84744200	-2.13794000
C	1.41514300	-1.05565300	-2.32688400
C	1.81835300	-1.15944400	-3.65391300
C	-0.74574800	-0.45501800	-2.98629700
C	0.90006600	-0.90088200	-4.66862500
H	2.84449800	-1.43767300	-3.89388100
C	-0.40028000	-0.54177700	-4.33066500
H	-1.75221600	-0.17742700	-2.66930700
H	1.20351900	-0.97793400	-5.71417600
H	-1.15056400	-0.32757000	-5.09251200
N	0.13023200	-0.67067500	2.02543300
N	1.70573700	-1.08798100	0.01032900
N	0.13334100	-0.70887900	-2.01435700
Ir	-0.19279100	-0.62354200	0.00471300

Cl	-0.64360000	-3.04073900	0.02706800
C	-0.04052900	1.38808700	-0.01314700
C	1.03608000	2.34607000	-0.02061000
C	-1.26314700	2.02682400	-0.01887600
C	0.55902200	3.68717000	-0.03166000
C	2.43092300	2.14197100	-0.01851500
S	-1.17934300	3.76957500	-0.03309500
C	-2.46756600	1.23587600	-0.01216700
C	1.42833300	4.78283000	-0.04014500
C	3.29368800	3.22637700	-0.02697700
H	2.83550900	1.13076500	-0.01044900
C	-3.78487900	1.71063800	-0.01621200
N	-2.21835500	-0.10250800	-0.00051800
C	2.79586300	4.54136900	-0.03766500
H	1.04053300	5.80390700	-0.04847100
H	4.37285200	3.05746200	-0.02530900
C	-4.84011700	0.81182900	-0.00806900
H	-3.97208400	2.78540500	-0.02561100
C	-3.22758000	-0.98170000	0.00746300
H	3.49066500	5.38449200	-0.04416300
C	-4.54321600	-0.54754100	0.00395100
H	-5.87945400	1.14525700	-0.01076800
H	-2.96187000	-2.04217400	0.01683600
F	-5.51703400	-1.44728900	0.01221300

Structure of Ir6, S_1 state

C	1.81474300	-1.12790600	3.68213300
C	1.42511800	-1.04060200	2.33647000
C	-0.76692900	-0.48299500	3.00596200
C	-0.42949000	-0.56229200	4.34268400
C	0.89391100	-0.89237200	4.68547200
H	2.84706000	-1.38112800	3.92556400
H	-1.77960400	-0.22821900	2.68837100
H	-1.18682900	-0.37015900	5.10295100
H	1.19443900	-0.96119000	5.73255600
C	2.30331500	-1.26465800	1.20614900
C	3.64277300	-1.63797800	1.21508900
C	4.31176600	-1.81029300	-0.00409300
H	4.16648400	-1.80224600	2.15717400
C	2.30271700	-1.25987600	-1.21139000
C	3.64240200	-1.63319800	-1.22206200
H	5.36233500	-2.10300600	-0.00485400
H	4.16576400	-1.79378500	-2.16499000
C	1.42427900	-1.03150200	-2.34023600

C	1.81338600	-1.11348500	-3.68655200
C	-0.76826200	-0.47176100	-3.00698900
C	0.89222000	-0.87435600	-4.68858100
H	2.84570000	-1.36546500	-3.93128800
C	-0.43131200	-0.54592500	-4.34406700
H	-1.78090600	-0.21841400	-2.68813400
H	1.19240300	-0.93902400	-5.73602800
H	-1.18897400	-0.35118600	-5.10334100
N	0.12076200	-0.71513600	2.02538000
N	1.70301100	-1.05543300	-0.00196400
N	0.11976700	-0.70738100	-2.02751100
Ir	-0.19877900	-0.60021700	-0.00087900
Cl	-0.66045400	-3.01062800	-0.00563800
C	-0.01376200	1.34392700	0.00248400
C	1.06713800	2.29665200	0.00378400
C	-1.26256400	2.03059600	0.00396300
C	0.60543900	3.63744600	0.00640100
C	2.45565300	2.07416200	0.00285900
S	-1.14743500	3.73279200	0.00715800
C	-2.47594200	1.25541100	0.00261600
C	1.46694500	4.72521100	0.00812000
C	3.32903700	3.15772700	0.00454000
H	2.84365900	1.05786000	0.00085200
C	-3.78315200	1.75144700	0.00340800
N	-2.23376700	-0.08453200	0.00022900
C	2.84202500	4.46817800	0.00714500
H	1.08975100	5.74949300	0.01015200
H	4.40600600	2.98016400	0.00381100
C	-4.84933800	0.86392300	0.00175000
H	-3.96020700	2.82791100	0.00534500
C	-3.24489900	-0.94947300	-0.00131700
H	3.54045400	5.30765800	0.00843300
C	-4.56260400	-0.49584800	-0.00062300
H	-5.88498500	1.20725200	0.00227900
H	-2.99237500	-2.01380100	-0.00305200
F	-5.53595600	-1.38373700	-0.00227100

Structure of Ir6, T_1 state

C	1.81699200	-1.13082000	3.68435600
C	1.43249900	-1.03578000	2.33707800
C	-0.76573400	-0.49200500	3.00309600
C	-0.43318600	-0.58062300	4.33990200
C	0.89074700	-0.90730700	4.68487100
H	2.84939100	-1.38136100	3.93023100

H	-1.77798700	-0.23886000	2.68281300
H	-1.19402800	-0.39764200	5.09901700
H	1.18727400	-0.98279800	5.73276300
C	2.31367900	-1.25081400	1.20898200
C	3.65393200	-1.62116200	1.21734900
C	4.32490100	-1.79251700	-0.00134300
H	4.17674000	-1.78587700	2.16006600
C	2.31327900	-1.24992300	-1.21062500
C	3.65353700	-1.62026100	-1.21967200
H	5.37629500	-2.08277500	-0.00163000
H	4.17604400	-1.78433700	-2.16267100
C	1.43166000	-1.03430900	-2.33823600
C	1.81559500	-1.12858600	-3.68573100
C	-0.76693200	-0.49045100	-3.00305400
C	0.88891400	-0.90460400	-4.68573500
H	2.84789900	-1.37895500	-3.93218800
C	-0.43491900	-0.57823700	-4.34004600
H	-1.77908800	-0.23762900	-2.68220700
H	1.18500700	-0.97954200	-5.73378900
H	-1.19609300	-0.39488400	-5.09873800
N	0.12797900	-0.71291200	2.02429500
N	1.71261200	-1.03831100	-0.00063900
N	0.12720000	-0.71183900	-2.02474500
Ir	-0.18972400	-0.59184100	-0.00013100
Cl	-0.64204900	-3.00642900	-0.00042400
C	-0.02387000	1.35109700	0.00036100
C	1.05137200	2.31038200	0.00072200
C	-1.27831100	2.02798700	0.00040900
C	0.57966300	3.64789000	0.00085600
C	2.44113000	2.09568500	0.00086700
S	-1.17481300	3.73315400	0.00062200
C	-2.48548200	1.24453000	0.00045000
C	1.43546300	4.74113500	0.00114200
C	3.30698700	3.18378400	0.00116600
H	2.83382300	1.08058700	0.00068800
C	-3.79673700	1.73076800	0.00061600
N	-2.23360700	-0.09387500	0.00036200
C	2.81082000	4.49218400	0.00131800
H	1.05210000	5.76325600	0.00124900
H	4.38528300	3.01372800	0.00127500
C	-4.85597900	0.83471200	0.00072900
H	-3.98198400	2.80589100	0.00060500
C	-3.23781600	-0.96661300	0.00045100
H	3.50451100	5.33582600	0.00158200

C	-4.55906700	-0.52295300	0.00064300
H	-5.89429000	1.17014700	0.00082700
H	-2.97712300	-2.02907500	0.00029700
F	-5.52569600	-1.41841000	0.00074600

Structure of Ir6, T_2 state

C	-1.78918800	-1.14715000	-3.70283600
C	-1.40641400	-1.05838900	-2.35518700
C	0.77505800	-0.45702100	-2.99373000
C	0.44642200	-0.53239100	-4.34151500
C	-0.86007800	-0.88565900	-4.69650500
H	-2.81438300	-1.41756800	-3.95631500
H	1.77964500	-0.18474300	-2.66539300
H	1.20616200	-0.31700600	-5.09307700
H	-1.14962500	-0.95279300	-5.74680500
C	-2.28318700	-1.29476000	-1.23231900
C	-3.61785000	-1.67486000	-1.23164300
C	-4.28727000	-1.85777700	-0.00044000
H	-4.14715600	-1.83626200	-2.17073600
C	-2.28303400	-1.29571200	1.23160500
C	-3.61775500	-1.67575300	1.23075400
H	-5.33620100	-2.15518200	-0.00050100
H	-4.14698200	-1.83775500	2.16978900
C	-1.40612800	-1.06030600	2.35452000
C	-1.78868200	-1.15024400	3.70217300
C	0.77543100	-0.45940600	2.99326700
C	-0.85944100	-0.88954200	4.69591700
H	-2.81380800	-1.42097400	3.95559900
C	0.44699400	-0.53589500	4.34103600
H	1.77996000	-0.18682400	2.66500700
H	-1.14882600	-0.95759100	5.74620200
H	1.20683300	-0.32109300	5.09266600
N	-0.11399000	-0.71655500	-2.03281800
N	-1.66091200	-1.08983700	-0.00034100
N	-0.11373500	-0.71818200	2.03226300
Ir	0.18225500	-0.64180600	-0.00026200
Cl	0.86560500	-2.97063600	-0.00127800
C	0.00789500	1.37215400	0.00052700
C	-1.11225900	2.27843800	0.00090800
C	1.20361900	2.05053800	0.00072000
C	-0.68286200	3.63568100	0.00137700
C	-2.49748900	2.02266600	0.00091100
S	1.05011500	3.78508800	0.00134900
C	2.43716000	1.30609100	0.00039400

C	-1.59183000	4.69856100	0.00181900
C	-3.39814100	3.07512200	0.00135400
H	-2.86433800	0.99779200	0.00057100
C	3.72927200	1.84291900	0.00054600
N	2.24328500	-0.03951700	-0.00009800
C	-2.94905000	4.40744600	0.00180000
H	-1.24063600	5.73263500	0.00217400
H	-4.47009100	2.86605000	0.00135600
C	4.82534400	0.99502700	0.00020300
H	3.86495200	2.92528400	0.00093300
C	3.29423300	-0.86850500	-0.00041800
H	-3.67421500	5.22447500	0.00214300
C	4.58935500	-0.37536200	-0.00027900
H	5.84808600	1.37609700	0.00030100
H	3.08971500	-1.94120100	-0.00080600
F	5.59965400	-1.23129800	-0.00062000

Structure of Ir7, S_0 state

C	1.85011000	-1.40871100	3.66363000
C	1.47302300	-1.23887800	2.33581700
C	-0.54378600	-0.25452300	2.99026700
C	-0.21991900	-0.39595100	4.33538900
C	0.99370500	-0.98327000	4.67621400
H	2.80816900	-1.86846100	3.90588100
H	-1.48365100	0.19844600	2.67140500
H	-0.91922500	-0.04598800	5.09546800
H	1.27779700	-1.10957200	5.72241100
C	2.30527400	-1.64054300	1.18680700
C	3.55107100	-2.26494400	1.21160700
C	4.17013600	-2.56542600	-0.00160900
H	4.03329900	-2.51614900	2.15583700
C	2.30564400	-1.63842000	-1.18892400
C	3.55144100	-2.26277100	-1.21447900
H	5.14718100	-3.05110500	-0.00189800
H	4.03395500	-2.51230000	-2.15901100
C	1.47372200	-1.23469400	-2.33744300
C	1.85116600	-1.40209200	-3.66545500
C	-0.54291600	-0.24913400	-2.99062700
C	0.99502400	-0.97482200	-4.67748700
H	2.80931100	-1.86136600	-3.90826800
C	-0.21869300	-0.38812800	-4.33591400
H	-1.48286100	0.20325100	-2.67118900
H	1.27940300	-1.09921100	-5.72383600
H	-0.91779500	-0.03678100	-5.09554200

N	0.27527400	-0.66714200	2.02038900
N	1.75320500	-1.33845200	-0.00087200
N	0.27589200	-0.66353900	-2.02128200
Ir	-0.03072200	-0.53776500	-0.00043500
Cl	-0.90303500	-2.83357300	-0.00271500
C	0.47493500	1.41171100	0.00128200
C	1.70414500	2.16154900	0.00185200
C	-0.61547600	2.26332400	0.00179100
C	1.47525500	3.56663200	0.00283000
C	3.03941800	1.70848900	0.00161900
S	-0.21829200	3.96326500	0.00307900
C	-1.93620700	1.70426800	0.00120100
C	2.52795200	4.48755600	0.00351000
C	4.08292400	2.61933400	0.00230300
H	3.25407800	0.64092200	0.00091500
C	-3.14692400	2.41012900	0.00178900
N	-1.93044000	0.33711100	0.00003300
C	3.82895700	4.00277300	0.00323500
H	2.33028800	5.56161500	0.00424200
H	5.11417500	2.25957300	0.00212200
C	-4.34139300	1.71188800	0.00115200
H	-3.13411700	3.50094700	0.00276500
C	-3.08225500	-0.33521100	-0.00056400
H	4.66435400	4.70688400	0.00376800
C	-4.31590000	0.30991700	-0.00004300
H	-5.29547700	2.24103100	0.00158500
H	-3.00854000	-1.42600000	-0.00150300
C	-5.53775700	-0.53258200	-0.00075900
O	-5.52295400	-1.74069900	-0.00149900
O	-6.65507300	0.19067600	-0.00045600
H	-7.40986000	-0.41979700	-0.00089600

Structure of Ir7, S_1 state

C	1.86504700	-1.37791300	3.68477400
C	1.49792600	-1.22448100	2.33859700
C	-0.57378700	-0.31408400	3.00659500
C	-0.25669800	-0.45151600	4.34344400
C	0.99381800	-0.99580200	4.68714100
H	2.84029500	-1.79980900	3.92947500
H	-1.53028900	0.10395800	2.68826000
H	-0.97378700	-0.14001800	5.10318300
H	1.27676900	-1.11599800	5.73448400
C	2.32736500	-1.59186500	1.20931700
C	3.58646800	-2.18234300	1.21913200

C	4.21718100	-2.46602200	0.00056500
H	4.07626200	-2.42917900	2.16141300
C	2.32698100	-1.59314000	-1.20843900
C	3.58601900	-2.18360600	-1.21815200
H	5.20465400	-2.92889800	0.00063400
H	4.07548500	-2.43140900	-2.16034700
C	1.49708100	-1.22698200	-2.33789600
C	1.86378900	-1.38183500	-3.68397700
C	-0.57486200	-0.31743600	-3.00612900
C	0.99218600	-1.00084400	-4.68648700
H	2.83898900	-1.80391400	-3.92854500
C	-0.25821100	-0.45629500	-4.34295100
H	-1.53127400	0.10090000	-2.68791500
H	1.27480000	-1.12213400	-5.73379400
H	-0.97558600	-0.14566500	-5.10277900
N	0.26607100	-0.68582400	2.02680000
N	1.77040600	-1.28818100	0.00034000
N	0.26536400	-0.68806500	-2.02624200
Ir	-0.02816500	-0.51928600	0.00026500
Cl	-0.88377000	-2.81472000	0.00179300
C	0.48357700	1.36395900	-0.00077500
C	1.71175400	2.11961200	-0.00103900
C	-0.62912600	2.25324500	-0.00124400
C	1.48346900	3.51894500	-0.00183100
C	3.04235300	1.66676500	-0.00062000
S	-0.22557600	3.90968000	-0.00219500
C	-1.95860000	1.69822100	-0.00082100
C	2.51562500	4.44700700	-0.00225000
C	4.08592100	2.58850000	-0.00103100
H	3.25446700	0.59977100	0.00001500
C	-3.15809200	2.41288300	-0.00123100
N	-1.94721200	0.33463500	0.00003600
C	3.82743600	3.96234200	-0.00184000
H	2.31387300	5.51959700	-0.00288500
H	5.11749200	2.23172100	-0.00071100
C	-4.35785700	1.71439700	-0.00068500
H	-3.14500800	3.50371800	-0.00198800
C	-3.09533200	-0.33608000	0.00057900
H	4.65759900	4.67179000	-0.00215400
C	-4.32943500	0.31769800	0.00025000
H	-5.31091000	2.24473800	-0.00098400
H	-3.02434400	-1.42730600	0.00127400
C	-5.55762000	-0.52699800	0.00087100
O	-5.53309400	-1.73289900	0.00161300

O	-6.66887400	0.19872000	0.00049900
H	-7.43043200	-0.40396500	0.00091400

Structure of Ir7, T_1 state

C	-1.85795300	-1.41445600	-3.67771800
C	-1.49732400	-1.24256000	-2.33323400
C	0.57661100	-0.33949600	-3.00149300
C	0.26665200	-0.49617400	-4.33806500
C	-0.98044000	-1.04521100	-4.68052800
H	-2.83140600	-1.84061600	-3.92184000
H	1.53068500	0.08373300	-2.68283400
H	0.98743000	-0.19448700	-5.09840800
H	-1.25746400	-1.18002600	-5.72777600
C	-2.33207400	-1.59900200	-1.20128200
C	-3.58679200	-2.19280000	-1.21073000
C	-4.22090800	-2.46936900	0.01187500
H	-4.07243100	-2.45029700	-2.15235900
C	-2.33118200	-1.58461300	1.21819500
C	-3.59134000	-2.17893200	1.22645000
H	-5.20729400	-2.93491200	0.01354000
H	-4.07996000	-2.42439100	2.17002700
C	-1.50060000	-1.21926100	2.34126800
C	-1.86005200	-1.37437900	3.69158000
C	0.57853900	-0.31133600	3.00365500
C	-0.98324900	-0.99655300	4.68859100
H	-2.83465900	-1.79540200	3.94062100
C	0.26843300	-0.45262100	4.34044100
H	1.53373800	0.10662700	2.68114800
H	-1.26074500	-1.11894700	5.73728700
H	0.98943600	-0.14449300	5.09789300
N	-0.27016300	-0.69865400	-2.02251000
N	-1.77660400	-1.27961000	0.00443200
N	-0.26756600	-0.67944900	2.02606500
Ir	0.02056500	-0.51102400	0.00359600
Cl	0.87884900	-2.80771200	0.00900600
C	-0.48097700	1.37259100	-0.00574400
C	-1.70798400	2.12987400	-0.00909200
C	0.63502300	2.25797800	-0.01115200
C	-1.47568100	3.52878800	-0.01744800
C	-3.03912100	1.67820600	-0.00450500
S	0.23511900	3.91775800	-0.02040200
C	1.96208500	1.69959600	-0.00791400
C	-2.50755500	4.45814100	-0.02193000
C	-4.08024400	2.60056900	-0.00891200

H	-3.25099700	0.61067400	0.00291600
C	3.16411600	2.41080300	-0.01243800
N	1.94729900	0.33575400	0.00035800
C	-3.81867700	3.97517700	-0.01769400
H	-2.30454400	5.53056000	-0.02840200
H	-5.11277000	2.24624100	-0.00532200
C	4.36166400	1.70840500	-0.00854200
H	3.15421500	3.50165400	-0.01896900
C	3.09299800	-0.33857300	0.00404300
H	-4.64820300	4.68565200	-0.02105700
C	4.32927600	0.31169100	-0.00020000
H	5.31640100	2.23582600	-0.01196600
H	3.01897600	-1.42961400	0.01030000
C	5.55467700	-0.53674500	0.00414900
O	5.52643200	-1.74261100	0.01165300
O	6.66825900	0.18547600	-0.00142600
H	7.42789900	-0.41962900	0.00164400

Structure of Ir7, T_2 state

C	1.93459000	-0.83012900	3.79629100
C	1.54245800	-0.88710000	2.44322700
C	-0.52202900	0.13104300	3.01112900
C	-0.17705800	0.19791000	4.34319700
C	1.08718200	-0.29628400	4.74197300
H	2.91564200	-1.21057600	4.08294300
H	-1.48397300	0.50216200	2.65303200
H	-0.87618100	0.62576800	5.06164600
H	1.39141300	-0.25381600	5.78931100
C	2.34151200	-1.41749700	1.37557800
C	3.60732700	-2.01647600	1.43824300
C	4.20689300	-2.47433100	0.27090300
H	4.11515000	-2.12967300	2.39662900
C	2.30345700	-1.76546500	-1.01384600
C	3.55179800	-2.36276900	-0.97354900
H	5.19129400	-2.94170100	0.31805300
H	4.01932100	-2.74643700	-1.87994700
C	1.44803900	-1.55305200	-2.17904800
C	1.79322400	-1.90156100	-3.48792000
C	-0.62397900	-0.72929500	-2.92809000
C	0.90415500	-1.65678600	-4.52291100
H	2.76043900	-2.36403900	-3.68563400
C	-0.33044400	-1.05896700	-4.23876200
H	-1.57154900	-0.26181100	-2.65576900
H	1.16698300	-1.92792300	-5.54700700

H	-1.05869800	-0.85042100	-5.02296600
N	0.29369600	-0.39329400	2.07837100
N	1.76754000	-1.29006000	0.13835300
N	0.23319000	-0.96675100	-1.92324600
Ir	-0.02708700	-0.51655300	0.07118200
Cl	-0.89021200	-2.78731700	0.39361800
C	0.48353800	1.35394800	-0.18753800
C	1.71313200	2.10119000	-0.28150000
C	-0.62620100	2.23002000	-0.30228500
C	1.48464100	3.48834300	-0.46846100
C	3.04371000	1.65304700	-0.21365800
S	-0.22314000	3.87545700	-0.52173500
C	-1.95607900	1.68258700	-0.21315500
C	2.51912800	4.40830300	-0.58794300
C	4.08686100	2.56607300	-0.33221900
H	3.25623100	0.59601100	-0.06815000
C	-3.15554400	2.39157000	-0.30372700
N	-1.94593700	0.33305500	-0.01904100
C	3.82914700	3.92870800	-0.51731100
H	2.31826400	5.47146300	-0.73134400
H	5.11839200	2.21293100	-0.27883000
C	-4.35517900	1.70183800	-0.19543200
H	-3.14174500	3.47138800	-0.45798600
C	-3.09446500	-0.32969700	0.08586300
H	4.66006700	4.63157700	-0.60753100
C	-4.32781200	0.31884400	0.00222000
H	-5.30812100	2.22808500	-0.26297800
H	-3.02406700	-1.40997000	0.23953800
C	-5.55634000	-0.51523300	0.12950800
O	-5.53336400	-1.70811500	0.30686600
O	-6.66709100	0.20394400	0.02456300
H	-7.42906800	-0.39132500	0.11506800

Structure of Ir8, S_0 state

C	1.73222900	1.34934000	3.66525100
C	1.34791000	1.19707700	2.33747800
C	-0.71099500	0.30428500	2.99167600
C	-0.38152000	0.43152900	4.33683600
C	0.85747300	0.96293200	4.67777500
H	2.71012700	1.76505300	3.90763300
H	-1.67026700	-0.10697200	2.67414900
H	-1.09622000	0.11375000	5.09671500
H	1.14702900	1.07612600	5.72396500
C	2.19668000	1.56277400	1.18871400

C	3.46944800	2.13007600	1.21410300
C	4.10130300	2.40393500	0.00120900
H	3.96283200	2.35748000	2.15860900
C	2.19684300	1.56374700	-1.18725200
C	3.46961800	2.13106500	-1.21199800
H	5.09940500	2.84468000	0.00145800
H	3.96314900	2.35922600	-2.15624600
C	1.34822200	1.19899100	-2.33642700
C	1.73271200	1.35235300	-3.66402500
C	-0.71062100	0.30679200	-2.99163200
C	0.85807500	0.96681200	-4.67698100
H	2.71064600	1.76825000	-3.90593900
C	-0.38097700	0.43516700	-4.33664300
H	-1.66994900	-0.10469300	-2.67457300
H	1.14776600	1.08087000	-5.72304000
H	-1.09559300	0.11805900	-5.09688000
N	0.12604200	0.67913300	2.02181300
N	1.63126700	1.28799900	0.00057900
N	0.12631100	0.68078900	-2.02134800
Ir	-0.18442700	0.56354800	0.00017000
Cl	-0.96677900	2.89027400	0.00102600
C	0.24165400	-1.40385100	-0.00052400
C	1.43835200	-2.20369200	-0.00083900
C	-0.88363200	-2.21127300	-0.00072400
C	1.15129400	-3.59819900	-0.00127700
C	2.79152000	-1.80628000	-0.00077600
S	-0.55666900	-3.92600600	-0.00129700
C	-2.17814000	-1.59938000	-0.00052100
C	2.16493100	-4.56193200	-0.00163400
C	3.79606700	-2.75948100	-0.00113800
H	3.05099900	-0.74881400	-0.00045500
C	-3.41787400	-2.25678800	-0.00066400
N	-2.11933900	-0.23370700	-0.00019800
C	3.48462600	-4.13123600	-0.00156100
H	1.92348600	-5.62688300	-0.00196100
H	4.84136000	-2.44302200	-0.00109000
C	-4.58308900	-1.51636800	-0.00051600
H	-3.45061900	-3.34707600	-0.00089600
C	-3.23873300	0.48977200	-0.00006900
H	4.29007500	-4.86939500	-0.00183700
C	-4.49958000	-0.11095700	-0.00023000
H	-5.55616300	-2.01008900	-0.00062700
H	-3.10422100	1.57528900	0.00016900
C	-5.66995000	0.70671300	-0.00009300

N	-6.62200600	1.36904700	0.00001100

Structure of Ir8, S_1 state

C	1.74076800	1.33029900	3.68427100
C	1.36697500	1.19066700	2.33852200
C	-0.73898700	0.36469200	3.00810100
C	-0.41626500	0.49136600	4.34456100
C	0.85536600	0.98468500	4.68739200
H	2.73247900	1.71253200	3.92787000
H	-1.71193200	-0.01542600	2.69221400
H	-1.14535600	0.21032200	5.10473400
H	1.14340000	1.09422800	5.73449900
C	2.20943100	1.52508900	1.20901800
C	3.49065500	2.06560100	1.21848400
C	4.13200200	2.32414200	-0.00009200
H	3.98968700	2.29286800	2.16081900
C	2.20884700	1.52600300	-1.20887900
C	3.49006900	2.06653000	-1.21854800
H	5.13695600	2.74766600	-0.00017200
H	3.98865300	2.29449000	-2.16095400
C	1.36586600	1.19240000	-2.33822000
C	1.73905400	1.33291400	-3.68404900
C	-0.74045500	0.36700000	-3.00739600
C	0.85316200	0.98804900	-4.68699400
H	2.73069700	1.71520400	-3.92783700
C	-0.41835600	0.49460400	-4.34391500
H	-1.71326600	-0.01328900	-2.69129600
H	1.14073200	1.09824800	-5.73416100
H	-1.14782500	0.21415700	-5.10394600
N	0.11498000	0.70058000	2.02727600
N	1.64035600	1.24368100	0.00010300
N	0.11400100	0.70212100	-2.02673500
Ir	-0.18503800	0.54335000	0.00027500
Cl	-0.95838000	2.86707100	0.00132800
C	0.25618700	-1.35735500	-0.00049100
C	1.45526100	-2.15805000	-0.00091500
C	-0.88881500	-2.20531700	-0.00061900
C	1.17488200	-3.54797300	-0.00133300
C	2.80176900	-1.75521000	-0.00095200
S	-0.54689000	-3.87529000	-0.00128600
C	-2.19598100	-1.60162900	-0.00026400
C	2.17170000	-4.51396400	-0.00175100
C	3.81027300	-2.71542400	-0.00137300
H	3.05428200	-0.69711900	-0.00064500

C	-3.42245000	-2.27152500	-0.00048900
N	-2.13577100	-0.23999000	0.00040700
C	3.50066300	-4.07848700	-0.00176500
H	1.93089700	-5.57832300	-0.00206700
H	4.85440000	-2.39738800	-0.00139500
C	-4.59526600	-1.53420700	-0.00011100
H	-3.45219100	-3.36182300	-0.00095700
C	-3.25349400	0.47888100	0.00075300
H	4.30360900	-4.81856000	-0.00209400
C	-4.51364800	-0.13389300	0.00049400
H	-5.56566500	-2.03240900	-0.00027200
H	-3.12474500	1.56535000	0.00127900
C	-5.68873000	0.67967800	0.00086400
N	-6.64171900	1.33908700	0.00115300

Structure of Ir8, T_1 state

C	1.75245200	-1.36918800	-3.66847200
C	1.37787500	-1.21037200	-2.32665200
C	-0.72766900	-0.39541000	-3.00605200
C	-0.40509600	-0.54215900	-4.34086800
C	0.86519100	-1.03855500	-4.67644200
H	2.74420700	-1.75447500	-3.90666900
H	-1.70038900	-0.01137800	-2.69437500
H	-1.13452100	-0.27275700	-5.10506500
H	1.15274300	-1.16326100	-5.72208100
C	2.22122400	-1.53171300	-1.18996200
C	3.49878200	-2.07310700	-1.19381800
C	4.13930800	-2.32079300	0.03234200
H	3.99805500	-2.31186800	-2.13318800
C	2.20981800	-1.51190300	1.22950000
C	3.49403800	-2.05368400	1.24308400
H	5.14411600	-2.74502300	0.03867000
H	3.98868000	-2.27615100	2.18924000
C	1.36156300	-1.17898400	2.34798200
C	1.72247000	-1.31630400	3.70013000
C	-0.75706300	-0.35975500	3.00187100
C	0.82690700	-0.97533500	4.69324200
H	2.71363300	-1.69425700	3.95289300
C	-0.44625300	-0.48658200	4.33965000
H	-1.72838500	0.01717300	2.67707000
H	1.10561500	-1.08399200	5.74311800
H	-1.18280900	-0.20923000	5.09399200
N	0.12890300	-0.71637100	-2.02231200
N	1.64744100	-1.23381900	0.01237500

N	0.10773400	-0.69164200	2.02719800
Ir	-0.17734200	-0.53592700	0.00365700
Cl	-0.95103100	-2.86213300	0.00604500
C	0.25190400	1.36524700	-0.00806200
C	1.44886000	2.16873700	-0.01251000
C	-0.89719600	2.20816000	-0.01330700
C	1.16311100	3.55783800	-0.01983500
C	2.79634100	1.76849500	-0.00919000
S	-0.56084600	3.88151800	-0.02157000
C	-2.20122100	1.59990300	-0.01216200
C	2.15851600	4.52611400	-0.02409700
C	3.80133000	2.73023900	-0.01362700
H	3.04985800	0.71015200	-0.00260600
C	-3.43076200	2.26511500	-0.01749000
N	-2.13637200	0.23819100	-0.00597400
C	3.48718200	4.09363200	-0.02112100
H	1.91549000	5.59003400	-0.02939700
H	4.84665200	2.41578400	-0.01103200
C	-4.60047600	1.52280500	-0.01703600
H	-3.46486700	3.35530400	-0.02198000
C	-3.25079000	-0.48529700	-0.00576700
H	4.28868500	4.83553900	-0.02445100
C	-4.51362200	0.12262400	-0.01133600
H	-5.57291700	2.01713400	-0.02108300
H	-3.11754000	-1.57126500	-0.00077500
C	-5.68541700	-0.69545000	-0.01091500
N	-6.63595000	-1.35850900	-0.01070900

Structure of Ir8, T_2 state

C	-1.81878700	-0.66330000	3.80780400
C	-1.41846600	-0.77677500	2.46024200
C	0.67527800	0.18934500	3.01380300
C	0.32196000	0.31152000	4.33962600
C	-0.96134200	-0.12806900	4.74331300
H	-2.81441000	-1.00096000	4.09768900
H	1.65157400	0.51800200	2.65339900
H	1.02896800	0.74022500	5.04981000
H	-1.27195700	-0.04157000	5.78605500
C	-2.22765800	-1.31011300	1.40281700
C	-3.51486700	-1.86201600	1.47239200
C	-4.12129500	-2.33416300	0.31488400
H	-4.03357100	-1.92785600	2.42937200
C	-2.18477000	-1.73190200	-0.97474500
C	-3.45332400	-2.28397300	-0.92700700

H	-5.12188100	-2.76509100	0.36789300
H	-3.92664200	-2.67944100	-1.82531100
C	-1.31439000	-1.58537500	-2.13914000
C	-1.66482400	-1.95665700	-3.44007800
C	0.79159400	-0.86159700	-2.89531300
C	-0.76038600	-1.77519300	-4.47496000
H	-2.64841900	-2.38587800	-3.63170400
C	0.49414800	-1.21713000	-4.19841200
H	1.75392900	-0.42136300	-2.62979600
H	-1.02705600	-2.06440800	-5.49310200
H	1.23482500	-1.05831800	-4.98262900
N	-0.14937100	-0.33925500	2.09099600
N	-1.64052700	-1.24061100	0.16674300
N	-0.08020100	-1.03836100	-1.89066400
Ir	0.18215500	-0.53834000	0.09238900
Cl	0.95877800	-2.82837000	0.48969700
C	-0.25249600	1.34169500	-0.22825300
C	-1.45102500	2.13244200	-0.35474900
C	0.89138900	2.17051800	-0.35835800
C	-1.16701400	3.50373400	-0.57947000
C	-2.79844600	1.73800800	-0.28544700
S	0.55405200	3.82336300	-0.62833800
C	2.19733900	1.57529400	-0.24019000
C	-2.16407200	4.45925400	-0.73445900
C	-3.80416600	2.68703600	-0.43935800
H	-3.05329000	0.69474800	-0.11111900
C	3.42547900	2.23488500	-0.33936200
N	2.13496200	0.23412900	-0.00661000
C	-3.49206300	4.03271200	-0.66139500
H	-1.92133800	5.50919100	-0.90668800
H	-4.84907000	2.37600400	-0.38473200
C	4.59616100	1.50827100	-0.19854900
H	3.45715300	3.30906300	-0.52554800
C	3.25119800	-0.47484900	0.13054900
H	-4.29425300	4.76427900	-0.77906700
C	4.51204900	0.12836900	0.04065500
H	5.56735400	1.99933300	-0.27205000
H	3.11985400	-1.54511200	0.31486800
C	5.68574700	-0.67252000	0.19423400
N	6.63806800	-1.32116800	0.31821900

Structure of Ir9, S_0 state

C	-1.86711500	-1.26434500	-3.70129400
C	-1.48252900	-1.14701600	-2.37003500

C	0.53884200	-0.15483200	-2.99757100
C	0.20822400	-0.24490600	-4.34537300
C	-1.01177200	-0.80909600	-4.70169900
H	-2.83044300	-1.70615800	-3.95563300
H	1.48355900	0.28003300	-2.66840600
H	0.90722100	0.12698500	-5.09522700
H	-1.30179800	-0.89422300	-5.75041000
C	-2.31230300	-1.58522200	-1.23287100
C	-3.55847600	-2.20786600	-1.27578300
C	-4.17403700	-2.55055000	-0.07213600
H	-4.04284700	-2.42674000	-2.22689200
C	-2.30530600	-1.66733300	1.14144800
C	-3.55151300	-2.29113200	1.14866200
H	-5.15098300	-3.03620900	-0.08590800
H	-4.03064700	-2.57472000	2.08522800
C	-1.46866200	-1.30828200	2.30100800
C	-1.84368500	-1.52039700	3.62317200
C	0.55385200	-0.35533300	2.98309900
C	-0.98303900	-1.13318600	4.64739900
H	-2.80380100	-1.98258100	3.85220600
C	0.23244200	-0.54035400	4.32343900
H	1.49461000	0.10579400	2.67900400
H	-1.26566000	-1.29264800	5.68945300
H	0.93505800	-0.21875100	5.09290300
N	-0.27921500	-0.59600700	-2.03945700
N	-1.75633800	-1.32556500	-0.03692100
N	-0.26891300	-0.73216700	2.00179200
Ir	0.03332800	-0.53768100	-0.01504100
Cl	0.89563200	-2.83332700	-0.09166100
C	-0.45036800	1.41345300	0.04739500
C	-1.66992100	2.17596100	0.06988900
C	0.65098700	2.25604000	0.06844400
C	-1.42600800	3.57814400	0.10735700
C	-3.00967600	1.73545800	0.06117300
S	0.27084500	3.95924800	0.11538400
C	1.96133300	1.68443300	0.04824500
C	-2.46942600	4.50904100	0.13423300
C	-4.04350200	2.65607500	0.08750700
H	-3.23438000	0.67033000	0.03402300
C	3.18207400	2.37972200	0.06625700
N	1.94157900	0.31598600	0.00738400
C	-3.77476900	4.03655900	0.12373400
H	-2.26176600	5.58071100	0.16285200
H	-5.07840100	2.30731300	0.08043200

C	4.36929300	1.67522800	0.04279600
H	3.18156400	3.46982400	0.09893900
C	3.08160000	-0.37330200	-0.01462500
H	-4.60308500	4.74866500	0.14423100
C	4.30457200	0.28041800	0.00223300
H	5.33786600	2.17554600	0.05553000
H	3.00093200	-1.46272800	-0.04606700
N	5.52364700	-0.51190400	-0.02413600
O	5.41233500	-1.71948700	-0.05391000
O	6.57835200	0.08609700	-0.01274600

Structure of Ir9, S_1 state

C	-1.86442300	-1.37056000	-3.68476600
C	-1.49604000	-1.21852800	-2.33880500
C	0.58144600	-0.32235000	-3.00787500
C	0.26325400	-0.45898300	-4.34434600
C	-0.99089600	-0.99511500	-4.68750500
H	-2.84245900	-1.78621200	-3.92886500
H	1.54101400	0.08985800	-2.69161000
H	0.98243800	-0.15299600	-5.10431700
H	-1.27472500	-1.11426800	-5.73470700
C	-2.32727100	-1.58013700	-1.20959300
C	-3.58996400	-2.16278900	-1.21917400
C	-4.22256300	-2.44258800	-0.00084600
H	-4.08108700	-2.40648300	-2.16155000
C	-2.32706900	-1.58145200	1.20840300
C	-3.58964900	-2.16408700	1.21777500
H	-5.21286700	-2.89929600	-0.00097800
H	-4.08054300	-2.40880600	2.15999700
C	-1.49550000	-1.22103900	2.33795800
C	-1.86363800	-1.37457800	3.68373200
C	0.58205600	-0.32564000	3.00749400
C	-0.98987100	-1.00022700	4.68674700
H	-2.84161800	-1.79051100	3.92756800
C	0.26413400	-0.46375100	4.34390900
H	1.54155400	0.08691200	2.69147300
H	-1.27348100	-1.12054500	5.73387400
H	0.98348800	-0.15858700	5.10405200
N	-0.26078300	-0.68756700	-2.02732800
N	-1.76819800	-1.27969700	-0.00042800
N	-0.26040800	-0.68977000	2.02676900
Ir	0.03415500	-0.52138700	-0.00026400
Cl	0.88619300	-2.81569100	-0.00163000
C	-0.46503400	1.36468000	0.00073200

C	-1.68794900	2.12850700	0.00101000
C	0.65341800	2.24720100	0.00125900
C	-1.44999000	3.52625100	0.00183100
C	-3.02123100	1.68476100	0.00057700
S	0.26039300	3.90541700	0.00220200
C	1.97889800	1.68414700	0.00089200
C	-2.47555600	4.46189700	0.00225800
C	-4.05844800	2.61418200	0.00099200
H	-3.24113000	0.61935000	-0.00009000
C	3.18411700	2.39298600	0.00128100
N	1.95829000	0.32047500	0.00005900
C	-3.79059300	3.98606600	0.00182900
H	-2.26641700	5.53300800	0.00290500
H	-5.09241200	2.26451000	0.00065300
C	4.37998600	1.69143400	0.00076200
H	3.17982800	3.48360300	0.00197900
C	3.09806100	-0.36474400	-0.00041600
H	-4.61585300	4.70115600	0.00214700
C	4.31732000	0.30228800	-0.00009400
H	5.34576400	2.19719600	0.00099700
H	3.02287300	-1.45536200	-0.00105900
N	5.54886800	-0.48862000	-0.00068000
O	5.43670900	-1.69372100	-0.00106700
O	6.59550200	0.11792800	-0.00075400

Structure of Ir9, T_1 state

C	-1.84469700	-1.40189500	-3.66572600
C	-1.47152000	-1.22246800	-2.33829100
C	0.57089300	-0.28937800	-2.99520800
C	0.25161600	-0.44343100	-4.33987800
C	-0.97352300	-1.00767800	-4.67853100
H	-2.80960800	-1.84682300	-3.90812400
H	1.51867400	0.14667200	-2.67568700
H	0.96285300	-0.12108900	-5.10102000
H	-1.25470100	-1.14232800	-5.72448000
C	-2.31322400	-1.60641600	-1.18872800
C	-3.56705300	-2.21470400	-1.21405000
C	-4.18910200	-2.50760900	-0.00031800
H	-4.05331100	-2.45941000	-2.15788600
C	-2.31281100	-1.60735600	1.18816700
C	-3.56664900	-2.21563100	1.21343300
H	-5.17251000	-2.98026400	-0.00033600
H	-4.05259900	-2.46107100	2.15723800
C	-1.47070300	-1.22436200	2.33775900

C	-1.84342500	-1.40487800	3.66517600
C	0.57193200	-0.29180800	2.99475800
C	-0.97192900	-1.01145300	4.67801200
H	-2.80823300	-1.85004000	3.90754700
C	0.25309000	-0.44692200	4.33941000
H	1.51961900	0.14447500	2.67528600
H	-1.25277000	-1.14693600	5.72394400
H	0.96458400	-0.12519700	5.10057300
N	-0.26488200	-0.66808400	-2.02643600
N	-1.75995500	-1.31307300	-0.00026400
N	-0.26415600	-0.66973600	2.02595500
Ir	0.03391500	-0.52601600	-0.00023300
Cl	0.88286000	-2.82148100	-0.00126100
C	-0.48837100	1.38856900	0.00057900
C	-1.69304700	2.14961900	0.00090600
C	0.67022300	2.26846800	0.00081800
C	-1.45682600	3.55510500	0.00138500
C	-3.03879700	1.72325300	0.00081500
S	0.27224300	3.93045500	0.00143800
C	1.96339200	1.70957100	0.00049600
C	-2.47047100	4.48995700	0.00174200
C	-4.07210400	2.65937900	0.00117100
H	-3.27746300	0.66131900	0.00045800
C	3.19982300	2.40148200	0.00072000
N	1.94425100	0.31792700	-0.00009200
C	-3.80064100	4.02780000	0.00162700
H	-2.25335000	5.56003400	0.00209900
H	-5.10746000	2.31227800	0.00108700
C	4.38148500	1.70427300	0.00035700
H	3.20048400	3.49308100	0.00119400
C	3.07433500	-0.36072500	-0.00045100
H	-4.61883300	4.75076100	0.00189500
C	4.31974400	0.28877800	-0.00024300
H	5.35050300	2.20133600	0.00051700
H	3.00447900	-1.45069000	-0.00090300
N	5.50094500	-0.49302900	-0.00062200
O	5.39567800	-1.71878700	-0.00113000
O	6.57936900	0.09625700	-0.00040700

Structure of Ir9, T_2 state

C	1.91115600	-0.84211400	3.80004300
C	1.52693200	-0.89388000	2.44347100
C	-0.54756600	0.11043900	3.00637100
C	-0.20965300	0.17201000	4.34024700

C	1.05607700	-0.31830900	4.74357400
H	2.89269300	-1.21890600	4.08973300
H	-1.50982100	0.47901800	2.64681900
H	-0.91466800	0.59253800	5.05723400
H	1.35408800	-0.27987800	5.79284100
C	2.33370000	-1.41284000	1.37862400
C	3.60363700	-2.00630900	1.44433300
C	4.21070900	-2.45551200	0.27905400
H	4.10707500	-2.12109800	2.40481300
C	2.31088000	-1.74923800	-1.01239900
C	3.56139500	-2.34105500	-0.96915700
H	5.19713900	-2.91830200	0.32888900
H	4.03534900	-2.71791000	-1.87495600
C	1.46124600	-1.53407200	-2.18237700
C	1.81703300	-1.87328600	-3.49026300
C	-0.60804200	-0.71362300	-2.93953800
C	0.93376000	-1.62531900	-4.52995000
H	2.78733400	-2.33068700	-3.68430500
C	-0.30418500	-1.03384300	-4.25048800
H	-1.55909500	-0.25075800	-2.67207000
H	1.20453800	-1.88897300	-5.55392300
H	-1.02778500	-0.82244000	-5.03822500
N	0.27526100	-0.40509900	2.07442100
N	1.76604100	-1.28241500	0.13809900
N	0.24303800	-0.95489000	-1.93070200
Ir	-0.03254300	-0.51961200	0.06711600
Cl	-0.88985900	-2.79361900	0.36560200
C	0.46337600	1.35722700	-0.18107400
C	1.68675900	2.11453200	-0.26605900
C	-0.65263100	2.22429500	-0.29749500
C	1.44731500	3.50062400	-0.44864900
C	3.02042900	1.67702800	-0.19252500
S	-0.26178100	3.87412500	-0.50811800
C	-1.97750100	1.66640800	-0.21411300
C	2.47499100	4.42995900	-0.55895400
C	4.05630000	2.59939000	-0.30191700
H	3.24118200	0.62131200	-0.04933600
C	-3.18382100	2.36835200	-0.30294500
N	-1.95692300	0.31581200	-0.02567100
C	3.78812500	3.96073600	-0.48309000
H	2.26605900	5.49193000	-0.69912800
H	5.09047400	2.25485200	-0.24411700
C	-4.37863700	1.67390700	-0.19707100
H	-3.17989600	3.44854700	-0.45299600

C	-3.09630100	-0.36312000	0.07719900
H	4.61374600	4.67070200	-0.56584400
C	-4.31550600	0.29755900	-0.00566200
H	-5.34500200	2.17478200	-0.25900000
H	-3.02073600	-1.44336800	0.22628100
N	-5.54628100	-0.48441500	0.11469100
O	-5.43416300	-1.67904000	0.27410700
O	-6.59315600	0.11799800	0.04626900

2.3 Frequency Calculation

Information of the first three frequencies of Ir1

S_0	1	2	3
	A	A	A
Frequencies --	23.9402	33.1201	39.5996
Red. masses --	6.7258	6.1580	5.2720
Frc consts --	0.0023	0.0040	0.0049
IR Inten --	0.1540	0.6186	0.3508

S_1	1	2	3
	A	A	A
Frequencies --	13.0644	28.5291	37.1253
Red. masses --	6.7735	6.3149	5.2720
Frc consts --	0.0007	0.0030	0.0043
IR Inten --	188.6179	8.0809	0.2363

T_1	1	2	3
	A	A	A
Frequencies --	21.8830	26.6586	35.8789
Red. masses --	6.4994	6.5728	5.3057
Frc consts --	0.0018	0.0028	0.0040
IR Inten --	8.9055	4.8482	36.3100

T_2	1	2	3
	A	A	A
Frequencies --	23.0791	30.2022	34.2470
Red. masses --	6.9995	5.9210	5.3090
Frc consts --	0.0022	0.0032	0.0037
IR Inten --	0.0009	2.8506	0.0381

Information of the first three frequencies of Ir2

S_0	1	2	3
	A	A	A
Frequencies --	16.8327	21.0196	28.3626
Red. masses --	16.3477	8.2767	7.9166
Frc consts --	0.0027	0.0022	0.0038
IR Inten --	0.0042	0.0416	0.0039

S_1	1	2	3
	A	A	A
Frequencies --	13.4491	17.3010	25.0073
Red. masses --	18.0706	7.0914	6.5090
Frc consts --	0.0019	0.0013	0.0024
IR Inten --	0.0561	85.6742	18.1002

T_1	1	2	3
	A	A	A
Frequencies --	10.4941	15.7228	19.7661
Red. masses --	17.2654	7.3348	5.9575
Frc consts --	0.0011	0.0011	0.0014
IR Inten --	38.5999	1500.8703	483.1275

T_2	1	2	3
	A	A	A
Frequencies --	12.1871	19.0229	25.9009
Red. masses --	17.6534	8.2779	5.8802
Frc consts --	0.0015	0.0018	0.0023
IR Inten --	0.0101	0.0977	0.3269

Information of the first three frequencies of Ir3

S_0	1	2	3
	A	A	A
Frequencies --	14.3018	16.7954	21.1105
Red. masses --	4.3440	6.1881	5.0765
Frc consts --	0.0005	0.0010	0.0013
IR Inten --	0.0473	0.0027	1.8216

S_1	1	2	3
	A	A	A
Frequencies --	15.7160	17.4220	20.7808
Red. masses --	4.2177	5.5199	5.0013
Frc consts --	0.0006	0.0010	0.0013
IR Inten --	0.0516	0.1035	1.4342

T_1	1	2	3
	A	A	A
Frequencies --	14.6471	16.3102	19.0092
Red. masses --	4.3024	5.4445	4.2914
Frc consts --	0.0005	0.0009	0.0009
IR Inten --	0.0503	0.0795	1.2167

T_2	1	2	3
	A	A	A
Frequencies --	14.5196	17.9715	19.6787
Red. masses --	4.2089	5.4982	5.1263
Frc consts --	0.0005	0.0010	0.0012
IR Inten --	0.0158	0.4077	0.8801

Information of the first three frequencies of Ir4

S_0	1	2	3
	A	A	A
Frequencies --	14.3835	16.2228	17.8350
Red. masses --	9.2674	4.4416	10.4443
Frc consts --	0.0011	0.0007	0.0020
IR Inten --	0.0862	0.0520	0.0195

S_1	1	2	3
	A	A	A
Frequencies --	14.6384	15.5314	16.5029
Red. masses --	18.1577	4.2869	6.6171
Frc consts --	0.0023	0.0006	0.0011
IR Inten --	0.0488	0.0958	0.0892

T_1	1	2	3
	A	A	A
Frequencies --	15.7699	16.3915	18.7606
Red. masses --	6.3299	4.4462	3.1720
Frc consts --	0.0009	0.0007	0.0007
IR Inten --	0.2332	0.0791	0.3595

T_2	1	2	3
	A	A	A
Frequencies --	15.0012	17.4247	20.7075
Red. masses --	7.5673	4.2556	14.0122
Frc consts --	0.0010	0.0008	0.0035
IR Inten --	0.1404	0.2712	0.0948

Information of the first three frequencies of Ir5

S_0	1	2	3
	A	A	A
Frequencies --	22.3804	31.2770	34.1198
Red. masses --	7.0521	7.5707	8.4948
Frc consts --	0.0021	0.0044	0.0058
IR Inten --	0.2299	0.6639	0.0066

S_1	1	2	3
	A	A	A
Frequencies --	16.0646	25.0481	32.2005
Red. masses --	6.8705	6.3386	11.5006
Frc consts --	0.0010	0.0023	0.0070
IR Inten --	147.4014	0.3974	18.3480

T_1	1	2	3

	A	A	A
Frequencies --	19.2865	24.9173	31.6203
Red. masses --	6.2010	7.2840	10.7534
Frc consts --	0.0014	0.0027	0.0063
IR Inten --	0.7681	40.1548	48.0645

T_2	1	2	3
	A	A	A
Frequencies --	23.9284	26.3150	33.2565
Red. masses --	7.9693	6.3375	9.0675
Frc consts --	0.0027	0.0026	0.0059
IR Inten --	0.0388	1.6530	0.1663

Information of the first three frequencies of Ir6

S_0	1	2	3
	A	A	A
Frequencies --	23.5597	32.9806	37.4632
Red. masses --	6.7695	6.5857	5.4055
Frc consts --	0.0022	0.0042	0.0045
IR Inten --	0.1130	0.8990	0.0074

S_1	1	2	3
	A	A	A
Frequencies --	17.3823	29.4560	37.8806
Red. masses --	6.8931	6.3638	9.4632
Frc consts --	0.0012	0.0033	0.0080
IR Inten --	129.3293	4.6326	14.4499

T_1	1	2	3
	A	A	A
Frequencies --	19.4024	23.9424	31.1873
Red. masses --	6.7259	6.6107	8.9596
Frc consts --	0.0015	0.0022	0.0051
IR Inten --	1118.1048	198.5853	867.4858

T_2	1	2	3
	A	A	A
Frequencies --	24.1091	29.2885	39.4860
Red. masses --	7.0551	6.6639	8.4383
Frc consts --	0.0024	0.0034	0.0078
IR Inten --	0.3365	2.1258	0.4110

Information of the first three frequencies of Ir7

S_0	1	2	3
	A	A	A
Frequencies --	17.1825	24.7678	31.6992
Red. masses --	7.5017	6.6227	5.8360
Frc consts --	0.0013	0.0024	0.0035
IR Inten --	0.0639	0.3208	0.7055

S_1	1	2	3
	A	A	A
Frequencies --	16.5041	23.4060	29.7548
Red. masses --	6.6376	6.7016	7.9138
Frc consts --	0.0011	0.0022	0.0041
IR Inten --	120.6687	0.0610	12.5747

T_1	1	2	3
	A	A	A
Frequencies --	13.7405	22.5398	27.7465
Red. masses --	6.4294	6.8293	7.9418
Frc consts --	0.0007	0.0020	0.0036
IR Inten --	161.9712	288.4797	269.0272

T_2	1	2	3
	A	A	A
Frequencies --	21.2476	29.3074	37.3681
Red. masses --	7.7499	7.4615	5.4316
Frc consts --	0.0021	0.0038	0.0045
IR Inten --	0.9506	0.3323	2.9301

Information of the first three frequencies of Ir8

S_0	1	2	3
	A	A	A
Frequencies --	22.6957	27.3971	32.9405
Red. masses --	7.0325	6.7364	8.1485
Frc consts --	0.0021	0.0030	0.0052
IR Inten --	0.0017	0.4917	0.7934

S_1	1	2	3
	A	A	A
Frequencies --	18.2823	24.6373	32.4479
Red. masses --	6.7444	6.3700	9.3917
Frc consts --	0.0013	0.0023	0.0058
IR Inten --	88.2239	0.2172	17.8587

T_1	1	2	3
	A	A	A
Frequencies --	8.9413	25.0041	31.3765
Red. masses --	6.1422	7.2201	9.1975
Frc consts --	0.0003	0.0027	0.0053
IR Inten --	44.2629	42.5267	50.1832

T_2	1	2	3
	A	A	A
Frequencies --	23.5716	30.6350	38.1688
Red. masses --	7.7311	8.0053	6.2556
Frc consts --	0.0025	0.0044	0.0054
IR Inten --	0.3560	0.0829	14.0804

Information of the first three frequencies of Ir9

S_0	1	2	3
	A	A	A
Frequencies --	22.0804	29.3699	30.9521
Red. masses --	7.1119	7.3678	7.8028
Frc consts --	0.0020	0.0037	0.0044
IR Inten --	0.0085	0.3404	0.6586

S_1	1	2	3
	A	A	A
Frequencies --	18.4757	23.5065	30.2912
Red. masses --	6.6991	6.5636	9.7131
Frc consts --	0.0013	0.0021	0.0053
IR Inten --	71.2214	1.4435	16.2754

T_1	1	2	3
	A	A	A
Frequencies --	21.1226	25.0045	30.5105
Red. masses --	7.4545	6.4932	8.4710
Frc consts --	0.0020	0.0024	0.0046
IR Inten --	0.9515	0.0003	0.8710

T_2	1	2	3
	A	A	A
Frequencies --	20.3558	27.0297	32.5528
Red. masses --	8.0482	7.9921	7.4562
Frc consts --	0.0020	0.0034	0.0047
IR Inten --	0.1396	0.7786	5.1674

2.4 Full CDA Results

Charge decomposition analysis is widespread adopted for structural analysis. It was firstly proposed by Dapprich et al.,[1] expanded by Gorelsky et al. (ECDA)[2] and generalized by Tian Lu et al. (GCDA)[3]. In this work, GCDA are used for studying electronic structure of **Ir1**.

Fragment orbitals that contribute over 1% to complex orbitals have been listed below for complex orbitals range from MO 101 to 150 and such range has already covered all orbitals that may be of importance to the coordinating structure of **Ir1**.

Occupation number of orbital 101 of the complex:2.00000000

Orbital	45 of fragment 1, Occ: 2.00000	Contribution:	4.52 %
Orbital	48 of fragment 1, Occ: 2.00000	Contribution:	10.31 %
Orbital	49 of fragment 1, Occ: 2.00000	Contribution:	6.30 %
Orbital	51 of fragment 1, Occ: 2.00000	Contribution:	7.74 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	2.38 %
Orbital	38 of fragment 4, Occ: 2.00000	Contribution:	14.18 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	37.31 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	9.65 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	1.58 %
Sum of values shown above:	93.96 %		

Occupation number of orbital 102 of the complex:2.00000000

Orbital	45 of fragment 1, Occ: 2.00000	Contribution:	2.97 %
Orbital	48 of fragment 1, Occ: 2.00000	Contribution:	16.98 %
Orbital	49 of fragment 1, Occ: 2.00000	Contribution:	2.18 %
Orbital	51 of fragment 1, Occ: 2.00000	Contribution:	25.41 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	3.81 %
Orbital	36 of fragment 4, Occ: 2.00000	Contribution:	1.43 %
Orbital	38 of fragment 4, Occ: 2.00000	Contribution:	4.05 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	32.99 %
Orbital	42 of fragment 4, Occ: 2.00000	Contribution:	3.59 %
Orbital	45 of fragment 4, Occ: 2.00000	Contribution:	1.55 %
Sum of values shown above:	94.97 %		

Occupation number of orbital 103 of the complex:2.00000000

Orbital	48 of fragment 1, Occ: 2.00000	Contribution:	3.62 %
Orbital	51 of fragment 1, Occ: 2.00000	Contribution:	11.91 %
Orbital	33 of fragment 4, Occ: 2.00000	Contribution:	1.95 %
Orbital	36 of fragment 4, Occ: 2.00000	Contribution:	4.09 %
Orbital	37 of fragment 4, Occ: 2.00000	Contribution:	1.85 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	7.36 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	1.82 %

Orbital 42 of fragment 4, Occ: 2.00000 Contribution: 50.42 %
Orbital 45 of fragment 4, Occ: 2.00000 Contribution: 2.73 %
Orbital 46 of fragment 4, Occ: 2.00000 Contribution: 7.11 %
Orbital 52 of fragment 4, Occ: 2.00000 Contribution: 1.43 %
Sum of values shown above: 94.29 %

Occupation number of orbital 104 of the complex:2.00000000
Orbital 47 of fragment 1, Occ: 2.00000 Contribution: 1.23 %
Orbital 50 of fragment 1, Occ: 2.00000 Contribution: 7.07 %
Orbital 52 of fragment 1, Occ: 2.00000 Contribution: 86.72 %
Sum of values shown above: 95.02 %

Occupation number of orbital 105 of the complex:2.00000000
Orbital 46 of fragment 1, Occ: 2.00000 Contribution: 3.15 %
Orbital 7 of fragment 2, Occ: 2.00000 Contribution: 1.22 %
Orbital 43 of fragment 4, Occ: 2.00000 Contribution: 81.45 %
Orbital 47 of fragment 4, Occ: 2.00000 Contribution: 5.63 %
Orbital 49 of fragment 4, Occ: 2.00000 Contribution: 1.15 %
Orbital 51 of fragment 4, Occ: 2.00000 Contribution: 1.57 %
Orbital 54 of fragment 4, Occ: 2.00000 Contribution: 1.22 %
Sum of values shown above: 95.39 %

Occupation number of orbital 106 of the complex:2.00000000
Orbital 45 of fragment 1, Occ: 2.00000 Contribution: 14.10 %
Orbital 48 of fragment 1, Occ: 2.00000 Contribution: 3.55 %
Orbital 51 of fragment 1, Occ: 2.00000 Contribution: 5.60 %
Orbital 57 of fragment 1, Occ: 2.00000 Contribution: 22.23 %
Orbital 61 of fragment 1, Occ: 2.00000 Contribution: 1.19 %
Orbital 8 of fragment 2, Occ: 0.00000 Contribution: 1.69 %
Orbital 9 of fragment 2, Occ: 0.00000 Contribution: 7.63 %
Orbital 36 of fragment 4, Occ: 2.00000 Contribution: 1.69 %
Orbital 37 of fragment 4, Occ: 2.00000 Contribution: 1.13 %
Orbital 40 of fragment 4, Occ: 2.00000 Contribution: 19.02 %
Orbital 42 of fragment 4, Occ: 2.00000 Contribution: 4.02 %
Orbital 44 of fragment 4, Occ: 2.00000 Contribution: 6.03 %
Orbital 55 of fragment 4, Occ: 2.00000 Contribution: 3.01 %
Sum of values shown above: 90.89 %

Occupation number of orbital 107 of the complex:2.00000000

Orbital	45 of fragment 1, Occ: 2.00000	Contribution:	5.05 %
Orbital	48 of fragment 1, Occ: 2.00000	Contribution:	21.13 %
Orbital	51 of fragment 1, Occ: 2.00000	Contribution:	31.25 %
Orbital	57 of fragment 1, Occ: 2.00000	Contribution:	12.91 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	13.38 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	3.76 %
Orbital	10 of fragment 2, Occ: 0.00000	Contribution:	1.30 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	3.46 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	1.51 %

Sum of values shown above: 93.73 %

Occupation number of orbital 108 of the complex:2.00000000

Orbital	45 of fragment 1, Occ: 2.00000	Contribution:	3.51 %
Orbital	49 of fragment 1, Occ: 2.00000	Contribution:	1.22 %
Orbital	51 of fragment 1, Occ: 2.00000	Contribution:	7.98 %
Orbital	57 of fragment 1, Occ: 2.00000	Contribution:	7.62 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	6.28 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	3.31 %
Orbital	10 of fragment 2, Occ: 0.00000	Contribution:	3.00 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	1.84 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	1.08 %
Orbital	36 of fragment 4, Occ: 2.00000	Contribution:	2.94 %
Orbital	37 of fragment 4, Occ: 2.00000	Contribution:	1.37 %
Orbital	38 of fragment 4, Occ: 2.00000	Contribution:	3.31 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	2.73 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	2.27 %
Orbital	42 of fragment 4, Occ: 2.00000	Contribution:	8.71 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	22.97 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	1.88 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	3.66 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	6.20 %

Sum of values shown above: 91.88 %

Occupation number of orbital 109 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	1.47 %
Orbital	34 of fragment 4, Occ: 2.00000	Contribution:	1.10 %
Orbital	35 of fragment 4, Occ: 2.00000	Contribution:	1.32 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	1.07 %
Orbital	42 of fragment 4, Occ: 2.00000	Contribution:	10.28 %

Orbital	45 of fragment 4, Occ: 2.00000	Contribution:	64.05 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	12.39 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	2.62 %

Sum of values shown above: 94.30 %

Occupation number of orbital 110 of the complex: 2.00000000

Orbital	46 of fragment 1, Occ: 2.00000	Contribution:	2.33 %
Orbital	47 of fragment 1, Occ: 2.00000	Contribution:	5.58 %
Orbital	50 of fragment 1, Occ: 2.00000	Contribution:	4.17 %
Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	14.40 %
Orbital	59 of fragment 1, Occ: 2.00000	Contribution:	43.12 %
Orbital	60 of fragment 1, Occ: 2.00000	Contribution:	1.57 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	2.81 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	7.01 %
Orbital	43 of fragment 4, Occ: 2.00000	Contribution:	8.61 %
Orbital	47 of fragment 4, Occ: 2.00000	Contribution:	2.33 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	1.26 %

Sum of values shown above: 93.21 %

Occupation number of orbital 111 of the complex:2.00000000

Orbital	44 of fragment 1, Occ: 2.00000	Contribution:	4.60 %
Orbital	49 of fragment 1, Occ: 2.00000	Contribution:	1.23 %
Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	53.16 %
Orbital	58 of fragment 1, Occ: 2.00000	Contribution:	5.55 %
Orbital	63 of fragment 1, Occ: 0.00000	Contribution:	1.32 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	2.20 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	3.00 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	2.47 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	1.15 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	1.18 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	1.24 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	4.75 %
Orbital	45 of fragment 4, Occ: 2.00000	Contribution:	9.62 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	1.16 %

Sum of values shown above: 92.62 %

Occupation number of orbital 112 of the complex:2.00000000

Orbital	46 of fragment 1, Occ: 2.00000	Contribution:	7.14 %
Orbital	47 of fragment 1, Occ: 2.00000	Contribution:	2.02 %
Orbital	50 of fragment 1, Occ: 2.00000	Contribution:	2.01 %
Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	32.58 %

Orbital	59 of fragment 1, Occ: 2.00000	Contribution:	24.58 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	10.90 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	2.36 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	2.03 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	1.28 %
Orbital	41 of fragment 4, Occ: 2.00000	Contribution:	2.23 %
Orbital	43 of fragment 4, Occ: 2.00000	Contribution:	2.16 %
Orbital	47 of fragment 4, Occ: 2.00000	Contribution:	3.74 %
Sum of values shown above:	93.03 %		

Occupation number of orbital 113 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	4.68 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	1.06 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	7.80 %
Orbital	10 of fragment 2, Occ: 0.00000	Contribution:	2.65 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	3.18 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	5.56 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	1.88 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	1.03 %
Orbital	42 of fragment 4, Occ: 2.00000	Contribution:	6.19 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	9.91 %
Orbital	45 of fragment 4, Occ: 2.00000	Contribution:	13.05 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	20.73 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	7.65 %
Orbital	52 of fragment 4, Occ: 2.00000	Contribution:	2.13 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	6.07 %
Sum of values shown above:	93.57 %		

Occupation number of orbital 114 of the complex:2.00000000

Orbital	46 of fragment 1, Occ: 2.00000	Contribution:	1.33 %
Orbital	53 of fragment 1, Occ: 2.00000	Contribution:	96.04 %
Sum of values shown above:	97.36 %		

Occupation number of orbital 115 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	6.04 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	4.53 %
Orbital	10 of fragment 2, Occ: 0.00000	Contribution:	1.40 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	1.18 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	2.97 %
Orbital	38 of fragment 4, Occ: 2.00000	Contribution:	1.99 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	39.11 %

Orbital	45 of fragment 4, Occ: 2.00000	Contribution:	2.67 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	26.14 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	1.42 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	5.06 %
Sum of values shown above:	92.53 %		

Occupation number of orbital 116 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	1.04 %
Orbital	57 of fragment 1, Occ: 2.00000	Contribution:	7.63 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	11.36 %
Orbital	39 of fragment 4, Occ: 2.00000	Contribution:	5.39 %
Orbital	40 of fragment 4, Occ: 2.00000	Contribution:	3.02 %
Orbital	42 of fragment 4, Occ: 2.00000	Contribution:	4.06 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	1.50 %
Orbital	52 of fragment 4, Occ: 2.00000	Contribution:	57.63 %
Sum of values shown above:	91.63 %		

Occupation number of orbital 117 of the complex:2.00000000

Orbital	49 of fragment 1, Occ: 2.00000	Contribution:	5.34 %
Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	4.13 %
Orbital	56 of fragment 1, Occ: 2.00000	Contribution:	80.11 %
Orbital	58 of fragment 1, Occ: 2.00000	Contribution:	5.39 %
Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	1.02 %
Sum of values shown above:	95.99 %		

Occupation number of orbital 118 of the complex:2.00000000

Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	11.66 %
Orbital	41 of fragment 4, Occ: 2.00000	Contribution:	2.49 %
Orbital	43 of fragment 4, Occ: 2.00000	Contribution:	2.28 %
Orbital	47 of fragment 4, Occ: 2.00000	Contribution:	76.32 %
Orbital	49 of fragment 4, Occ: 2.00000	Contribution:	1.38 %
Orbital	50 of fragment 4, Occ: 2.00000	Contribution:	1.23 %
Sum of values shown above:	95.36 %		

Occupation number of orbital 119 of the complex:2.00000000

Orbital	44 of fragment 4, Occ: 2.00000	Contribution:	3.34 %
Orbital	46 of fragment 4, Occ: 2.00000	Contribution:	18.87 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	73.91 %
Sum of values shown above:	96.12 %		

Occupation number of orbital 120 of the complex:2.00000000

Orbital	59 of fragment 1, Occ: 2.00000	Contribution:	5.60 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	2.14 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	6.17 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	1.83 %
Orbital	41 of fragment 4, Occ: 2.00000	Contribution:	6.21 %
Orbital	43 of fragment 4, Occ: 2.00000	Contribution:	1.82 %
Orbital	47 of fragment 4, Occ: 2.00000	Contribution:	1.70 %
Orbital	49 of fragment 4, Occ: 2.00000	Contribution:	64.58 %
Orbital	50 of fragment 4, Occ: 2.00000	Contribution:	3.55 %
Sum of values shown above:	93.60 %		

Occupation number of orbital 121 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	15.30 %
Orbital	56 of fragment 1, Occ: 2.00000	Contribution:	11.62 %
Orbital	57 of fragment 1, Occ: 2.00000	Contribution:	1.20 %
Orbital	58 of fragment 1, Occ: 2.00000	Contribution:	63.67 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	1.09 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	1.48 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	1.22 %
Sum of values shown above:	95.57 %		

Occupation number of orbital 122 of the complex:2.00000000

Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	12.77 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	5.54 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	2.91 %
Orbital	47 of fragment 4, Occ: 2.00000	Contribution:	5.12 %
Orbital	49 of fragment 4, Occ: 2.00000	Contribution:	1.51 %
Orbital	50 of fragment 4, Occ: 2.00000	Contribution:	57.79 %
Orbital	51 of fragment 4, Occ: 2.00000	Contribution:	5.91 %
Orbital	53 of fragment 4, Occ: 2.00000	Contribution:	1.26 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	2.87 %
Sum of values shown above:	95.69 %		

Occupation number of orbital 123 of the complex:2.00000000

Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	15.36 %
Orbital	60 of fragment 1, Occ: 2.00000	Contribution:	11.20 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	8.73 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	4.12 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	1.35 %

Orbital	43 of fragment 4, Occ: 2.00000	Contribution:	1.08 %
Orbital	49 of fragment 4, Occ: 2.00000	Contribution:	2.20 %
Orbital	50 of fragment 4, Occ: 2.00000	Contribution:	31.99 %
Orbital	51 of fragment 4, Occ: 2.00000	Contribution:	17.49 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	2.30 %
Sum of values shown above:	95.82 %		

Occupation number of orbital 124 of the complex:2.00000000

Orbital	54 of fragment 1, Occ: 2.00000	Contribution:	3.35 %
Orbital	58 of fragment 1, Occ: 2.00000	Contribution:	13.50 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	9.55 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	13.01 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	10.70 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	2.15 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	2.48 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	3.00 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	11.19 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	15.87 %
Orbital	48 of fragment 4, Occ: 2.00000	Contribution:	3.56 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	4.99 %
Sum of values shown above:	93.35 %		

Occupation number of orbital 125 of the complex:2.00000000

Orbital	60 of fragment 1, Occ: 2.00000	Contribution:	65.81 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	1.27 %
Orbital	51 of fragment 4, Occ: 2.00000	Contribution:	25.60 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	1.65 %
Sum of values shown above:	94.33 %		

Occupation number of orbital 126 of the complex:2.00000000

Orbital	55 of fragment 1, Occ: 2.00000	Contribution:	5.06 %
Orbital	60 of fragment 1, Occ: 2.00000	Contribution:	18.03 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	2.32 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	6.00 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	17.11 %
Orbital	13 of fragment 2, Occ: 0.00000	Contribution:	1.79 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	1.73 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	14.04 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	6.62 %
Orbital	49 of fragment 4, Occ: 2.00000	Contribution:	2.68 %
Orbital	50 of fragment 4, Occ: 2.00000	Contribution:	2.22 %

Orbital 51 of fragment 4, Occ: 2.00000 Contribution: 20.15 %

Sum of values shown above: 97.76 %

Occupation number of orbital 127 of the complex:2.00000000

Orbital 59 of fragment 1, Occ: 2.00000 Contribution: 6.92 %

Orbital 5 of fragment 2, Occ: 2.00000 Contribution: 15.47 %

Orbital 6 of fragment 2, Occ: 2.00000 Contribution: 32.06 %

Orbital 7 of fragment 2, Occ: 2.00000 Contribution: 6.37 %

Orbital 49 of fragment 4, Occ: 2.00000 Contribution: 17.52 %

Orbital 51 of fragment 4, Occ: 2.00000 Contribution: 16.09 %

Sum of values shown above: 94.42 %

Occupation number of orbital 128 of the complex:2.00000000

Orbital 54 of fragment 1, Occ: 2.00000 Contribution: 4.53 %

Orbital 56 of fragment 1, Occ: 2.00000 Contribution: 1.16 %

Orbital 58 of fragment 1, Occ: 2.00000 Contribution: 2.85 %

Orbital 63 of fragment 1, Occ: 0.00000 Contribution: 1.35 %

Orbital 7 of fragment 3, Occ: 2.00000 Contribution: 36.20 %

Orbital 9 of fragment 3, Occ: 2.00000 Contribution: 18.14 %

Orbital 55 of fragment 4, Occ: 2.00000 Contribution: 27.31 %

Sum of values shown above: 91.54 %

Occupation number of orbital 129 of the complex:2.00000000

Orbital 55 of fragment 1, Occ: 2.00000 Contribution: 1.20 %

Orbital 59 of fragment 1, Occ: 2.00000 Contribution: 1.40 %

Orbital 5 of fragment 2, Occ: 2.00000 Contribution: 5.24 %

Orbital 7 of fragment 2, Occ: 2.00000 Contribution: 8.91 %

Orbital 13 of fragment 2, Occ: 0.00000 Contribution: 2.43 %

Orbital 7 of fragment 3, Occ: 2.00000 Contribution: 4.45 %

Orbital 8 of fragment 3, Occ: 2.00000 Contribution: 36.11 %

Orbital 9 of fragment 3, Occ: 2.00000 Contribution: 17.03 %

Orbital 51 of fragment 4, Occ: 2.00000 Contribution: 9.31 %

Orbital 54 of fragment 4, Occ: 2.00000 Contribution: 10.09 %

Sum of values shown above: 96.17 %

Occupation number of orbital 130 of the complex:2.00000000

Orbital 54 of fragment 1, Occ: 2.00000 Contribution: 1.17 %

Orbital 58 of fragment 1, Occ: 2.00000 Contribution: 1.47 %

Orbital 63 of fragment 1, Occ: 0.00000 Contribution: 2.14 %

Orbital 5 of fragment 2, Occ: 2.00000 Contribution: 6.56 %

Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	8.94 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	7.35 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	2.23 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	1.79 %
Orbital	11 of fragment 2, Occ: 0.00000	Contribution:	2.57 %
Orbital	7 of fragment 3, Occ: 2.00000	Contribution:	33.36 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	18.08 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	10.49 %
Sum of values shown above:	96.13 %		

Occupation number of orbital 131 of the complex:2.00000000

Orbital	53 of fragment 4, Occ: 2.00000	Contribution:	94.92 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	1.70 %
Sum of values shown above:	96.63 %		

Occupation number of orbital 132 of the complex:2.00000000

Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	7.50 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	6.11 %
Orbital	17 of fragment 2, Occ: 0.00000	Contribution:	-1.08 %
Orbital	8 of fragment 3, Occ: 2.00000	Contribution:	3.88 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	1.83 %
Orbital	51 of fragment 4, Occ: 2.00000	Contribution:	1.76 %
Orbital	53 of fragment 4, Occ: 2.00000	Contribution:	1.28 %
Orbital	54 of fragment 4, Occ: 2.00000	Contribution:	74.96 %
Sum of values shown above:	96.23 %		

Occupation number of orbital 133 of the complex:0.00000000

Orbital	63 of fragment 1, Occ: 0.00000	Contribution:	90.24 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	1.07 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	1.46 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	1.20 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	1.14 %
Orbital	9 of fragment 3, Occ: 2.00000	Contribution:	1.54 %
Sum of values shown above:	96.66 %		

Occupation number of orbital 134 of the complex:0.00000000

Orbital	62 of fragment 1, Occ: 0.00000	Contribution:	97.42 %
Sum of values shown above:	97.42 %		

Occupation number of orbital 135 of the complex:0.00000000

Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	1.71 %
Orbital	6 of fragment 2, Occ: 2.00000	Contribution:	1.10 %
Orbital	56 of fragment 4, Occ: 0.00000	Contribution:	88.95 %
Orbital	57 of fragment 4, Occ: 0.00000	Contribution:	2.06 %
Orbital	65 of fragment 4, Occ: 0.00000	Contribution:	2.53 %
Sum of values shown above:	96.35 %		

Occupation number of orbital 136 of the complex:0.00000000

Orbital	65 of fragment 1, Occ: 0.00000	Contribution:	92.54 %
Orbital	66 of fragment 1, Occ: 0.00000	Contribution:	5.11 %
Sum of values shown above:	97.65 %		

Occupation number of orbital 137 of the complex:0.00000000

Orbital	64 of fragment 1, Occ: 0.00000	Contribution:	93.27 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	1.96 %
Orbital	7 of fragment 2, Occ: 2.00000	Contribution:	1.87 %
Orbital	57 of fragment 4, Occ: 0.00000	Contribution:	1.31 %
Sum of values shown above:	98.41 %		

Occupation number of orbital 138 of the complex:0.00000000

Orbital	64 of fragment 1, Occ: 0.00000	Contribution:	1.56 %
Orbital	56 of fragment 4, Occ: 0.00000	Contribution:	1.86 %
Orbital	57 of fragment 4, Occ: 0.00000	Contribution:	92.79 %
Sum of values shown above:	96.20 %		

Occupation number of orbital 139 of the complex:0.00000000

Orbital	65 of fragment 1, Occ: 0.00000	Contribution:	5.45 %
Orbital	66 of fragment 1, Occ: 0.00000	Contribution:	92.46 %
Sum of values shown above:	97.91 %		

Occupation number of orbital 140 of the complex:0.00000000

Orbital	57 of fragment 1, Occ: 2.00000	Contribution:	5.00 %
Orbital	61 of fragment 1, Occ: 2.00000	Contribution:	27.27 %
Orbital	70 of fragment 1, Occ: 0.00000	Contribution:	5.26 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	34.72 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	25.57 %
Orbital	18 of fragment 2, Occ: 0.00000	Contribution:	-4.08 %
Orbital	19 of fragment 2, Occ: 0.00000	Contribution:	-6.31 %

Orbital 52 of fragment 4, Occ: 2.00000 Contribution: 4.29 %

Orbital 55 of fragment 4, Occ: 2.00000 Contribution: 1.63 %

Sum of values shown above: 93.36 %

Occupation number of orbital 141 of the complex:0.00000000

Orbital 67 of fragment 1, Occ: 0.00000 Contribution: 75.27 %

Orbital 58 of fragment 4, Occ: 0.00000 Contribution: 23.09 %

Sum of values shown above: 98.36 %

Occupation number of orbital 142 of the complex:0.00000000

Orbital 67 of fragment 1, Occ: 0.00000 Contribution: 23.17 %

Orbital 58 of fragment 4, Occ: 0.00000 Contribution: 74.06 %

Sum of values shown above: 97.23 %

Occupation number of orbital 143 of the complex:0.00000000

Orbital 57 of fragment 1, Occ: 2.00000 Contribution: 4.87 %

Orbital 61 of fragment 1, Occ: 2.00000 Contribution: 2.85 %

Orbital 68 of fragment 1, Occ: 0.00000 Contribution: 2.03 %

Orbital 5 of fragment 2, Occ: 2.00000 Contribution: 2.14 %

Orbital 6 of fragment 2, Occ: 2.00000 Contribution: 2.88 %

Orbital 7 of fragment 2, Occ: 2.00000 Contribution: 2.40 %

Orbital 8 of fragment 2, Occ: 0.00000 Contribution: 20.51 %

Orbital 9 of fragment 2, Occ: 0.00000 Contribution: 19.74 %

Orbital 15 of fragment 2, Occ: 0.00000 Contribution: -1.00 %

Orbital 18 of fragment 2, Occ: 0.00000 Contribution: -6.11 %

Orbital 19 of fragment 2, Occ: 0.00000 Contribution: -2.66 %

Orbital 7 of fragment 3, Occ: 2.00000 Contribution: 3.31 %

Orbital 9 of fragment 3, Occ: 2.00000 Contribution: 4.42 %

Orbital 52 of fragment 4, Occ: 2.00000 Contribution: 3.39 %

Orbital 55 of fragment 4, Occ: 2.00000 Contribution: 28.49 %

Orbital 60 of fragment 4, Occ: 0.00000 Contribution: 7.29 %

Orbital 62 of fragment 4, Occ: 0.00000 Contribution: 1.43 %

Sum of values shown above: 96.00 %

Occupation number of orbital 144 of the complex:0.00000000

Orbital 59 of fragment 4, Occ: 0.00000 Contribution: 95.69 %

Orbital 70 of fragment 4, Occ: 0.00000 Contribution: 1.08 %

Sum of values shown above: 96.77 %

Occupation number of orbital 145 of the complex:0.00000000

Orbital	68 of fragment 1, Occ: 0.00000	Contribution:	29.05 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	1.23 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	1.10 %
Orbital	14 of fragment 2, Occ: 0.00000	Contribution:	1.37 %
Orbital	60 of fragment 4, Occ: 0.00000	Contribution:	44.33 %
Orbital	61 of fragment 4, Occ: 0.00000	Contribution:	6.31 %
Orbital	62 of fragment 4, Occ: 0.00000	Contribution:	8.90 %
Orbital	64 of fragment 4, Occ: 0.00000	Contribution:	2.36 %
Sum of values shown above:	94.64 %		

Occupation number of orbital 146 of the complex:0.00000000

Orbital	68 of fragment 1, Occ: 0.00000	Contribution:	63.84 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	1.28 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	4.16 %
Orbital	55 of fragment 4, Occ: 2.00000	Contribution:	2.61 %
Orbital	60 of fragment 4, Occ: 0.00000	Contribution:	17.97 %
Orbital	61 of fragment 4, Occ: 0.00000	Contribution:	2.06 %
Orbital	62 of fragment 4, Occ: 0.00000	Contribution:	4.16 %
Sum of values shown above:	96.09 %		

Occupation number of orbital 147 of the complex:0.00000000

Orbital	69 of fragment 1, Occ: 0.00000	Contribution:	90.60 %
Orbital	71 of fragment 1, Occ: 0.00000	Contribution:	1.62 %
Orbital	13 of fragment 2, Occ: 0.00000	Contribution:	2.43 %
Orbital	65 of fragment 4, Occ: 0.00000	Contribution:	3.53 %
Sum of values shown above:	98.17 %		

Occupation number of orbital 148 of the complex:0.00000000

Orbital	69 of fragment 1, Occ: 0.00000	Contribution:	4.93 %
Orbital	5 of fragment 2, Occ: 2.00000	Contribution:	1.15 %
Orbital	13 of fragment 2, Occ: 0.00000	Contribution:	1.79 %
Orbital	56 of fragment 4, Occ: 0.00000	Contribution:	3.62 %
Orbital	65 of fragment 4, Occ: 0.00000	Contribution:	79.69 %
Orbital	72 of fragment 4, Occ: 0.00000	Contribution:	6.05 %
Sum of values shown above:	97.24 %		

Occupation number of orbital 149 of the complex:0.00000000

Orbital	70 of fragment 1, Occ: 0.00000	Contribution:	61.65 %
Orbital	72 of fragment 1, Occ: 0.00000	Contribution:	4.14 %

Orbital	73 of fragment 1, Occ: 0.00000	Contribution:	2.87 %
Orbital	75 of fragment 1, Occ: 0.00000	Contribution:	1.60 %
Orbital	76 of fragment 1, Occ: 0.00000	Contribution:	1.17 %
Orbital	8 of fragment 2, Occ: 0.00000	Contribution:	3.15 %
Orbital	9 of fragment 2, Occ: 0.00000	Contribution:	2.39 %
Orbital	10 of fragment 2, Occ: 0.00000	Contribution:	2.39 %
Orbital	11 of fragment 2, Occ: 0.00000	Contribution:	5.68 %
Orbital	14 of fragment 2, Occ: 0.00000	Contribution:	4.96 %
Orbital	19 of fragment 2, Occ: 0.00000	Contribution:	-1.16 %
Orbital	20 of fragment 2, Occ: 0.00000	Contribution:	1.16 %
Orbital	52 of fragment 4, Occ: 2.00000	Contribution:	1.98 %
Orbital	60 of fragment 4, Occ: 0.00000	Contribution:	1.58 %
Orbital	61 of fragment 4, Occ: 0.00000	Contribution:	4.43 %
Sum of values shown above:	97.98 %		

Occupation number of orbital 150 of the complex:0.00000000

Orbital	63 of fragment 1, Occ: 0.00000	Contribution:	1.07 %
Orbital	70 of fragment 1, Occ: 0.00000	Contribution:	4.14 %
Orbital	73 of fragment 1, Occ: 0.00000	Contribution:	91.33 %
Sum of values shown above:	96.53 %		

2.5 Calculated Fluorescence Emission Rates

Table S2. Calculated oscillator strength (f), fluorescence emission rates (k_f) and Emission lifetime (τ).

Mol.	Ir1	Ir2	Ir3	Ir4	Ir5	Ir6	Ir7	Ir8	Ir9
f//a. u.	0.0062	0.0060	0.0078	0.0082	0.0059	0.0058	0.0061	0.0058	0.0058
$k_f/10^6$ s^{-1}	1.19	1.25	1.70	1.92	1.14	1.10	1.26	1.24	1.28
τ/μs	0.838	0.803	0.589	0.521	0.875	0.910	0.791	0.807	0.782

2.6 Calculated Phosphorescence Lifetime

Table S3. Calculated phosphorescence emission lifetime (τ).

Mol.	initial minimum point	τ/s [a]
Ir1	T_1	0.200
	T_2	0.018
Ir2	T_1	0.677
	T_2	0.298

[a] Phosphorescence emission lifetime is calculated by the Dalton program.

2.7 Calculated Excitation Energies and Oscillator Strengths

Table S4. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir1.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	537.59	2.3063	0.0049	**T_1**	555.73	2.2310	0
S_2	466.32	2.6588	0.0037	**T_2**	554.95	2.2341	0
S_3	390.81	3.1725	0.1846	**T_3**	490.47	2.5279	0
S_4	385.30	3.2178	0.0072	**T_4**	464.01	2.6720	0
S_5	381.53	3.2497	0.0000	**T_5**	412.09	3.0087	0
S_6	379.00	3.2713	0.0008	**T_6**	409.81	3.0254	0
S_7	357.62	3.4669	0.0186	**T_7**	382.41	3.2421	0
S_8	349.85	3.5440	0.0001	**T_8**	379.02	3.2712	0
S_9	343.73	3.6070	0.0001	**T_9**	373.48	3.3197	0
S_{10}	339.51	3.6519	0.0137	**T_{10}**	365.23	3.3946	0
S_{11}	337.84	3.6699	0.0144	**T_{11}**	365.05	3.3964	0
S_{12}	333.86	3.7137	0.0193	**T_{12}**	353.38	3.5085	0
S_{13}	319.54	3.8801	0.0772	**T_{13}**	348.24	3.5603	0
S_{14}	312.68	3.9652	0.2770	**T_{14}**	346.37	3.5795	0
S_{15}	311.14	3.9849	0.2036	**T_{15}**	344.61	3.5978	0

Table S5. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir2.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	519.50	2.3866	0.0048	**T_1**	581.40	2.1325	0
S_2	451.21	2.7478	0.0049	**T_2**	537.08	2.3085	0
S_3	414.88	2.9885	0.1736	**T_3**	481.75	2.5736	0
S_4	381.28	3.2518	0.0196	**T_4**	454.31	2.7291	0

S_5	376.45	3.2935	0.0001	T_5	408.58	3.0345	0
S_6	370.95	3.3424	0.0003	T_6	405.50	3.0575	0
S_7	353.11	3.5112	0.0177	T_7	388.86	3.1884	0
S_8	342.87	3.6161	0.0004	T_8	378.41	3.2764	0
S_9	338.86	3.6588	0.0199	T_9	375.97	3.2977	0
S_{10}	337.04	3.6787	0.0016	T_{10}	371.28	3.3394	0
S_{11}	331.79	3.7368	0.0054	T_{11}	361.46	3.4301	0
S_{12}	330.37	3.7529	0.0219	T_{12}	357.73	3.4658	0
S_{13}	329.27	3.7654	0.0010	T_{13}	342.40	3.6210	0
S_{14}	328.62	3.7728	0.2075	T_{14}	341.00	3.6359	0
S_{15}	320.71	3.8659	0.0492	T_{15}	339.72	3.6496	0

Table S6. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir3.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	503.90	2.4605	0.0093	T_1	2227.56	0.5566	0
S_2	449.24	2.7599	0.0051	T_2	1309.00	0.9472	0
S_3	393.08	3.1541	0.1719	T_3	800.08	1.5496	0
S_4	375.05	3.3058	0.0312	T_4	668.33	1.8551	0
S_5	365.18	3.3951	0.0031	T_5	605.34	2.0482	0
S_6	360.62	3.4381	0.0015	T_6	578.74	2.1423	0
S_7	353.37	3.5086	0.0216	T_7	507.26	2.4442	0
S_8	337.62	3.6723	0.0000	T_8	467.19	2.6538	0
S_9	336.26	3.6872	0.0162	T_9	429.51	2.8867	0
S_{10}	333.91	3.7131	0.0104	T_{10}	399.30	3.1050	0
S_{11}	331.79	3.7368	0.0104	T_{11}	396.26	3.1288	0
S_{12}	328.52	3.7740	0.0233	T_{12}	393.25	3.1528	0
S_{13}	319.36	3.8823	0.0752	T_{13}	383.98	3.2289	0
S_{14}	317.61	3.9037	0.0002	T_{14}	383.34	3.2343	0
S_{15}	311.25	3.9834	0.1758	T_{15}	370.78	3.3439	0

Table S7. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir4.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	487.92	2.5411	0.0093	T_1	573.88	2.1605	0
S_2	435.20	2.8489	0.0095	T_2	569.86	2.1757	0
S_3	417.65	2.9686	0.1660	T_3	560.98	2.2101	0
S_4	370.85	3.3432	0.0381	T_4	460.25	2.6938	0
S_5	360.46	3.4396	0.0022	T_5	434.12	2.8560	0
S_6	352.82	3.5141	0.0019	T_6	403.98	3.0691	0
S_7	348.72	3.5554	0.0202	T_7	400.90	3.0927	0
S_8	339.29	3.6542	0.0166	T_8	386.79	3.2055	0
S_9	337.47	3.6739	0.0000	T_9	381.83	3.2471	0
S_{10}	331.29	3.7424	0.0027	T_{10}	378.41	3.2765	0
S_{11}	328.92	3.7695	0.0040	T_{11}	371.98	3.3331	0
S_{12}	328.21	3.7776	0.1766	T_{12}	356.37	3.4791	0

S_{13}	324.93	3.8158	0.0183	T_{13}	350.54	3.5370	0
S_{14}	324.08	3.8258	0.0188	T_{14}	347.36	3.5694	0
S_{15}	318.17	3.8968	0.0303	T_{15}	341.14	3.6344	0

Table S8. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir5.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	535.73	2.3143	0.0048	T_1	602.31	2.0585	0
S_2	463.87	2.6728	0.0034	T_2	576.44	2.1508	0
S_3	400.04	3.0993	0.1860	T_3	561.54	2.2079	0
S_4	388.06	3.1950	0.0139	T_4	489.86	2.5310	0
S_5	381.85	3.2469	0.0012	T_5	442.42	2.8024	0
S_6	379.63	3.2660	0.0001	T_6	426.39	2.9078	0
S_7	358.25	3.4608	0.0181	T_7	412.76	3.0038	0
S_8	348.90	3.5536	0.0004	T_8	403.05	3.0762	0
S_9	338.12	3.6668	0.0311	T_9	390.80	3.1726	0
S_{10}	337.97	3.6685	0.0111	T_{10}	385.32	3.2177	0
S_{11}	334.21	3.7098	0.0126	T_{11}	375.95	3.2979	0
S_{12}	333.28	3.7202	0.0025	T_{12}	358.12	3.4620	0
S_{13}	323.37	3.8342	0.0617	T_{13}	354.10	3.5014	0
S_{14}	318.45	3.8933	0.0007	T_{14}	352.90	3.5133	0
S_{15}	316.84	3.9132	0.2779	T_{15}	348.21	3.5607	0

Table S9. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir6.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	540.49	2.2939	0.0048	T_1	2174.94	0.5701	0
S_2	467.80	2.6504	0.0031	T_2	1375.57	0.9013	0
S_3	393.91	3.1476	0.1343	T_3	810.15	1.5304	0
S_4	388.91	3.1880	0.0127	T_4	678.90	1.8262	0
S_5	382.63	3.2403	0.0012	T_5	606.05	2.0458	0
S_6	380.66	3.2571	0.0001	T_6	603.10	2.0558	0
S_7	359.18	3.4519	0.0183	T_7	512.02	2.4215	0
S_8	349.92	3.5432	0.0004	T_8	462.52	2.6806	0
S_9	339.78	3.6490	0.0123	T_9	426.55	2.9067	0
S_{10}	338.91	3.6583	0.0278	T_{10}	424.05	2.9238	0
S_{11}	334.06	3.7115	0.0026	T_{11}	403.42	3.0733	0
S_{12}	333.88	3.7135	0.0150	T_{12}	395.21	3.1371	0
S_{13}	321.76	3.8533	0.0802	T_{13}	389.20	3.1856	0
S_{14}	314.12	3.9470	0.1636	T_{14}	377.35	3.2856	0
S_{15}	313.37	3.9565	0.0073	T_{15}	368.76	3.3622	0

Table S10. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir7.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	520.20	2.3834	0.0050	T_1	599.53	2.0680	0
S_2	451.90	2.7436	0.0061	T_2	537.83	2.3053	0

S_3	421.21	2.9435	0.2416	T_3	482.47	2.5698	0
S_4	388.24	3.1935	0.0127	T_4	455.48	2.7220	0
S_5	379.07	3.2707	0.0008	T_5	408.78	3.0331	0
S_6	370.71	3.3445	0.0002	T_6	406.29	3.0516	0
S_7	358.58	3.4576	0.0186	T_7	398.77	3.1091	0
S_8	341.29	3.6328	0.0006	T_8	379.24	3.2692	0
S_9	340.00	3.6465	0.0000	T_9	371.92	3.3336	0
S_{10}	337.55	3.6731	0.0785	T_{10}	370.44	3.3470	0
S_{11}	336.23	3.6874	0.0498	T_{11}	364.43	3.4022	0
S_{12}	333.18	3.7212	0.0002	T_{12}	362.65	3.4188	0
S_{13}	330.80	3.7480	0.0070	T_{13}	343.41	3.6104	0
S_{14}	330.23	3.7544	0.1405	T_{14}	343.37	3.6108	0
S_{15}	319.57	3.8798	0.0189	T_{15}	341.77	3.6277	0

Table S11. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir8.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	513.67	2.4137	0.0048	T_1	1033.35	1.1998	0
S_2	446.23	2.7785	0.0097	T_2	776.44	1.5968	0
S_3	429.95	2.8837	0.2268	T_3	665.90	1.8619	0
S_4	384.76	3.2224	0.0157	T_4	568.77	2.1799	0
S_5	376.44	3.2936	0.0006	T_5	496.89	2.4952	0
S_6	368.86	3.3613	0.0002	T_6	489.44	2.5332	0
S_7	354.85	3.4940	0.0176	T_7	434.51	2.8534	0
S_8	345.69	3.5865	0.0001	T_8	420.42	2.9491	0
S_9	345.00	3.5937	0.0724	T_9	409.43	3.0282	0
S_{10}	339.40	3.6530	0.0026	T_{10}	392.38	3.1598	0
S_{11}	336.99	3.6791	0.1891	T_{11}	390.99	3.1710	0
S_{12}	333.78	3.7146	0.0137	T_{12}	382.50	3.2414	0
S_{13}	329.54	3.7623	0.0001	T_{13}	371.45	3.3379	0
S_{14}	327.15	3.7898	0.0048	T_{14}	357.87	3.4645	0
S_{15}	321.86	3.8522	0.3066	T_{15}	348.39	3.5588	0

Table S12. Excitation energies and oscillator strengths obtained from TD-DFT calculation for Ir9.

State	*E* / nm	*E* / eV	*f*	State	*E* / nm	*E* / eV	*f*
S_1	506.24	2.4491	0.0048	T_1	1375.57	0.9013	0
S_2	473.42	2.6189	0.2364	T_2	1251.10	0.9910	0
S_3	439.77	2.8193	0.0012	T_3	717.02	1.7292	0
S_4	383.32	3.2345	0.0159	T_4	689.11	1.7992	0
S_5	375.64	3.3006	0.0001	T_5	621.73	1.9942	0
S_6	375.25	3.3040	0.0005	T_6	595.63	2.0816	0
S_7	368.17	3.3676	0.1898	T_7	533.32	2.3248	0
S_8	364.06	3.4056	0.0002	T_8	488.27	2.5392	0
S_9	357.91	3.4641	0.0207	T_9	442.39	2.8026	0
S_{10}	353.33	3.5090	0.0175	T_{10}	422.62	2.9337	0

$\mathbf{S_{11}}$	349.32	3.5493	0.2871	$\mathbf{T_{11}}$	418.75	2.9608	0
$\mathbf{S_{12}}$	336.01	3.6899	0.0045	$\mathbf{T_{12}}$	407.27	3.0443	0
$\mathbf{S_{13}}$	331.93	3.7353	0.0172	$\mathbf{T_{13}}$	400.08	3.0989	0
$\mathbf{S_{14}}$	327.14	3.7900	0.0003	$\mathbf{T_{14}}$	398.07	3.1146	0
$\mathbf{S_{15}}$	324.72	3.8181	0.0015	$\mathbf{T_{15}}$	383.82	3.2303	0

3. References

1. Dapprich, S.; Frenking, G., Investigation of Donor-Acceptor Interactions: A Charge Decomposition Analysis Using Fragment Molecular Orbitals. *The Journal of Physical Chemistry* **1995**, *99*, 9352-9362.
2. Gorelsky, S. I.; Ghosh, S.; Solomon, E. I., Mechanism of N2o Reduction by the M4-S Tetranuclear Cuz Cluster of Nitrous Oxide Reductase. *Journal of the American Chemical Society* **2006**, *128*, 278-290.
3. Meng Xiao, T. L., Generalized Charge Decomposition Analysis (Gcda) Method. *Journal of Advances in Physical Chemistry* **2015**, *4*.