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Cyclometalated cinchophen ligands on iridium(III): towards water soluble complexes with visible luminescence

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Table S1. Parameters associated with the single crystal diffraction data collection for complexes **3b** and **3e.**

	3b	**3e**
Formula	$C_{50}H_{45}F_6IrN_4O_{4.5}P$	$C_{66}H_{57}F_6IrN_5O_5P$
Formula weight	1111.07	1337.34
Temperature / K	293(2)	293(2)
Wavelength / Å	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	P2(1)/a
a/Å	31.7884(9)	15.3862(3)
b/Å	16.8473(5)	20.0202(4)
c/Å	18.0766(4)	19.0094(3)
α/°	90	90
β/°	94.354(2)	96.3930(10)
γ/°	90	90
Volume/Å^3	9653.0(4)	5819.14(19)
Z	8	4
F000	4440	2696
μ/mm^{-1}	2.871	2.397
Reflections collected	16579	21056
Independent reflections (R_{int})	8543 (0.0862)	11600 (0.0688)
Final *R*1 [$I>2\sigma(I)$]: R_1, wR_2	0.0818, 0.1392	0.0730, 0.1262

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Electrochemistry

Table S2. Electrochemical properties of $[Ir(epqc)_2(N^N)]PF_6$ (**3a-h**) complexes.[a]

Complex	*Oxidation*			*Reduction 1*			*Reduction 2*		
	E_p^{ox}/V	E_p^{red}/V	$E^0_{(ox)}$/V	E_p^{red}/V	E_p^{ox}/V	$E^0_{(red\ 1)}$/V	E_p^{red}/V	E_p^{ox}/V	$E^0_{(red\ 2)}$/V
3a	1.48	1.38	1.43	-1.20	-1.14	-1.17	-	-	-
3b	1.42	1.33	1.38	-1.11	-1.05	-1.08	-1.50	-1.41	-1.46
3c	1.56	1.39	1.48	-0.95	-0.89	-0.92	-1.32	-1.23	-1.28
3d	1.48	1.39	1.44	-1.20	-1.15	-1.18	-	-	-
3e	1.46	1.41	1.44	-1.13	-1.10	-1.12	-1.36	-1.30	-1.33
3f	1.51	1.45	1.48	-0.99	-0.95	-0.97	-1.41	-1.19	-1.30
3g	1.56	1.42	1.49	-1.24	-1.12	-1.18	-	-	-
3h	1.52	1.41	1.47	-0.44	-0.39	-0.42	-0.99	-0.89	-0.95

[a] Oxidation and reduction potentials measured in CH_2Cl_2 solutions at 200 mVs^{-1} with 0.1 M $[NBu_4][PF_6]$ as supporting electrolyte calibrated with Fc/Fc^+.

Table S3. Absorption and electrochemical properties of $[Ir(epqc)_2(N^N)]PF_6$ (**3a-h**) complexes.

Complex	E_{ox} / V	HOMO / eV[b]	$E_{bandgap}$ / eV[c]	LUMO / eV[d]
3a	1.43	-5.77	2.15	-3.62
3b	1.38	-5.72	2.15	-3.57
3c	1.48	-5.82	2.17	-3.65
3d	1.44	-5.78	2.14	-3.64
3e	1.44	-5.78	2.16	-3.62
3f	1.48	-5.82	2.16	-3.66
3g	1.49	-5.83	2.14	-3.69
3h	1.47	-5.81	2.14	-3.67

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DFT calculations

Figure S1. Frontier orbitals of **[Ir(epqc)$_2$(N^N)]$^+$** (**3a-h**) complexes.

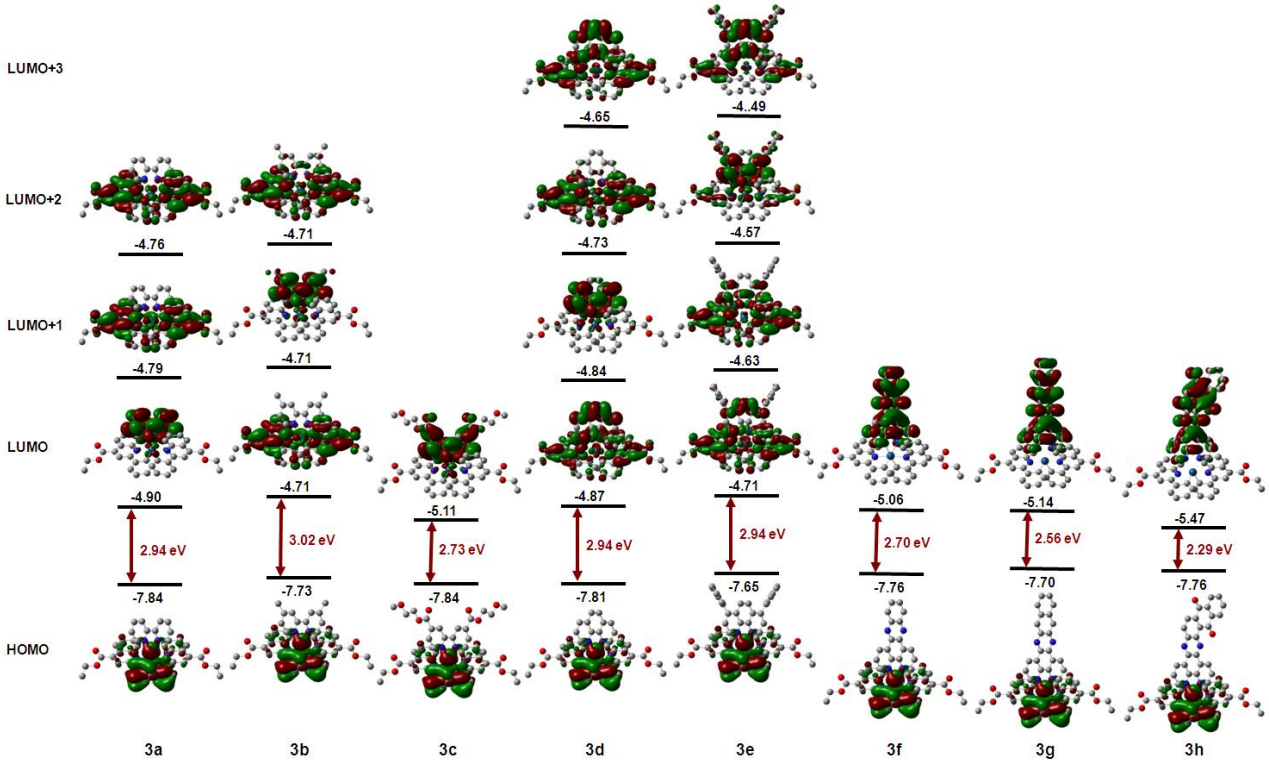
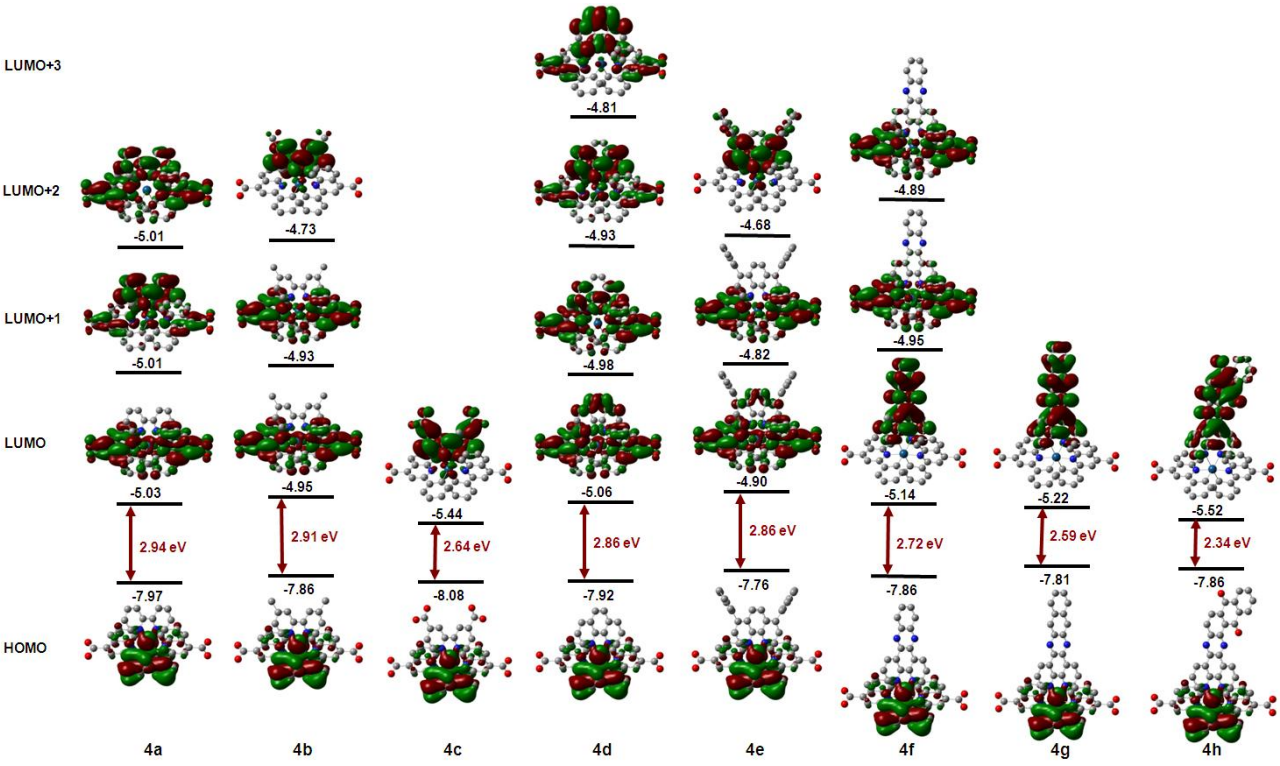


Figure S2. Frontier orbitals of **[Ir(epqc)$_2$(N^N)]$^+$** (**4a-h**) complexes.



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Luminescence Spectroscopy

Cartesian coordinates

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.664569	1.724717	1.159796
2	7	0	2.065846	-0.197114	0.388136
3	7	0	-2.066225	-0.196594	-0.388126
4	7	0	0.665203	1.724863	-1.159567
5	6	0	1.449551	1.652510	-2.252639
6	1	0	1.603192	0.658826	-2.658374
7	6	0	2.028158	2.773935	-2.840503
8	1	0	2.647899	2.662105	-3.721865
9	6	0	1.796896	4.025633	-2.268367
10	1	0	2.239869	4.920623	-2.689978
11	6	0	0.991763	4.105153	-1.135165
12	1	0	0.820679	5.063215	-0.661483
13	6	0	0.430523	2.939163	-0.599130
14	6	0	-0.428765	2.939162	0.600158
15	6	0	-0.989068	4.105294	1.136869
16	1	0	-0.817080	5.063513	0.663833
17	6	0	-1.794455	4.025739	2.269887
18	1	0	-2.236710	4.920842	2.692011
19	6	0	-2.026947	2.773866	2.841146
20	1	0	-2.646973	2.662003	3.722303
21	6	0	-1.449205	1.652325	2.252659
22	1	0	-1.603774	0.658508	2.657724
23	6	0	6.393487	-0.363684	0.268150
24	8	0	7.163420	0.422009	0.793756
25	8	0	6.797148	-1.389371	-0.512098
26	6	0	8.251037	-1.494672	-0.691778
27	1	0	8.603753	-0.572255	-1.162910
28	1	0	8.710279	-1.565771	0.298325
29	6	0	8.507802	-2.720439	-1.542256
30	1	0	8.029390	-2.630371	-2.522319
31	1	0	9.584433	-2.840664	-1.700244
32	1	0	8.133166	-3.624643	-1.053362
33	6	0	-0.499712	-1.461003	1.320373
34	6	0	0.364324	-2.188780	2.152994
35	1	0	1.437535	-2.055144	2.071352
36	6	0	-0.134143	-3.094899	3.092414
37	1	0	0.555764	-3.647610	3.723199
38	6	0	-1.513939	-3.303307	3.224254
39	1	0	-1.893885	-4.010788	3.953178
40	6	0	-2.391941	-2.606224	2.403410
41	1	0	-3.458334	-2.785579	2.496783
42	6	0	-1.890397	-1.695911	1.451581
43	6	0	-2.725363	-0.959339	0.512875
44	6	0	-4.139646	-1.021763	0.522709
45	1	0	-4.635552	-1.622609	1.270930
46	6	0	-2.788909	0.432149	-1.390809
47	6	0	-2.103787	1.057779	-2.457615
48	1	0	-1.028724	0.989258	-2.480837
49	6	0	-2.791178	1.695198	-3.470654
50	1	0	-2.242484	2.150926	-4.288370
51	6	0	-4.200153	1.742417	-3.456436
52	1	0	-4.734677	2.253907	-4.249342
53	6	0	-4.902164	1.115554	-2.447108
54	1	0	-5.982946	1.132145	-2.433734

55	6	0	-4.227057	0.428628	-1.404068
56	6	0	-4.897507	-0.317681	-0.381677
57	6	0	2.103152	1.055512	2.458694
58	1	0	1.028095	0.986862	2.481809
59	6	0	2.790430	1.692119	3.472318
60	1	0	2.241648	2.147121	4.290379
61	6	0	4.199404	1.739425	3.458252
62	1	0	4.733837	2.250294	4.251619
63	6	0	4.901532	1.113392	2.448490
64	1	0	5.982314	1.130010	2.435248
65	6	0	4.226545	0.427275	1.404839
66	6	0	2.788397	0.430808	1.391422
67	6	0	4.897110	-0.318271	0.381966
68	6	0	4.139354	-1.021730	-0.522998
69	1	0	4.635348	-1.622055	-1.271579
70	6	0	2.725073	-0.959277	-0.513294
71	6	0	1.890183	-1.695250	-1.452548
72	6	0	2.391793	-2.605029	-2.404851
73	1	0	3.458189	-2.784370	-2.498217
74	6	0	0.499488	-1.460383	-1.321358
75	6	0	-0.364493	-2.187648	-2.154475
76	1	0	-1.437707	-2.053988	-2.072848
77	6	0	0.134039	-3.093241	-3.094370
78	1	0	-0.555815	-3.645569	-3.725548
79	6	0	1.513844	-3.301613	-3.226182
80	1	0	1.893843	-4.008692	-3.955470
81	6	0	-6.393870	-0.363205	-0.267729
82	8	0	-7.163880	0.422845	-0.792689
83	8	0	-6.797412	-1.389452	0.511847
84	6	0	-8.251275	-1.494960	0.691597
85	1	0	-8.710685	-1.564643	-0.298526
86	1	0	-8.603877	-0.573192	1.164090
87	6	0	-8.507947	-2.721899	1.540410
88	1	0	-9.584528	-2.842032	1.698807
89	1	0	-8.133840	-3.625502	1.050002
90	1	0	-8.028981	-2.633400	2.520346
91	77	0	-0.000135	-0.048020	-0.000180

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.693240	1.528784	1.140586
2	7	0	2.055305	-0.389967	0.440438
3	7	0	-2.054559	-0.390625	-0.440935
4	7	0	0.692395	1.529862	-1.139774
5	6	0	1.505810	1.468273	-2.212948
6	1	0	1.675976	0.477803	-2.620312
7	6	0	2.092233	2.591105	-2.782023
8	1	0	2.733360	2.477698	-3.649211
9	6	0	1.855062	3.858145	-2.226525
10	6	0	1.013289	3.910231	-1.111270
11	1	0	0.822822	4.865880	-0.638332
12	6	0	0.442708	2.744052	-0.589053
13	6	0	-0.447281	2.743173	0.588891
14	6	0	-1.021722	3.908080	1.110013
15	1	0	-0.835767	4.863650	0.635178
16	6	0	-1.862035	3.854583	2.226144
17	6	0	-2.096042	2.587074	2.782244
18	1	0	-2.737982	2.472163	3.648641
19	6	0	-1.506445	1.465632	2.213962

20	1	0	-1.674721	0.474792	2.621196
21	6	0	6.384987	-0.539024	0.423030
22	8	0	7.139676	0.248417	0.968101
23	8	0	6.811680	-1.560274	-0.351388
24	6	0	8.269267	-1.657014	-0.499518
25	1	0	8.627958	-0.729618	-0.956210
26	1	0	8.707251	-1.733116	0.499830
27	6	0	8.550888	-2.875354	-1.352956
28	1	0	8.093587	-2.780324	-2.342592
29	1	0	9.631306	-2.989472	-1.488044
30	1	0	8.169784	-3.784816	-0.879045
31	6	0	-0.534419	-1.656473	1.307049
32	6	0	0.306540	-2.385871	2.162110
33	1	0	1.381819	-2.254157	2.107758
34	6	0	-0.217302	-3.290212	3.089120
35	1	0	0.455283	-3.843861	3.737622
36	6	0	-1.600526	-3.495953	3.186098
37	1	0	-2.000225	-4.202354	3.905493
38	6	0	-2.455901	-2.797620	2.342843
39	1	0	-3.524733	-2.974769	2.408983
40	6	0	-1.928492	-1.888852	1.403607
41	6	0	-2.737857	-1.150665	0.444131
42	6	0	-4.152272	-1.207933	0.420214
43	1	0	-4.667971	-1.805550	1.157592
44	6	0	-2.750764	0.239537	-1.461189
45	6	0	-2.037628	0.862482	-2.511162
46	1	0	-0.962296	0.793459	-2.506210
47	6	0	-2.698202	1.500582	-3.541426
48	1	0	-2.128083	1.954290	-4.345503
49	6	0	-4.106959	1.551511	-3.562192
50	1	0	-4.620399	2.063248	-4.368820
51	6	0	-4.835470	0.928156	-2.569601
52	1	0	-5.916204	0.947868	-2.582938
53	6	0	-4.188186	0.240564	-1.509547
54	6	0	-4.885786	-0.501896	-0.502481
55	6	0	2.037837	0.862214	2.511214
56	1	0	0.962504	0.793277	2.505863
57	6	0	2.698140	1.499764	3.541994
58	1	0	2.127809	1.953021	4.346177
59	6	0	4.106891	1.550682	3.563180
60	1	0	4.620114	2.061933	4.370255
61	6	0	4.835661	0.927943	2.570393
62	1	0	5.916394	0.947700	2.583984
63	6	0	4.188653	0.240941	1.509790
64	6	0	2.751247	0.239793	1.461122
65	6	0	4.886560	-0.500839	0.502436
66	6	0	4.153335	-1.206365	-0.420865
67	1	0	4.669262	-1.803470	-1.158499
68	6	0	2.738909	-1.149312	-0.445000
69	6	0	1.929878	-1.887068	-1.405065
70	6	0	2.457660	-2.794904	-2.345001
71	1	0	3.526562	-2.971578	-2.411275
72	6	0	0.535718	-1.655290	-1.308369
73	6	0	-0.304949	-2.384366	-2.163998
74	1	0	-1.380277	-2.253113	-2.109557
75	6	0	0.219266	-3.287774	-3.091700
76	1	0	-0.453092	-3.841174	-3.740648
77	6	0	1.602576	-3.492898	-3.188821
78	1	0	2.002558	-4.198569	-3.908775
79	6	0	-6.384197	-0.540313	-0.422772
80	8	0	-7.139149	0.246944	-0.967734
81	8	0	-6.810595	-1.561592	0.351799
82	6	0	-8.268141	-1.658547	0.500127

83	1	0	-8.706255	-1.734754	-0.499156
84	1	0	-8.626913	-0.731184	0.956824
85	6	0	-8.549474	-2.876890	1.353656
86	1	0	-9.629859	-2.991158	1.488887
87	1	0	-8.168301	-3.786318	0.879734
88	1	0	-8.092060	-2.781751	2.343230
89	77	0	0.000342	-0.244664	-0.000181
90	6	0	-2.493208	5.090521	2.800747
91	1	0	-2.183006	5.241088	3.841383
92	1	0	-2.220229	5.984741	2.235065
93	1	0	-3.586247	5.009674	2.798612
94	6	0	2.492008	5.094304	-2.794211
95	1	0	2.326593	5.162849	-3.874892
96	1	0	2.096987	6.002199	-2.331654
97	1	0	3.576935	5.081081	-2.633688

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.091081	0.518464	0.774055
2	7	0	1.713308	-1.399508	1.220480
3	7	0	-1.713300	-1.399496	-1.220496
4	7	0	1.091082	0.518478	-0.774045
5	6	0	2.260634	0.450640	-1.439657
6	1	0	2.575579	-0.541888	-1.740863
7	6	0	3.025971	1.573113	-1.740542
8	1	0	3.957085	1.473816	-2.282912
9	6	0	2.566935	2.826065	-1.325407
10	6	0	1.361170	2.900273	-0.629146
11	1	0	1.022201	3.872402	-0.293248
12	6	0	0.638689	1.733636	-0.367422
13	6	0	-0.638694	1.733629	0.367447
14	6	0	-1.361178	2.900260	0.629187
15	1	0	-1.022213	3.872395	0.293301
16	6	0	-2.566942	2.826038	1.325449
17	6	0	-3.025974	1.573079	1.740567
18	1	0	-3.957086	1.473772	2.282937
19	6	0	-2.260632	0.450613	1.439667
20	1	0	-2.575573	-0.541920	1.740860
21	6	0	5.693513	-1.574322	2.925935
22	8	0	6.165158	-0.817487	3.757150
23	8	0	6.398080	-2.571099	2.347422
24	6	0	7.793415	-2.680641	2.791772
25	1	0	8.296594	-1.734223	2.572297
26	1	0	7.793325	-2.820048	3.876641
27	6	0	8.405384	-3.852602	2.054219
28	1	0	8.386129	-3.693096	0.971746
29	1	0	9.449182	-3.976536	2.360257
30	1	0	7.872984	-4.781530	2.279281
31	6	0	-1.010371	-2.659230	0.992847
32	6	0	-0.578913	-3.383084	2.115071
33	1	0	0.428012	-3.248712	2.494686
34	6	0	-1.427786	-4.286404	2.759730
35	1	0	-1.068656	-4.835816	3.624886
36	6	0	-2.734232	-4.496076	2.297752
37	1	0	-3.386593	-5.201537	2.800704
38	6	0	-3.183406	-3.802609	1.180653
39	1	0	-4.189751	-3.982511	0.816113
40	6	0	-2.326742	-2.895038	0.526264
41	6	0	-2.689625	-2.160570	-0.677751
42	6	0	-3.977663	-2.223531	-1.261083

43	1	0	-4.741582	-2.822682	-0.787837
44	6	0	-1.950476	-0.768543	-2.432415
45	6	0	-0.883305	-0.135530	-3.109775
46	1	0	0.101852	-0.200218	-2.678242
47	6	0	-1.084148	0.506796	-4.314838
48	1	0	-0.245284	0.970832	-4.823073
49	6	0	-2.368704	0.550294	-4.894021
50	1	0	-2.522932	1.066576	-5.835081
51	6	0	-3.427205	-0.084064	-4.276227
52	1	0	-4.413381	-0.069942	-4.718525
53	6	0	-3.250500	-0.774702	-3.048367
54	6	0	-4.287143	-1.522323	-2.401648
55	6	0	0.883311	-0.135577	3.109782
56	1	0	-0.101847	-0.200263	2.678251
57	6	0	1.084153	0.506730	4.314855
58	1	0	0.245289	0.970754	4.823100
59	6	0	2.368710	0.550224	4.894037
60	1	0	2.522938	1.066491	5.835105
61	6	0	3.427213	-0.084120	4.276231
62	1	0	4.413390	-0.070000	4.718526
63	6	0	3.250508	-0.774738	3.048360
64	6	0	1.950483	-0.768574	2.432409
65	6	0	4.287153	-1.522345	2.401629
66	6	0	3.977674	-2.223537	1.261053
67	1	0	4.741595	-2.822679	0.787798
68	6	0	2.689636	-2.160571	0.677723
69	6	0	2.326755	-2.895023	-0.526303
70	6	0	3.183421	-3.802582	-1.180705
71	1	0	4.189767	-3.982486	-0.816169
72	6	0	1.010383	-2.659213	-0.992880
73	6	0	0.578925	-3.383053	-2.115113
74	1	0	-0.428000	-3.248679	-2.494726
75	6	0	1.427801	-4.286362	-2.759787
76	1	0	1.068672	-4.835763	-3.624950
77	6	0	2.734248	-4.496035	-2.297813
78	1	0	3.386611	-5.201486	-2.800776
79	6	0	-5.693503	-1.574296	-2.925956
80	8	0	-6.165145	-0.817466	-3.757177
81	8	0	-6.398074	-2.571071	-2.347441
82	6	0	-7.793407	-2.680612	-2.791796
83	1	0	-7.793313	-2.820030	-3.876663
84	1	0	-8.296584	-1.734191	-2.572332
85	6	0	-8.405382	-3.852564	-2.054234
86	1	0	-9.449180	-3.976499	-2.360276
87	1	0	-7.872983	-4.781497	-2.279285
88	1	0	-8.386132	-3.693048	-0.971762
89	77	0	0.000004	-1.248541	-0.000007
90	6	0	-3.307309	4.101705	1.581757
91	8	0	-2.910153	5.186415	1.200208
92	8	0	-4.442842	3.895091	2.275709
93	6	0	3.307297	4.101738	-1.581698
94	8	0	2.910131	5.186443	-1.200146
95	8	0	4.442827	3.895138	-2.275659
96	6	0	-5.216014	5.103186	2.563121
97	1	0	-5.521982	5.567504	1.622396
98	1	0	-4.591087	5.809660	3.114643
99	6	0	-6.416606	4.665771	3.383296
100	1	0	-7.022258	3.937588	2.819532
101	1	0	-6.086595	4.179800	4.315914
102	6	0	5.215987	5.103242	-2.563067
103	1	0	4.591050	5.809716	-3.114577
104	1	0	5.521960	5.567553	-1.622340
105	6	0	6.416575	4.665845	-3.383257

106	1	0	6.086560	4.179879	-4.315876
107	1	0	7.022239	3.937661	-2.819505
108	8	0	-7.149317	5.852314	3.649426
109	8	0	7.149275	5.852395	-3.649382
110	6	0	-8.319459	5.597691	4.429081
111	1	0	-8.064161	5.161450	5.405805
112	1	0	-8.807454	6.561738	4.582415
113	1	0	-9.011142	4.920792	3.906650
114	6	0	8.319413	5.597789	-4.429048
115	1	0	8.807399	6.561841	-4.582377
116	1	0	9.011105	4.920891	-3.906627
117	1	0	8.064112	5.161554	-5.405774

3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.668714	1.533662	1.174638
2	7	0	2.063242	-0.374742	0.404926
3	7	0	-2.064164	-0.373732	-0.404508
4	7	0	0.669905	1.532712	-1.175491
5	6	0	6.392661	-0.441604	0.280419
6	8	0	7.144809	0.347648	0.826115
7	8	0	6.819579	-1.436735	-0.526846
8	6	0	8.275317	-1.503579	-0.708720
9	1	0	8.606451	-0.561532	-1.156096
10	1	0	8.736444	-1.589157	0.279365
11	6	0	8.560298	-2.700993	-1.590083
12	1	0	8.079914	-2.596977	-2.567800
13	1	0	9.639413	-2.792396	-1.750435
14	1	0	8.206489	-3.625721	-1.124611
15	6	0	-0.523344	-1.636695	1.323497
16	6	0	0.328992	-2.378023	2.156325
17	1	0	1.404524	-2.269036	2.067020
18	6	0	-0.184859	-3.265404	3.105325
19	1	0	0.495693	-3.829542	3.736183
20	6	0	-1.568424	-3.440757	3.246678
21	1	0	-1.960184	-4.133597	3.983399
22	6	0	-2.435151	-2.731547	2.424013
23	1	0	-3.504812	-2.887383	2.522665
24	6	0	-1.918102	-1.841033	1.461977
25	6	0	-2.739201	-1.102626	0.512372
26	6	0	-4.154438	-1.132898	0.524565
27	1	0	-4.663117	-1.704472	1.287135
28	6	0	-2.772874	0.243328	-1.423717
29	6	0	-2.073709	0.821505	-2.508001
30	1	0	-1.000805	0.723244	-2.530858
31	6	0	-2.746645	1.446396	-3.538198
32	1	0	-2.188392	1.864870	-4.369225
33	6	0	-4.154174	1.528384	-3.524291
34	1	0	-4.677001	2.030594	-4.330819
35	6	0	-4.870171	0.946362	-2.498155
36	1	0	-5.950249	0.988825	-2.485335
37	6	0	-4.210600	0.272040	-1.436976
38	6	0	-4.896891	-0.432439	-0.395581
39	6	0	2.072789	0.819546	2.508955
40	1	0	0.999879	0.721367	2.531733
41	6	0	2.745737	1.443881	3.539477
42	1	0	2.187483	1.862078	4.370643
43	6	0	4.153281	1.525622	3.525726
44	1	0	4.676129	2.027419	4.332499
45	6	0	4.869278	0.943809	2.499471

46	1	0	5.949369	0.985954	2.486827
47	6	0	4.209701	0.270006	1.437962
48	6	0	2.771957	0.241701	1.424491
49	6	0	4.895954	-0.434290	0.396405
50	6	0	4.153420	-1.134332	-0.524008
51	1	0	4.662042	-1.705779	-1.286709
52	6	0	2.738197	-1.103679	-0.511988
53	6	0	1.916998	-1.841718	-1.461823
54	6	0	2.433896	-2.732293	-2.423883
55	1	0	3.503521	-2.888480	-2.522391
56	6	0	0.522276	-1.636950	-1.323583
57	6	0	-0.330190	-2.377859	-2.156630
58	1	0	-1.405697	-2.268432	-2.067456
59	6	0	0.183513	-3.265307	-3.105654
60	1	0	-0.497111	-3.829138	-3.736709
61	6	0	1.567048	-3.441116	-3.246768
62	1	0	1.958699	-4.134009	-3.983498
63	6	0	-6.393571	-0.439387	-0.279418
64	8	0	-7.145441	0.351138	-0.823646
65	8	0	-6.820708	-1.435713	0.526244
66	6	0	-8.276432	-1.502329	0.708328
67	1	0	-8.737913	-1.584620	-0.279863
68	1	0	-8.606898	-0.561463	1.158694
69	6	0	-8.561805	-2.702250	1.586149
70	1	0	-9.640877	-2.793203	1.747036
71	1	0	-8.209148	-3.625830	1.117538
72	1	0	-8.080588	-2.601707	2.563820
73	77	0	-0.000360	-0.237164	-0.000139
74	6	0	-0.373809	5.199665	0.568592
75	1	0	-0.680139	6.134719	1.025700
76	6	0	0.381704	5.199115	-0.568538
77	1	0	0.689746	6.133720	-1.025414
78	6	0	-0.373737	2.739490	0.611590
79	6	0	-0.772416	3.970437	1.192233
80	6	0	-1.543931	3.917531	2.374185
81	1	0	-1.871889	4.837998	2.845711
82	6	0	-1.870564	2.685827	2.912030
83	1	0	-2.465949	2.607391	3.813632
84	6	0	-1.408195	1.514930	2.287020
85	1	0	-1.625885	0.536181	2.700626
86	6	0	0.777991	3.969317	-1.192531
87	6	0	0.377163	2.738951	-0.612136
88	6	0	1.549167	3.915305	-2.374654
89	1	0	1.878719	4.835292	-2.846006
90	6	0	1.873353	2.683147	-2.912929
91	1	0	2.468326	2.603853	-3.814729
92	6	0	1.409016	1.512927	-2.288101
93	1	0	1.624866	0.533891	-2.701976

3e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.867968	0.579953	1.021883
2	7	0	1.956920	-1.319650	0.768289
3	7	0	-1.957059	-1.319561	-0.768298
4	7	0	0.867984	0.579889	-1.021967
5	6	0	6.242630	-1.347509	1.398368
6	8	0	6.882154	-0.570506	2.086927
7	8	0	6.815029	-2.314427	0.647898
8	6	0	8.280545	-2.362083	0.713464
9	1	0	8.668994	-1.393452	0.384868

10	1	0	8.568664	-2.504895	1.758983
11	6	0	8.729290	-3.503040	-0.174920
12	1	0	8.422689	-3.340598	-1.212791
13	1	0	9.821030	-3.581537	-0.151944
14	1	0	8.312870	-4.455455	0.166433
15	6	0	-0.753584	-2.593187	1.202135
16	6	0	-0.066321	-3.342250	2.170454
17	1	0	1.007503	-3.232912	2.279615
18	6	0	-0.743027	-4.238044	3.001809
19	1	0	-0.187947	-4.808598	3.740665
20	6	0	-2.129175	-4.414123	2.887892
21	1	0	-2.647097	-5.114211	3.534427
22	6	0	-2.833159	-3.695677	1.929257
23	1	0	-3.902970	-3.851384	1.831287
24	6	0	-2.150627	-2.796710	1.085598
25	6	0	-2.787157	-2.047780	0.011239
26	6	0	-4.183062	-2.065196	-0.223601
27	1	0	-4.820965	-2.632937	0.437833
28	6	0	-2.472206	-0.692851	-1.891888
29	6	0	-1.588436	-0.113154	-2.830813
30	1	0	-0.529378	-0.217279	-2.660566
31	6	0	-2.064811	0.523495	-3.958639
32	1	0	-1.365926	0.944150	-4.674151
33	6	0	-3.452209	0.615076	-4.192923
34	1	0	-3.821446	1.126101	-5.075373
35	6	0	-4.342172	0.031909	-3.313930
36	1	0	-5.407105	0.081834	-3.492494
37	6	0	-3.884962	-0.653473	-2.157665
38	6	0	-4.748706	-1.354537	-1.255016
39	6	0	1.588283	-0.113313	2.830844
40	1	0	0.529227	-0.217409	2.660575
41	6	0	2.064652	0.523279	3.958705
42	1	0	1.365762	0.943922	4.674220
43	6	0	3.452047	0.614817	4.193021
44	1	0	3.821280	1.125799	5.075498
45	6	0	4.342012	0.031658	3.314025
46	1	0	5.406943	0.081547	3.492614
47	6	0	3.884809	-0.653670	2.157726
48	6	0	2.472057	-0.692996	1.891915
49	6	0	4.748553	-1.354731	1.255075
50	6	0	4.182913	-2.065345	0.223627
51	1	0	4.820814	-2.633088	-0.437806
52	6	0	2.787014	-2.047875	-0.011247
53	6	0	2.150484	-2.796767	-1.085635
54	6	0	2.833006	-3.695740	-1.929295
55	1	0	3.902811	-3.851479	-1.831310
56	6	0	0.753449	-2.593205	-1.202197
57	6	0	0.066182	-3.342230	-2.170541
58	1	0	-1.007636	-3.232853	-2.279724
59	6	0	0.742878	-4.238031	-3.001898
60	1	0	0.187798	-4.808557	-3.740775
61	6	0	2.129019	-4.414151	-2.887955
62	1	0	2.646934	-5.114244	-3.534492
63	6	0	-6.242785	-1.347269	-1.398276
64	8	0	-6.882302	-0.570240	-2.086813
65	8	0	-6.815197	-2.314179	-0.647805
66	6	0	-8.280717	-2.361787	-0.713337
67	1	0	-8.568860	-2.504687	-1.758837
68	1	0	-8.669125	-1.393111	-0.384825
69	6	0	-8.729486	-3.502646	0.175161
70	1	0	-9.821228	-3.581113	0.152203
71	1	0	-8.313098	-4.455106	-0.166105
72	1	0	-8.422869	-3.340112	1.213013

73	77	0	-0.000055	-1.187172	-0.000037
74	6	0	-0.494521	4.240164	0.470940
75	1	0	-0.879940	5.179188	0.848202
76	6	0	0.494875	4.240126	-0.470962
77	1	0	0.880373	5.179121	-0.848212
78	6	0	-0.494796	1.792589	0.522424
79	6	0	-1.030215	3.018777	0.996939
80	6	0	-2.050613	2.968776	1.995775
81	6	0	-2.407968	1.711365	2.476954
82	1	0	-3.182762	1.620043	3.229159
83	6	0	-1.800230	0.553976	1.977994
84	1	0	-2.074124	-0.425217	2.355769
85	6	0	1.030459	3.018699	-0.996981
86	6	0	0.494930	1.792552	-0.522484
87	6	0	2.050847	2.968619	-1.995827
88	6	0	2.408076	1.711183	-2.477033
89	1	0	3.182857	1.619800	-3.229246
90	6	0	1.800232	0.553843	-1.978089
91	1	0	2.074032	-0.425370	-2.355883
92	6	0	-2.727311	4.177957	2.520090
93	6	0	-2.812138	4.386500	3.908379
94	6	0	-3.342444	5.101067	1.653886
95	6	0	-3.482363	5.499393	4.417699
96	1	0	-2.333393	3.685530	4.585746
97	6	0	-4.020309	6.207539	2.167803
98	1	0	-3.318319	4.932736	0.581491
99	6	0	-4.088022	6.412046	3.549130
100	1	0	-3.530574	5.654707	5.490406
101	1	0	-4.502435	6.904759	1.490530
102	1	0	-4.612690	7.274733	3.945946
103	6	0	2.727669	4.177742	-2.520117
104	6	0	2.812520	4.386305	-3.908401
105	6	0	3.342900	5.100770	-1.653894
106	6	0	3.482859	5.499141	-4.417698
107	1	0	2.333703	3.685399	-4.585783
108	6	0	4.020879	6.207183	-2.167787
109	1	0	3.318758	4.932418	-0.581503
110	6	0	4.088613	6.411713	-3.549110
111	1	0	3.531086	5.654473	-5.490401
112	1	0	4.503078	6.904340	-1.490500
113	1	0	4.613371	7.274354	-3.945907

3f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.682343	0.695717	-1.163741
2	7	0	-2.066521	-1.200885	-0.421203
3	7	0	2.053783	-1.218977	0.422418
4	7	0	-0.676000	0.702904	1.164645
5	6	0	-6.397584	-1.266722	-0.337378
6	8	0	-7.147144	-0.485994	-0.898737
7	8	0	-6.830365	-2.254009	0.476818
8	6	0	-8.287341	-2.321808	0.645549
9	1	0	-8.625292	-1.373935	1.075154
10	1	0	-8.738859	-2.423908	-0.345433
11	6	0	-8.577806	-3.506238	1.542626
12	1	0	-8.107940	-3.385212	2.523497
13	1	0	-9.658241	-3.598781	1.693190
14	1	0	-8.216142	-4.436956	1.095446
15	6	0	0.519604	-2.478006	-1.314983
16	6	0	-0.330031	-3.213814	-2.155543

17	1	0	-1.405455	-3.094637	-2.078810
18	6	0	0.186206	-4.108483	-3.096298
19	1	0	-0.492398	-4.667954	-3.733405
20	6	0	1.569607	-4.297011	-3.221566
21	1	0	1.963225	-4.995550	-3.951905
22	6	0	2.433521	-3.592934	-2.391621
23	1	0	3.502803	-3.758183	-2.478376
24	6	0	1.913921	-2.694818	-1.438068
25	6	0	2.731554	-1.957887	-0.484331
26	6	0	4.146569	-1.997892	-0.484252
27	1	0	4.657438	-2.576817	-1.239702
28	6	0	2.758277	-0.600031	1.443426
29	6	0	2.053865	-0.008947	2.517334
30	1	0	0.980127	-0.099124	2.531633
31	6	0	2.722028	0.619522	3.548491
32	1	0	2.159285	1.048748	4.370942
33	6	0	4.130081	0.691814	3.545967
34	1	0	4.649432	1.197152	4.352798
35	6	0	4.850940	0.096746	2.530718
36	1	0	5.931323	0.131286	2.527138
37	6	0	4.196159	-0.581244	1.468928
38	6	0	4.886439	-1.297244	0.437864
39	6	0	-2.055807	0.010066	-2.515627
40	1	0	-0.982802	-0.088146	-2.529161
41	6	0	-2.718337	0.644117	-3.547007
42	1	0	-2.151660	1.069492	-4.368758
43	6	0	-4.125794	0.727118	-3.545615
44	1	0	-4.640631	1.236801	-4.352604
45	6	0	-4.851945	0.137027	-2.531241
46	1	0	-5.932045	0.179734	-2.528416
47	6	0	-4.203167	-0.546411	-1.469259
48	6	0	-2.765471	-0.576156	-1.442538
49	6	0	-4.899792	-1.257578	-0.439146
50	6	0	-4.166069	-1.963681	0.483693
51	1	0	-4.682014	-2.538871	1.238547
52	6	0	-2.750802	-1.934436	0.485030
53	6	0	-1.939856	-2.677776	1.439507
54	6	0	-2.467447	-3.570915	2.393332
55	1	0	-3.538111	-3.727226	2.479504
56	6	0	-0.543723	-2.472656	1.317129
57	6	0	0.299248	-3.214780	2.158895
58	1	0	1.375679	-3.104459	2.082904
59	6	0	-0.224978	-4.104415	3.099992
60	1	0	0.448575	-4.668890	3.738047
61	6	0	-1.609962	-4.281500	3.224392
62	1	0	-2.009846	-4.976219	3.954969
63	6	0	6.384005	-1.316883	0.334281
64	8	0	7.139643	-0.541538	0.894955
65	8	0	6.808982	-2.306861	-0.480746
66	6	0	8.265287	-2.384590	-0.651128
67	1	0	8.717155	-2.490596	0.339284
68	1	0	8.609303	-1.438723	-1.080337
69	6	0	8.546623	-3.570268	-1.549454
70	1	0	9.626247	-3.670217	-1.701109
71	1	0	8.178893	-4.498810	-1.102703
72	1	0	8.076705	-3.445142	-2.529785
73	77	0	-0.005741	-1.071680	0.000846
74	6	0	0.428554	4.385429	-0.590049
75	6	0	-0.383970	4.389743	0.590190
76	6	0	0.396604	1.904521	-0.613523
77	6	0	0.819096	3.115639	-1.196451
78	6	0	1.600337	3.056684	-2.361919
79	1	0	1.934322	3.981537	-2.816742

80	6	0	1.919690	1.815616	-2.893511
81	1	0	2.525315	1.728725	-3.787546
82	6	0	1.436986	0.658290	-2.271452
83	1	0	1.644969	-0.327235	-2.673294
84	6	0	-0.787471	3.124174	1.196994
85	6	0	-0.377603	1.908617	0.614304
86	6	0	-1.569316	3.073583	2.362453
87	1	0	-1.893661	4.001952	2.817090
88	6	0	-1.901716	1.835992	2.894156
89	1	0	-2.508334	1.755542	3.788119
90	6	0	-1.431174	0.673583	2.272246
91	1	0	-1.649635	-0.309588	2.674291
92	6	0	0.443808	6.672993	-0.592053
93	6	0	-0.376366	6.677356	0.591137
94	6	0	0.451729	9.093571	-0.585956
95	1	0	0.758377	10.038725	-1.020784
96	6	0	-0.360399	9.097897	0.583661
97	1	0	-0.657751	10.046272	1.017931
98	6	0	-0.768036	7.917658	1.163010
99	1	0	-1.386296	7.898075	2.053238
100	6	0	0.847703	7.909042	-1.164627
101	1	0	1.465691	7.882836	-2.054874
102	7	0	-0.778049	5.520255	1.166207
103	7	0	0.833946	5.511676	-1.166563

3g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.187987	0.633565	1.195978
2	7	0	-1.932513	-1.940027	0.445527
3	7	0	-1.569556	2.156333	-0.437143
4	7	0	0.105526	-0.730665	-1.125461
5	6	0	-2.326408	-6.253183	0.370927
6	8	0	-1.625781	-7.057316	0.961669
7	8	0	-3.309129	-6.614213	-0.483141
8	6	0	-3.471680	-8.062302	-0.661554
9	1	0	-2.510973	-8.478439	-0.978447
10	1	0	-3.724044	-8.496076	0.310593
11	6	0	-4.565144	-8.264764	-1.688946
12	1	0	-4.290454	-7.822441	-2.651474
13	1	0	-4.732926	-9.335579	-1.843105
14	1	0	-5.506613	-7.817871	-1.355849
15	6	0	-2.989952	0.765123	1.297280
16	6	0	-3.818109	-0.001182	2.132615
17	1	0	-3.802473	-1.083861	2.066960
18	6	0	-4.673453	0.608051	3.053993
19	1	0	-5.306058	-0.007254	3.686994
20	6	0	-4.729334	2.004336	3.164973
21	1	0	-5.398314	2.470657	3.880037
22	6	0	-3.931556	2.788016	2.340161
23	1	0	-3.994313	3.869043	2.415055
24	6	0	-3.072874	2.175047	1.406150
25	6	0	-2.248012	2.909685	0.456926
26	6	0	-2.150203	4.321925	0.447369
27	1	0	-2.684872	4.892835	1.192480
28	6	0	-0.876571	2.789505	-1.457264
29	6	0	-0.350283	2.023837	-2.522775
30	1	0	-0.548479	0.964718	-2.534072
31	6	0	0.350120	2.620751	-3.551394
32	1	0	0.727544	2.013621	-4.367631
33	6	0	0.562673	4.014697	-3.554813

34	1	0	1.124740	4.476324	-4.359191
35	6	0	0.033061	4.796855	-2.548720
36	1	0	0.176437	5.868384	-2.549294
37	6	0	-0.715927	4.218070	-1.490635
38	6	0	-1.371205	4.982261	-0.472054
39	6	0	-0.778407	-2.009828	2.569632
40	1	0	-0.791733	-0.932187	2.573976
41	6	0	-0.225625	-2.712903	3.620662
42	1	0	0.222913	-2.175862	4.449945
43	6	0	-0.255261	-4.122529	3.628874
44	1	0	0.190831	-4.670187	4.451765
45	6	0	-0.874012	-4.807394	2.602882
46	1	0	-0.916115	-5.887455	2.607479
47	6	0	-1.475664	-4.114580	1.519462
48	6	0	-1.391697	-2.679202	1.485859
49	6	0	-2.209049	-4.759959	0.471603
50	6	0	-2.832635	-3.978734	-0.471646
51	1	0	-3.424088	-4.452624	-1.241325
52	6	0	-2.695398	-2.569928	-0.475798
53	6	0	-3.352406	-1.707552	-1.448147
54	6	0	-4.269495	-2.166538	-2.414713
55	1	0	-4.508511	-3.221829	-2.501456
56	6	0	-3.039179	-0.331547	-1.325965
57	6	0	-3.701231	0.564810	-2.179161
58	1	0	-3.508744	1.629438	-2.101860
59	6	0	-4.615789	0.109302	-3.132041
60	1	0	-5.117582	0.823193	-3.778573
61	6	0	-4.898134	-1.258064	-3.257626
62	1	0	-5.611034	-1.604175	-3.998111
63	6	0	-1.243471	6.474593	-0.377915
64	8	0	-0.363599	7.140133	-0.896707
65	8	0	-2.229383	7.005448	0.377786
66	6	0	-2.167308	8.463001	0.542083
67	1	0	-2.189704	8.917295	-0.452701
68	1	0	-1.209321	8.714082	1.007239
69	6	0	-3.353263	8.866092	1.392579
70	1	0	-3.350713	9.951013	1.539174
71	1	0	-4.295776	8.590411	0.910250
72	1	0	-3.313967	8.390641	2.377433
73	77	0	-1.618105	0.095955	0.009840
74	6	0	3.856411	0.135577	0.627431
75	6	0	3.805866	-0.686755	-0.556911
76	6	0	1.375297	0.263976	0.650330
77	6	0	2.611361	0.603918	1.234507
78	6	0	2.603039	1.385847	2.400345
79	1	0	3.548063	1.656710	2.855700
80	6	0	1.385394	1.787944	2.931035
81	1	0	1.338504	2.396762	3.825934
82	6	0	0.199700	1.388490	2.305030
83	1	0	-0.769844	1.667002	2.702760
84	6	0	2.512051	-1.010869	-1.155363
85	6	0	1.327987	-0.514398	-0.575820
86	6	0	2.406475	-1.796702	-2.313802
87	1	0	3.310480	-2.187335	-2.765443
88	6	0	1.148587	-2.047317	-2.843731
89	1	0	1.026585	-2.654572	-3.732577
90	6	0	0.022476	-1.490725	-2.227802
91	1	0	-0.973522	-1.640295	-2.629437
92	6	0	6.143603	0.017819	0.614043
93	6	0	6.092474	-0.812171	-0.570821
94	6	0	8.576913	-0.100162	0.594404
95	6	0	8.525407	-0.934483	-0.593732
96	6	0	7.284371	-1.270678	-1.146581

97	1	0	7.223248	-1.891800	-2.034094
98	6	0	7.384713	0.354640	1.169605
99	1	0	7.400713	0.978721	2.056973
100	7	0	4.899620	-1.149000	-1.135760
101	7	0	4.999780	0.476431	1.194630
102	6	0	9.754927	-1.388517	-1.166941
103	1	0	9.714938	-2.012062	-2.054677
104	6	0	10.958669	-1.043372	-0.607802
105	1	0	11.885348	-1.392585	-1.050677
106	6	0	11.009359	-0.223231	0.559750
107	1	0	11.973697	0.036441	0.983359
108	6	0	9.855268	0.234029	1.142735
109	1	0	9.892627	0.857979	2.030323

3h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.184821	0.523812	-0.905933
2	7	0	2.834487	-1.622408	-0.582435
3	7	0	1.895135	2.353908	0.425229
4	7	0	0.910133	-0.796719	1.332965
5	6	0	4.044527	-5.781196	-0.682977
6	8	0	3.406541	-6.711979	-1.144588
7	8	0	5.227935	-5.935536	-0.050073
8	6	0	5.698485	-7.322799	0.050396
9	1	0	4.950451	-7.897242	0.605055
10	1	0	5.758790	-7.734194	-0.961252
11	6	0	7.042610	-7.288749	0.746165
12	1	0	6.957916	-6.864452	1.751337
13	1	0	7.435426	-8.306358	0.839615
14	1	0	7.765645	-6.696393	0.177552
15	6	0	3.225715	1.215325	-1.548554
16	6	0	4.015279	0.594844	-2.529306
17	1	0	4.192864	-0.474349	-2.486514
18	6	0	4.585569	1.334386	-3.568352
19	1	0	5.194855	0.831230	-4.313347
20	6	0	4.385913	2.719113	-3.655390
21	1	0	4.834638	3.287480	-4.462774
22	6	0	3.619722	3.361273	-2.690316
23	1	0	3.484679	4.436506	-2.751258
24	6	0	3.048724	2.617571	-1.638449
25	6	0	2.281511	3.206433	-0.550036
26	6	0	1.951716	4.581825	-0.492627
27	1	0	2.253233	5.230108	-1.302294
28	6	0	1.276979	2.865667	1.555670
29	6	0	1.056187	2.024283	2.670230
30	1	0	1.419023	1.010955	2.620512
31	6	0	0.441428	2.498255	3.811367
32	1	0	0.300942	1.837400	4.660434
33	6	0	0.010747	3.838711	3.884354
34	1	0	-0.482173	4.202981	4.778997
35	6	0	0.238488	4.696383	2.827436
36	1	0	-0.073172	5.730170	2.878326
37	6	0	0.891745	4.248247	1.649222
38	6	0	1.236535	5.107736	0.556288
39	6	0	1.339908	-1.938899	-2.458036
40	1	0	1.146806	-0.878929	-2.439660
41	6	0	0.744608	-2.748192	-3.404277
42	1	0	0.056840	-2.317251	-4.124402
43	6	0	1.037253	-4.126728	-3.448606
44	1	0	0.557736	-4.760114	-4.186794

45	6	0	1.952939	-4.667871	-2.569286
46	1	0	2.196153	-5.720528	-2.604185
47	6	0	2.603752	-3.858690	-1.601101
48	6	0	2.258796	-2.464709	-1.520997
49	6	0	3.628245	-4.339334	-0.722824
50	6	0	4.255636	-3.442500	0.108168
51	1	0	5.058619	-3.785810	0.743858
52	6	0	3.856842	-2.085769	0.171163
53	6	0	4.502272	-1.105569	1.033371
54	6	0	5.644663	-1.374929	1.813270
55	1	0	6.091157	-2.364197	1.826868
56	6	0	3.918058	0.184441	1.005239
57	6	0	4.535672	1.194907	1.758562
58	1	0	4.134144	2.202468	1.747889
59	6	0	5.671886	0.927886	2.526420
60	1	0	6.133075	1.727775	3.098181
61	6	0	6.227247	-0.358710	2.560719
62	1	0	7.111519	-0.557761	3.156307
63	6	0	0.855329	6.559566	0.519632
64	8	0	0.018646	7.087874	1.231833
65	8	0	1.553501	7.228039	-0.424037
66	6	0	1.228965	8.655205	-0.539578
67	1	0	1.392541	9.120067	0.436924
68	1	0	0.166126	8.744974	-0.783395
69	6	0	2.125709	9.230045	-1.615486
70	1	0	1.921175	10.298993	-1.734165
71	1	0	3.181260	9.113233	-1.352440
72	1	0	1.950494	8.742307	-2.579298
73	77	0	2.234898	0.328861	-0.059332
74	6	0	-3.166450	-0.657681	0.255691
75	6	0	-2.771262	-1.450319	1.376792
76	6	0	-0.801644	-0.061130	-0.177848
77	6	0	-2.159182	0.041056	-0.535344
78	6	0	-2.505469	0.809650	-1.658763
79	1	0	-3.551676	0.892299	-1.933379
80	6	0	-1.491961	1.432648	-2.373281
81	1	0	-1.712731	2.039380	-3.243182
82	6	0	-0.161415	1.261580	-1.971485
83	1	0	0.655607	1.714359	-2.522530
84	6	0	-1.362489	-1.527043	1.750711
85	6	0	-0.405698	-0.815794	0.997986
86	6	0	-0.921681	-2.276717	2.852708
87	1	0	-1.647497	-2.830631	3.436102
88	6	0	0.431423	-2.283594	3.160603
89	1	0	0.811753	-2.854171	3.999250
90	6	0	1.314907	-1.525606	2.383531
91	1	0	2.374249	-1.483674	2.611555
92	6	0	-5.367746	-1.192869	0.609927
93	6	0	-4.965277	-1.996046	1.737724
94	6	0	-7.678558	-1.796570	1.057941
95	6	0	-5.940501	-2.690017	2.502355
96	1	0	-5.602798	-3.286328	3.342180
97	6	0	-6.764822	-1.100191	0.268648
98	7	0	-3.666872	-2.109773	2.101909
99	7	0	-4.434659	-0.536243	-0.110428
100	6	0	-8.720772	-0.246098	-1.143968
101	6	0	-9.155255	-1.759307	0.797012
102	6	0	-9.634817	-0.948125	-0.336300
103	6	0	-7.250180	-0.288284	-0.898229
104	6	0	-7.263847	-2.586692	2.165830
105	1	0	-8.038046	-3.097832	2.726229
106	6	0	-11.007872	-0.882193	-0.605343
107	1	0	-11.688382	-1.434651	0.033095

108	6	0	-11.472110	-0.118595	-1.675010
109	1	0	-12.535489	-0.067062	-1.882968
110	6	0	-10.564590	0.581309	-2.481033
111	1	0	-10.926334	1.175339	-3.313729
112	6	0	-9.196541	0.517246	-2.217242
113	1	0	-8.478679	1.050676	-2.829860
114	8	0	-9.920580	-2.392588	1.522738
115	8	0	-6.490333	0.327247	-1.642613

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.536339	1.560422	-1.226782
2	7	0	-2.095814	-0.363678	-0.160914
3	7	0	2.095790	-0.363720	0.160894
4	7	0	-0.536308	1.560328	1.226908
5	6	0	-1.201296	1.489505	2.396327
6	1	0	-1.308416	0.496659	2.818307
7	6	0	-1.717748	2.611409	3.038878
8	1	0	-2.241185	2.500831	3.980768
9	6	0	-1.551078	3.861830	2.441887
10	1	0	-1.949596	4.757156	2.905080
11	6	0	-0.869679	3.939597	1.230002
12	1	0	-0.752438	4.896502	0.737945
13	6	0	-0.364367	2.773396	0.641453
14	6	0	0.364484	2.773439	-0.641195
15	6	0	0.869874	3.939668	-1.229621
16	1	0	0.752704	4.896528	-0.737460
17	6	0	1.551259	3.861985	-2.441520
18	1	0	1.949838	4.757332	-2.904617
19	6	0	1.717832	2.611617	-3.038649
20	1	0	2.241251	2.501105	-3.980558
21	6	0	1.201306	1.489681	-2.396216
22	1	0	1.308354	0.496872	-2.818303
23	6	0	-6.379390	-0.548776	0.424536
24	8	0	-7.243523	0.105794	-0.128958
25	6	0	0.352835	-1.627013	-1.369524
26	6	0	-0.595858	-2.357583	-2.101172
27	1	0	-1.653869	-2.228642	-1.901269
28	6	0	-0.201391	-3.262637	-3.089762
29	1	0	-0.955054	-3.818135	-3.639903
30	6	0	1.155972	-3.466825	-3.373811
31	1	0	1.454839	-4.173489	-4.140196
32	6	0	2.117445	-2.767011	-2.655571
33	1	0	3.167139	-2.944370	-2.867187
34	6	0	1.721137	-1.858057	-1.653685
35	6	0	2.651623	-1.122682	-0.810143
36	6	0	4.056535	-1.183643	-0.974995
37	1	0	4.463961	-1.775385	-1.781429
38	6	0	2.923812	0.259719	1.081836
39	6	0	2.355232	0.890501	2.211803
40	1	0	1.287033	0.831612	2.339682
41	6	0	3.146337	1.523448	3.148938
42	1	0	2.687429	1.984313	4.017426
43	6	0	4.546718	1.559874	2.990671
44	1	0	5.163242	2.066707	3.724829
45	6	0	5.138329	0.929058	1.914849
46	1	0	6.212559	0.933857	1.795918
47	6	0	4.355928	0.248103	0.945845
48	6	0	4.909557	-0.490698	-0.149782
49	6	0	-2.355221	0.890851	-2.211635

50	1	0	-1.287015	0.831997	-2.339491
51	6	0	-3.146309	1.523932	-3.148691
52	1	0	-2.687386	1.984933	-4.017099
53	6	0	-4.546695	1.560324	-2.990450
54	1	0	-5.163207	2.067262	-3.724545
55	6	0	-5.138325	0.929349	-1.914731
56	1	0	-6.212556	0.934132	-1.795818
57	6	0	-4.355940	0.248259	-0.945809
58	6	0	-2.923823	0.259895	-1.081777
59	6	0	-4.909584	-0.490692	0.149709
60	6	0	-4.056573	-1.183742	0.974845
61	1	0	-4.464011	-1.775587	1.781200
62	6	0	-2.651658	-1.122762	0.810020
63	6	0	-1.721180	-1.858228	1.653492
64	6	0	-2.117495	-2.767293	2.655273
65	1	0	-3.167192	-2.944684	2.866854
66	6	0	-0.352876	-1.627140	1.369377
67	6	0	0.595812	-2.357781	2.100961
68	1	0	1.653826	-2.228812	1.901088
69	6	0	0.201338	-3.262944	3.089447
70	1	0	0.954997	-3.818494	3.639540
71	6	0	-1.156028	-3.467176	3.373453
72	1	0	-1.454901	-4.173926	4.139757
73	6	0	6.379359	-0.548749	-0.424637
74	8	0	7.243505	0.105720	0.128955
75	77	0	-0.000014	-0.214579	-0.000005
76	8	0	-6.677652	-1.437829	1.409021
77	1	0	-7.646394	-1.399838	1.518177
78	8	0	6.677603	-1.437650	-1.409264
79	1	0	7.646346	-1.399655	-1.518419

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.577119	1.364515	1.206978
2	7	0	2.087599	-0.558446	0.237825
3	7	0	-2.087409	-0.558637	-0.237970
4	7	0	0.576955	1.364912	-1.206626
5	6	0	1.284696	1.304623	-2.349803
6	1	0	1.410845	0.315669	-2.776082
7	6	0	1.824594	2.428523	-2.965915
8	1	0	2.382406	2.316336	-3.888686
9	6	0	1.651024	3.691638	-2.384920
10	6	0	0.918157	3.742475	-1.192010
11	1	0	0.783724	4.695550	-0.694391
12	6	0	0.388178	2.579278	-0.627754
13	6	0	-0.388922	2.579028	0.628241
14	6	0	-0.919541	3.741905	1.192577
15	1	0	-0.785717	4.695067	0.694966
16	6	0	-1.652336	3.690594	2.385503
17	6	0	-1.825336	2.427320	2.966343
18	1	0	-2.383261	2.314738	3.888998
19	6	0	-1.284855	1.303760	2.350141
20	1	0	-1.410640	0.314680	2.776234
21	6	0	6.390313	-0.742878	-0.181927
22	8	0	7.232491	-0.089179	0.405789
23	6	0	-0.404370	-1.821355	1.356514
24	6	0	0.515658	-2.554487	2.121844
25	1	0	1.580383	-2.430057	1.957360
26	6	0	0.084172	-3.455136	3.098722
27	1	0	0.816314	-4.012439	3.675532

28	6	0	-1.283046	-3.652712	3.337386
29	1	0	-1.610720	-4.355762	4.095326
30	6	0	-2.216570	-2.951426	2.584652
31	1	0	-3.273663	-3.123952	2.760738
32	6	0	-1.782520	-2.047076	1.594221
33	6	0	-2.680074	-1.313154	0.714695
34	6	0	-4.090316	-1.373510	0.825846
35	1	0	-4.528172	-1.960839	1.619489
36	6	0	-2.879622	0.057939	-1.194335
37	6	0	-2.267828	0.681316	-2.305791
38	1	0	-1.195169	0.625238	-2.389809
39	6	0	-3.022366	1.304094	-3.279080
40	1	0	-2.529902	1.758611	-4.132428
41	6	0	-4.428030	1.337993	-3.177361
42	1	0	-5.016066	1.836187	-3.940314
43	6	0	-5.060592	0.715558	-2.120093
44	1	0	-6.138697	0.718894	-2.043759
45	6	0	-4.315954	0.044820	-1.114931
46	6	0	-4.911209	-0.686572	-0.036108
47	6	0	2.267848	0.681009	2.305958
48	1	0	1.195185	0.624884	2.389885
49	6	0	3.022302	1.303564	3.279454
50	1	0	2.529769	1.757841	4.132890
51	6	0	4.427971	1.337542	3.177831
52	1	0	5.015942	1.835550	3.940955
53	6	0	5.060620	0.715421	2.120430
54	1	0	6.138729	0.718830	2.044156
55	6	0	4.316068	0.044921	1.115045
56	6	0	2.879732	0.057939	1.194380
57	6	0	4.911421	-0.686142	0.036052
58	6	0	4.090611	-1.372886	-0.826133
59	1	0	4.528540	-1.959971	-1.619917
60	6	0	2.680359	-1.312657	-0.715025
61	6	0	1.782898	-2.046417	-1.594778
62	6	0	2.217055	-2.950423	-2.585477
63	1	0	3.274168	-3.122772	-2.761613
64	6	0	0.404722	-1.820924	-1.357013
65	6	0	-0.515220	-2.553937	-2.122560
66	1	0	-1.579960	-2.429677	-1.958041
67	6	0	-0.083628	-3.454245	-3.099705
68	1	0	-0.815703	-4.011460	-3.676683
69	6	0	1.283615	-3.651591	-3.338424
70	1	0	1.611372	-4.354374	-4.096575
71	6	0	-6.390088	-0.743451	0.181932
72	8	0	-7.232339	-0.089681	-0.405602
73	77	0	0.000088	-0.411524	-0.000057
74	8	0	6.727602	-1.629423	-1.156350
75	1	0	7.699817	-1.590100	-1.226911
76	8	0	-6.727273	-1.630241	1.156168
77	1	0	-7.699488	-1.591004	1.226774
78	6	0	2.225854	4.936755	-2.998317
79	1	0	1.432909	5.643161	-3.271061
80	1	0	2.890623	5.451378	-2.295024
81	1	0	2.799325	4.711664	-3.900524
82	6	0	-2.226928	4.935467	2.999619
83	1	0	-1.432651	5.634686	3.286910
84	1	0	-2.879366	5.459157	2.291611
85	1	0	-2.812815	4.708385	3.893311

4c

Center	Atomic	Atomic	Coordinates (Angstroms)		

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Number	Number	Type	X	Y	Z
1	7	0	0.689110	1.029684	-1.145870
2	7	0	-2.057866	-0.890438	-0.431051
3	7	0	2.057880	-0.890409	0.431037
4	7	0	-0.689127	1.029665	1.145870
5	6	0	-1.494188	0.959078	2.223904
6	1	0	-1.660154	-0.033783	2.626286
7	6	0	-2.078676	2.080341	2.805351
8	1	0	-2.715840	1.978924	3.674404
9	6	0	-1.825142	3.333143	2.240552
10	6	0	-0.997267	3.411141	1.121526
11	1	0	-0.821277	4.383590	0.678633
12	6	0	-0.438331	2.245254	0.592404
13	6	0	0.438294	2.245265	-0.592395
14	6	0	0.997211	3.411164	-1.121510
15	1	0	0.821206	4.383608	-0.678610
16	6	0	1.825088	3.333188	-2.240536
17	6	0	2.078642	2.080393	-2.805344
18	1	0	2.715808	1.978993	-3.674397
19	6	0	1.494172	0.959118	-2.223905
20	1	0	1.660153	-0.033738	-2.626294
21	6	0	-6.380931	-1.069494	-0.394452
22	8	0	-7.166507	-0.412398	-1.051892
23	6	0	0.524831	-2.151489	-1.312054
24	6	0	-0.322716	-2.877856	-2.161905
25	1	0	-1.397333	-2.744445	-2.102450
26	6	0	0.194580	-3.783784	-3.091584
27	1	0	-0.482643	-4.335965	-3.736257
28	6	0	1.576582	-3.992790	-3.195628
29	1	0	1.970837	-4.700167	-3.916842
30	6	0	2.438311	-3.296644	-2.357121
31	1	0	3.506082	-3.477189	-2.429360
32	6	0	1.917754	-2.386538	-1.415083
33	6	0	2.733147	-1.651244	-0.459253
34	6	0	4.147526	-1.711666	-0.443177
35	1	0	4.655291	-2.306135	-1.188414
36	6	0	2.760335	-0.264600	1.450115
37	6	0	2.053522	0.361887	2.501870
38	1	0	0.978219	0.293721	2.503494
39	6	0	2.719688	0.999332	3.528973
40	1	0	2.154640	1.456568	4.334491
41	6	0	4.128495	1.044958	3.544209
42	1	0	4.646697	1.556887	4.347454
43	6	0	4.851609	0.415578	2.551257
44	1	0	5.932249	0.425313	2.565997
45	6	0	4.198581	-0.271287	1.494472
46	6	0	4.887515	-1.012880	0.480360
47	6	0	-2.053529	0.361881	-2.501872
48	1	0	-0.978224	0.293736	-2.503496
49	6	0	-2.719707	0.999325	-3.528968
50	1	0	-2.154667	1.456580	-4.334480
51	6	0	-4.128514	1.044925	-3.544204
52	1	0	-4.646726	1.556853	-4.347443
53	6	0	-4.851617	0.415522	-2.551258
54	1	0	-5.932258	0.425234	-2.565995
55	6	0	-4.198576	-0.271343	-1.494482
56	6	0	-2.760330	-0.264632	-1.450124
57	6	0	-4.887498	-1.012958	-0.480379
58	6	0	-4.147499	-1.711737	0.443155
59	1	0	-4.655255	-2.306221	1.188387
60	6	0	-2.733121	-1.651292	0.459232
61	6	0	-1.917716	-2.386579	1.415058
62	6	0	-2.438258	-3.296700	2.357089

63	1	0	-3.506026	-3.477262	2.429326
64	6	0	-0.524796	-2.151507	1.312031
65	6	0	0.322762	-2.877866	2.161877
66	1	0	1.397377	-2.744438	2.102423
67	6	0	-0.194519	-3.783809	3.091549
68	1	0	0.482712	-4.335983	3.736219
69	6	0	-1.576518	-3.992838	3.195592
70	1	0	-1.970762	-4.700226	3.916801
71	6	0	6.380949	-1.069388	0.394421
72	8	0	7.166523	-0.412381	1.051954
73	77	0	0.000006	-0.738608	-0.000007
74	6	0	2.406599	4.601813	-2.772824
75	8	0	2.197981	5.694316	-2.283984
76	6	0	-2.406673	4.601755	2.772849
77	8	0	-2.198073	5.694265	2.284017
78	8	0	-6.802103	-1.960147	0.542166
79	1	0	-7.776958	-1.921645	0.528151
80	8	0	-3.188544	4.393945	3.857258
81	1	0	-3.522737	5.267868	4.135219
82	8	0	3.188474	4.394023	-3.857233
83	1	0	3.522652	5.267953	-4.135189
84	8	0	6.802132	-1.960175	-0.542063
85	1	0	7.776990	-1.921745	-0.527970

4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.530833	1.373973	1.245458
2	7	0	2.097078	-0.536099	0.163205
3	7	0	-2.097022	-0.536149	-0.163217
4	7	0	0.530776	1.374015	-1.245393
5	6	0	6.377885	-0.624981	-0.458536
6	8	0	7.233297	0.034301	0.102948
7	6	0	-0.365527	-1.797474	1.376606
8	6	0	0.577604	-2.540182	2.103248
9	1	0	1.635418	-2.432585	1.889446
10	6	0	0.176949	-3.429404	3.103651
11	1	0	0.925789	-3.995372	3.649721
12	6	0	-1.180923	-3.604669	3.404760
13	1	0	-1.484469	-4.298941	4.180607
14	6	0	-2.137275	-2.893802	2.690288
15	1	0	-3.187902	-3.050681	2.913436
16	6	0	-1.734751	-2.001751	1.675873
17	6	0	-2.659249	-1.264561	0.827174
18	6	0	-4.063626	-1.295384	1.004005
19	1	0	-4.475602	-1.861044	1.826781
20	6	0	-2.920210	0.078557	-1.093679
21	6	0	-2.348152	0.666663	-2.244605
22	1	0	-1.282702	0.579386	-2.380215
23	6	0	-3.133967	1.290389	-3.192096
24	1	0	-2.673372	1.717677	-4.076691
25	6	0	-4.532008	1.360264	-3.023386
26	1	0	-5.144163	1.860412	-3.765746
27	6	0	-5.127507	0.769755	-1.927094
28	1	0	-6.200451	0.799305	-1.800327
29	6	0	-4.351033	0.097911	-0.946875
30	6	0	-4.909770	-0.603692	0.170389
31	6	0	2.348204	0.666724	2.244588
32	1	0	1.282756	0.579433	2.380203
33	6	0	3.134016	1.290465	3.192072
34	1	0	2.673420	1.717749	4.076669

35	6	0	4.532053	1.360362	3.023353
36	1	0	5.144207	1.860520	3.765709
37	6	0	5.127555	0.769863	1.927056
38	1	0	6.200496	0.799433	1.800280
39	6	0	4.351084	0.098007	0.946843
40	6	0	2.920263	0.078626	1.093658
41	6	0	4.909825	-0.603585	-0.170426
42	6	0	4.063688	-1.295291	-1.004037
43	1	0	4.475668	-1.860942	-1.826817
44	6	0	2.659312	-1.264496	-0.827194
45	6	0	1.734822	-2.001700	-1.675887
46	6	0	2.137354	-2.893740	-2.690308
47	1	0	3.187983	-3.050597	-2.913466
48	6	0	0.365598	-1.797451	-1.376604
49	6	0	-0.577526	-2.540174	-2.103241
50	1	0	-1.635339	-2.432600	-1.889429
51	6	0	-0.176863	-3.429385	-3.103651
52	1	0	-0.925697	-3.995365	-3.649716
53	6	0	1.181009	-3.604622	-3.404774
54	1	0	1.484561	-4.298885	-4.180627
55	6	0	-6.377831	-0.625116	0.458488
56	8	0	-7.233257	0.034122	-0.103026
57	77	0	0.000026	-0.397341	0.000010
58	6	0	-0.310467	5.040041	0.608038
59	1	0	-0.563502	5.974769	1.097228
60	6	0	0.310024	5.040066	-0.608016
61	1	0	0.562962	5.974815	-1.097216
62	6	0	-0.303172	2.579359	0.650704
63	6	0	-0.633472	3.810368	1.272977
64	6	0	-1.265349	3.757664	2.535159
65	1	0	-1.537894	4.678273	3.040476
66	6	0	-1.527857	2.526318	3.107776
67	1	0	-2.016368	2.448228	4.071495
68	6	0	-1.139117	1.355370	2.434627
69	1	0	-1.306939	0.376654	2.870679
70	6	0	0.633161	3.810420	-1.272938
71	6	0	0.302986	2.579384	-0.650654
72	6	0	1.265054	3.757768	-2.535115
73	1	0	1.537505	4.678399	-3.040442
74	6	0	1.527701	2.526442	-3.107713
75	1	0	2.016233	2.448392	-4.071424
76	6	0	1.139078	1.355462	-2.434554
77	1	0	1.307009	0.376758	-2.870591
78	8	0	6.685978	-1.484696	-1.465928
79	1	0	7.652778	-1.424019	-1.581676
80	8	0	-6.685909	-1.484807	1.465905
81	1	0	-7.652713	-1.424155	1.581640

4e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.890692	0.394021	1.002937
2	7	0	1.939171	-1.505473	0.812627
3	7	0	-1.937408	-1.507113	-0.812945
4	7	0	0.890575	0.395341	-1.002650
5	6	0	6.201808	-1.553520	1.545981
6	8	0	6.837613	-0.872070	2.329240
7	6	0	-0.778083	-2.779040	1.185541
8	6	0	-0.112118	-3.527708	2.168650
9	1	0	0.958969	-3.418474	2.301640
10	6	0	-0.806877	-4.423772	2.984690

11	1	0	-0.268159	-4.994471	3.735377
12	6	0	-2.190268	-4.600190	2.840411
13	1	0	-2.722043	-5.300328	3.475414
14	6	0	-2.873295	-3.882324	1.866600
15	1	0	-3.940634	-4.038978	1.745839
16	6	0	-2.172100	-2.983259	1.037930
17	6	0	-2.783278	-2.236320	-0.051357
18	6	0	-4.173476	-2.257043	-0.319155
19	1	0	-4.823693	-2.822930	0.331795
20	6	0	-2.426861	-0.884943	-1.950757
21	6	0	-1.521912	-0.303276	-2.867786
22	1	0	-0.467218	-0.401775	-2.669933
23	6	0	-1.971623	0.328860	-4.009015
24	1	0	-1.256390	0.750966	-4.707206
25	6	0	-3.352776	0.413900	-4.278926
26	1	0	-3.701535	0.921003	-5.171852
27	6	0	-4.262876	-0.171546	-3.422095
28	1	0	-5.322317	-0.130721	-3.632243
29	6	0	-3.832770	-0.852522	-2.253273
30	6	0	-4.715117	-1.552642	-1.367725
31	6	0	1.522367	-0.303150	2.868106
32	1	0	0.467778	-0.402666	2.670217
33	6	0	1.971389	0.328881	4.009665
34	1	0	1.255696	0.749834	4.708080
35	6	0	3.352447	0.415307	4.279610
36	1	0	3.700655	0.922334	5.172794
37	6	0	4.263182	-0.168698	3.422473
38	1	0	5.322578	-0.126834	3.632642
39	6	0	3.833820	-0.849562	2.253308
40	6	0	2.427943	-0.883347	1.950765
41	6	0	4.716927	-1.548315	1.367431
42	6	0	4.176042	-2.252802	0.318530
43	1	0	4.826862	-2.817713	-0.332665
44	6	0	2.785837	-2.233406	0.050703
45	6	0	2.175483	-2.980438	-1.038987
46	6	0	2.877646	-3.878334	-1.868102
47	1	0	3.945146	-4.033933	-1.747394
48	6	0	0.781256	-2.777619	-1.186533
49	6	0	0.116110	-3.526462	-2.170051
50	1	0	-0.955086	-3.418285	-2.303010
51	6	0	0.811833	-4.421374	-2.986542
52	1	0	0.273737	-4.992247	-3.737542
53	6	0	2.195401	-4.596414	-2.842307
54	1	0	2.727934	-5.295666	-3.477652
55	6	0	-6.199991	-1.559308	-1.546264
56	8	0	-6.836550	-0.877684	-2.328758
57	77	0	0.000831	-1.372686	-0.000131
58	6	0	-0.508267	4.054399	0.459373
59	1	0	-0.903330	4.993104	0.827274
60	6	0	0.503641	4.055124	-0.458304
61	1	0	0.897538	4.994395	-0.826006
62	6	0	-0.507544	1.606848	0.511319
63	6	0	-1.055455	2.832662	0.972506
64	6	0	-2.100029	2.782170	1.946238
65	6	0	-2.465651	1.524540	2.421040
66	1	0	-3.258013	1.432472	3.154618
67	6	0	-1.843995	0.367778	1.938303
68	1	0	-2.124341	-0.611169	2.311918
69	6	0	1.052325	2.834169	-0.971701
70	6	0	0.505948	1.607585	-0.510754
71	6	0	2.096909	2.785160	-1.945499
72	6	0	2.464064	1.528088	-2.420587
73	1	0	3.256482	1.437166	-3.154248

74	6	0	1.843871	0.370452	-1.938045
75	1	0	2.125410	-0.608085	-2.311829
76	8	0	6.813465	-2.426189	0.700961
77	1	0	7.768169	-2.350632	0.886589
78	8	0	-6.810730	-2.432981	-0.701620
79	1	0	-7.765543	-2.358085	-0.886956
80	6	0	-2.793410	3.990084	2.450749
81	6	0	-2.920736	4.197138	3.836095
82	6	0	-3.383919	4.912903	1.567112
83	6	0	-3.608276	5.308206	4.325774
84	1	0	-2.461437	3.496642	4.527270
85	6	0	-4.079327	6.017464	2.061210
86	1	0	-3.327406	4.745663	0.495755
87	6	0	-4.189310	6.220431	3.440051
88	1	0	-3.689372	5.462421	5.396631
89	1	0	-4.542246	6.714280	1.370283
90	1	0	-4.727697	7.081529	3.821585
91	6	0	2.788706	3.994057	-2.449846
92	6	0	2.915454	4.201652	-3.835161
93	6	0	3.378315	4.917331	-1.566085
94	6	0	3.601522	5.313700	-4.324683
95	1	0	2.456859	3.500781	-4.526424
96	6	0	4.072261	6.022879	-2.060030
97	1	0	3.322255	4.749713	-0.494762
98	6	0	4.181657	6.226379	-3.438840
99	1	0	3.682176	5.468318	-5.395515
100	1	0	4.534502	6.720056	-1.369013
101	1	0	4.718904	7.088239	-3.820259

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.501119	0.540798	-1.236377
2	7	0	1.410376	-2.094773	-0.185653
3	7	0	1.409862	2.095102	0.185687
4	7	0	-0.500992	-0.540866	1.236425
5	6	0	1.509556	-6.382454	0.385403
6	8	0	0.856164	-7.233963	-0.188856
7	8	0	2.366754	-6.699776	1.392286
8	6	0	2.673923	0.379959	-1.370207
9	6	0	3.416595	-0.555507	-2.106883
10	1	0	3.307070	-1.615626	-1.905718
11	6	0	4.307787	-0.144371	-3.101185
12	1	0	4.873441	-0.887501	-3.655353
13	6	0	4.485332	1.216742	-3.386058
14	1	0	5.181084	1.528464	-4.157343
15	6	0	3.774500	2.165543	-2.661610
16	1	0	3.932694	3.218520	-2.872448
17	6	0	2.880288	1.752294	-1.653415
18	6	0	2.141650	2.667767	-0.796250
19	6	0	2.174675	4.074023	-0.956793
20	1	0	2.742715	4.494608	-1.773527
21	6	0	0.794091	2.908411	1.124154
22	6	0	0.202360	2.324058	2.267069
23	1	0	0.287471	1.257071	2.390772
24	6	0	-0.422896	3.099611	3.221975
25	1	0	-0.853525	2.629144	4.099710
26	6	0	-0.490462	4.499547	3.069174
27	1	0	-0.992136	5.103727	3.817028
28	6	0	0.103926	5.106867	1.981467
29	1	0	0.076339	6.181238	1.867147

30	6	0	0.777270	4.340946	0.994049
31	6	0	1.482398	4.911556	-0.115008
32	6	0	0.202785	-2.324008	-2.266949
33	1	0	0.287544	-1.256987	-2.390599
34	6	0	-0.422309	-3.099710	-3.221840
35	1	0	-0.853156	-2.629336	-4.099518
36	6	0	-0.489433	-4.499673	-3.069097
37	1	0	-0.990982	-5.103972	-3.816938
38	6	0	0.105224	-5.106859	-1.981463
39	1	0	0.077981	-6.181244	-1.867187
40	6	0	0.778409	-4.340776	-0.994062
41	6	0	0.794783	-2.908230	-1.124106
42	6	0	1.483777	-4.911224	0.114926
43	6	0	2.175821	-4.073509	0.956724
44	1	0	2.744033	-4.493953	1.773409
45	6	0	2.142362	-2.667257	0.796240
46	6	0	2.880765	-1.751601	1.653411
47	6	0	3.775098	-2.164628	2.661588
48	1	0	3.933558	-3.217566	2.872423
49	6	0	2.674043	-0.379319	1.370215
50	6	0	3.416497	0.556333	2.106878
51	1	0	3.306708	1.616424	1.905719
52	6	0	4.307816	0.145417	3.101158
53	1	0	4.873298	0.888687	3.655313
54	6	0	4.485707	-1.215652	3.386025
55	1	0	5.181551	-1.527202	4.157297
56	6	0	1.507675	6.382765	-0.385587
57	8	0	0.854016	7.234096	0.188635
58	8	0	2.364710	6.700270	-1.392549
59	77	0	1.271185	0.000153	0.000019
60	6	0	-4.189349	0.333620	-0.633547
61	6	0	-4.189268	-0.334588	0.633592
62	6	0	-1.707684	0.313209	-0.654552
63	6	0	-2.921601	0.657314	-1.281871
64	6	0	-2.867936	1.298582	-2.530179
65	1	0	-3.795197	1.571313	-3.019669
66	6	0	-1.629323	1.562714	-3.096544
67	1	0	-1.546581	2.061500	-4.054653
68	6	0	-0.468824	1.163185	-2.423515
69	1	0	0.515247	1.329505	-2.847322
70	6	0	-2.921441	-0.657963	1.281921
71	6	0	-1.707609	-0.313558	0.654602
72	6	0	-2.867621	-1.299226	2.530224
73	1	0	-3.794815	-1.572184	3.019711
74	6	0	-1.628944	-1.563064	3.096587
75	1	0	-1.546082	-2.061835	4.054693
76	6	0	-0.468542	-1.163255	2.423556
77	1	0	0.515571	-1.329343	2.847357
78	6	0	-6.476892	0.336562	-0.636024
79	6	0	-6.476810	-0.338116	0.636053
80	6	0	-8.897442	0.332764	-0.628883
81	6	0	-7.714969	-0.665087	1.251541
82	1	0	-7.692190	-1.173170	2.208848
83	6	0	-7.715131	0.663212	-1.251521
84	7	0	-5.317567	-0.663534	1.253310
85	7	0	-5.317728	0.662277	-1.253273
86	6	0	-8.897361	-0.334945	0.628893
87	1	0	-9.844104	-0.583370	1.096161
88	1	0	2.308903	-7.668118	1.495636
89	1	0	2.306505	7.668579	-1.495996
90	1	0	-9.844246	0.580943	-1.096159
91	1	0	-7.692477	1.171302	-2.208828

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.057404	0.547048	-1.233066
2	7	0	1.968652	-2.093555	-0.197796
3	7	0	1.968426	2.093688	0.197836
4	7	0	0.057443	-0.547062	1.233060
5	6	0	2.072164	-6.384766	0.345841
6	8	0	1.422688	-7.234066	-0.236187
7	8	0	2.926538	-6.707280	1.353642
8	6	0	3.232593	0.387499	-1.367654
9	6	0	3.975163	-0.543733	-2.109878
10	1	0	3.865140	-1.605018	-1.915143
11	6	0	4.866603	-0.127015	-3.101590
12	1	0	5.432043	-0.867034	-3.660147
13	6	0	5.044622	1.235727	-3.378353
14	1	0	5.740506	1.551844	-4.147746
15	6	0	4.333981	2.180385	-2.648338
16	1	0	4.492383	3.234560	-2.852995
17	6	0	3.439508	1.761405	-1.642759
18	6	0	2.700890	2.671934	-0.780336
19	6	0	2.735145	4.079119	-0.932083
20	1	0	3.303578	4.504153	-1.746224
21	6	0	1.353202	2.901756	1.141229
22	6	0	0.760376	2.310857	2.280203
23	1	0	0.843505	1.242974	2.396955
24	6	0	0.135771	3.080976	3.239886
25	1	0	-0.296057	2.605192	4.114150
26	6	0	0.070041	4.481930	3.096180
27	1	0	-0.431261	5.081884	3.847685
28	6	0	0.665451	5.095501	2.012554
29	1	0	0.639254	6.170602	1.905042
30	6	0	1.338073	4.335150	1.020382
31	6	0	2.043855	4.912097	-0.085006
32	6	0	0.760525	-2.310843	-2.280105
33	1	0	0.843438	-1.242936	-2.396791
34	6	0	0.136011	-3.081025	-3.239795
35	1	0	-0.295955	-2.605273	-4.114008
36	6	0	0.070543	-4.481999	-3.096158
37	1	0	-0.430685	-5.082006	-3.847670
38	6	0	0.666109	-5.095515	-2.012588
39	1	0	0.640117	-6.170626	-1.905121
40	6	0	1.338637	-4.335092	-1.020407
41	6	0	1.353516	-2.901689	-1.141191
42	6	0	2.044535	-4.911969	0.084942
43	6	0	2.735689	-4.078908	0.932049
44	1	0	3.304199	-4.503878	1.746169
45	6	0	2.701217	-2.671724	0.780348
46	6	0	3.439720	-1.761115	1.642781
47	6	0	4.334250	-2.179992	2.648352
48	1	0	4.492780	-3.234150	2.853003
49	6	0	3.232632	-0.387232	1.367690
50	6	0	3.975096	0.544085	2.109913
51	1	0	3.864948	1.605357	1.915184
52	6	0	4.866594	0.127468	3.101616
53	1	0	5.431949	0.867553	3.660172
54	6	0	5.044779	-1.235253	3.378371
55	1	0	5.740704	-1.551291	4.147759
56	6	0	2.071202	6.384887	-0.345985
57	8	0	1.421430	7.234072	0.235877
58	8	0	2.925675	6.707532	-1.353661
59	77	0	1.829459	0.000057	0.000018

60	6	0	-3.633803	0.339329	-0.636315
61	6	0	-3.633779	-0.339582	0.636321
62	6	0	-1.149228	0.317079	-0.653809
63	6	0	-2.362301	0.664879	-1.280165
64	6	0	-2.306468	1.312149	-2.524787
65	1	0	-3.233506	1.587581	-3.013220
66	6	0	-1.067055	1.578824	-3.089279
67	1	0	-0.983648	2.082523	-4.044790
68	6	0	0.092158	1.175704	-2.417634
69	1	0	1.076955	1.343619	-2.838943
70	6	0	-2.362254	-0.665045	1.280169
71	6	0	-1.149206	-0.317165	0.653810
72	6	0	-2.306375	-1.312317	2.524788
73	1	0	-3.233393	-1.587807	3.013224
74	6	0	-1.066943	-1.578916	3.089273
75	1	0	-0.983501	-2.082615	4.044782
76	6	0	0.092242	-1.175722	2.417625
77	1	0	1.077052	-1.343579	2.838928
78	6	0	-5.923913	0.341444	-0.638216
79	6	0	-5.923889	-0.341855	0.638223
80	6	0	-8.360087	0.342150	-0.640681
81	6	0	-8.360063	-0.342733	0.640686
82	6	0	-7.141968	-0.668034	1.248380
83	1	0	-7.119256	-1.179812	2.204794
84	6	0	-7.142014	0.667538	-1.248373
85	1	0	-7.119338	1.179318	-2.204787
86	7	0	-4.753987	-0.670223	1.253687
87	7	0	-4.754034	0.669893	-1.253680
88	6	0	-9.615462	-0.665810	1.245659
89	1	0	-9.614348	-1.177532	2.203047
90	6	0	-10.795759	-0.336735	0.629685
91	1	0	-11.742348	-0.586514	1.096965
92	6	0	-10.795782	0.335974	-0.629685
93	1	0	-11.742389	0.585684	-1.096966
94	6	0	-9.615508	0.665136	-1.245656
95	1	0	-9.614430	1.176859	-2.203043
96	1	0	2.870030	-7.676407	1.449899
97	1	0	2.868968	7.676641	-1.449987

4h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.465535	0.454844	0.969502
2	7	0	-2.956421	-1.828067	0.448475
3	7	0	-2.301761	2.271500	-0.209606
4	7	0	-1.098513	-0.697142	-1.389336
5	6	0	-3.868233	-6.049352	0.196336
6	8	0	-3.269167	-6.979578	0.703774
7	8	0	-4.935573	-6.249657	-0.622230
8	6	0	-3.545971	0.880233	1.652416
9	6	0	-4.303727	0.128651	2.563513
10	1	0	-4.427746	-0.938901	2.416862
11	6	0	-4.912401	0.734801	3.665448
12	1	0	-5.496294	0.131959	4.354602
13	6	0	-4.783913	2.113060	3.887118
14	1	0	-5.261534	2.576875	4.743196
15	6	0	-4.053258	2.884521	2.991887
16	1	0	-3.976394	3.954747	3.156126
17	6	0	-3.444913	2.275532	1.875890
18	6	0	-2.720347	3.005162	0.845591
19	6	0	-2.460919	4.395214	0.916779

20	1	0	-2.777116	4.943080	1.792372
21	6	0	-1.739530	2.920813	-1.297535
22	6	0	-1.504840	2.200748	-2.491142
23	1	0	-1.818769	1.170534	-2.531584
24	6	0	-0.943025	2.812027	-3.593491
25	1	0	-0.791087	2.243308	-4.504913
26	6	0	-0.582372	4.174205	-3.545606
27	1	0	-0.130742	4.646959	-4.410776
28	6	0	-0.828886	4.916184	-2.408093
29	1	0	-0.577017	5.966565	-2.370216
30	6	0	-1.430453	4.325291	-1.266166
31	6	0	-1.792764	5.054727	-0.087300
32	6	0	-1.469367	-2.183707	2.321203
33	1	0	-1.354198	-1.114362	2.386803
34	6	0	-0.831518	-3.019253	3.215241
35	1	0	-0.187075	-2.597962	3.979687
36	6	0	-1.025931	-4.414140	3.149045
37	1	0	-0.513927	-5.067276	3.847064
38	6	0	-1.888136	-4.949549	2.213557
39	1	0	-2.059993	-6.015685	2.169286
40	6	0	-2.581034	-4.116245	1.296743
41	6	0	-2.334699	-2.699229	1.329426
42	6	0	-3.551969	-4.596126	0.358699
43	6	0	-4.230706	-3.682978	-0.412619
44	1	0	-4.994877	-4.028283	-1.093441
45	6	0	-3.935083	-2.299678	-0.356316
46	6	0	-4.649767	-1.300658	-1.137414
47	6	0	-5.766028	-1.586335	-1.949147
48	1	0	-6.133757	-2.601859	-2.057434
49	6	0	-4.168515	0.023113	-0.987106
50	6	0	-4.862968	1.047167	-1.649294
51	1	0	-4.542240	2.077915	-1.542877
52	6	0	-5.973772	0.763464	-2.447834
53	1	0	-6.496560	1.573856	-2.947106
54	6	0	-6.425353	-0.554308	-2.605429
55	1	0	-7.290138	-0.766422	-3.224522
56	6	0	-1.486944	6.508714	0.087755
57	8	0	-0.786740	7.191232	-0.637194
58	8	0	-2.083613	7.024454	1.195514
59	77	0	-2.499599	0.196855	0.095009
60	6	0	2.958816	-0.381988	-0.274523
61	6	0	2.619991	-1.088385	-1.468912
62	6	0	0.558237	0.007842	0.196947
63	6	0	1.905601	0.167484	0.571987
64	6	0	2.198797	0.847992	1.765220
65	1	0	3.236938	0.974549	2.053521
66	6	0	1.145253	1.331035	2.528322
67	1	0	1.323804	1.866249	3.453125
68	6	0	-0.170259	1.110426	2.102122
69	1	0	-1.015814	1.455004	2.687208
70	6	0	1.219976	-1.224502	-1.858715
71	6	0	0.215540	-0.656405	-1.048420
72	6	0	0.833647	-1.893870	-3.030745
73	1	0	1.597054	-2.337633	-3.658672
74	6	0	-0.515354	-1.965129	-3.347825
75	1	0	-0.854885	-2.478117	-4.239502
76	6	0	-1.449912	-1.348422	-2.507968
77	1	0	-2.509125	-1.360485	-2.739799
78	6	0	5.191891	-0.729006	-0.661686
79	6	0	4.846542	-1.447627	-1.863319
80	6	0	7.539047	-1.127608	-1.147162
81	6	0	5.867989	-1.999350	-2.681613
82	1	0	5.573179	-2.536458	-3.575761

83	6	0	6.578872	-0.572381	-0.303338
84	7	0	3.559306	-1.613599	-2.246594
85	7	0	4.215360	-0.209310	0.110677
86	6	0	8.469663	0.290899	1.189834
87	6	0	9.009586	-1.011894	-0.873760
88	6	0	9.430779	-0.269554	0.327870
89	6	0	7.005723	0.160211	0.936861
90	6	0	7.180701	-1.838375	-2.326372
91	1	0	7.988770	-2.242170	-2.925289
92	6	0	10.795920	-0.125829	0.606645
93	1	0	11.513772	-0.569379	-0.074416
94	6	0	11.205272	0.575589	1.739490
95	1	0	12.262516	0.687751	1.954715
96	6	0	10.250864	1.135023	2.599293
97	1	0	10.570181	1.680996	3.480777
98	6	0	8.890547	0.992368	2.326407
99	1	0	8.136826	1.416206	2.980169
100	8	0	9.817167	-1.525577	-1.646565
101	8	0	6.203905	0.643188	1.733219
102	1	0	-5.057501	-7.216461	-0.668561
103	1	0	-1.820315	7.963293	1.226937

TD-DFT calculations

3a in MeCN

HOMO-4 metal d + quinoline pi — HOMO-3 metal d + phenyl pi

HOMO-2 metal d + quinoline pi — HOMO-1 metal d + quinoline pi

HOMO metal d + phenyl pi — LUMO quinoline pi*

LUMO+1 quinoline pi* — LUMO+2 bipy pi*

Excited State 1: Singlet-A	2.3472 eV	528.21 nm	f=0.0422	<S**2>=0.000
HOMO ->LUMO+1	0.70070			
Excited State 2: Singlet-A	2.3578 eV	525.84 nm	f=0.0027	<S**2>=0.000
HOMO ->LUMO	0.70239			
Excited State 3: Singlet-A	2.6638 eV	465.45 nm	f=0.0007	<S**2>=0.000
HOMO ->LUMO+2	0.70218			
Excited State 4: Singlet-A	**3.0181 eV**	**410.81 nm**	**f=0.0538**	**<S**2>=0.000**
HOMO-1 ->LUMO	0.65151			
Excited State 5: Singlet-A	3.0537 eV	406.01 nm	f=0.0158	<S**2>=0.000
HOMO-1 ->LUMO+1	0.64790			
Excited State 6: Singlet-A	**3.2009 eV**	**387.34 nm**	**f=0.1495**	**<S**2>=0.000**
HOMO-2 ->LUMO+1	0.63944			
Excited State 7: Singlet-A	**3.2195 eV**	**385.10 nm**	**f=0.0469**	**<S**2>=0.000**

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HOMO-2 ->LUMO	0.59534			
Excited State 8: Singlet-A	**3.3052 eV**	**375.12 nm**	**f=0.1743**	**<S**2>=0.000**
HOMO-3 ->LUMO	0.67090			
Excited State 9:Singlet-A	3.3127 eV	374.27 nm	f=0.0010	<S**2>=0.000
HOMO-3 ->LUMO+1	0.45466			
HOMO-1 ->LUMO+2	0.50237			
Excited State 10: Singlet-A	3.3881 eV	365.94 nm	f=0.0045	<S**2>=0.000
HOMO-3 ->LUMO+1	0.47788			
HOMO-1 ->LUMO+2	-0.43694			
Excited State 11: Singlet-A	**3.4507 eV**	**359.30 nm**	**f=0.1040**	**<S**2>=0.000**
HOMO-4 ->LUMO	-0.35805			
HOMO-4 ->LUMO+1	0.45453			
Excited State 12: Singlet-A	**3.4509 eV**	**359.28 nm**	**f=0.0815**	**<S**2>=0.000**
HOMO-4 ->LUMO	0.53006			
HOMO-4 ->LUMO+1	0.30659			

Emission

Excited State 1: Triplet-A	1.8706 eV	662.81 nm	f=0.0000	<S**2>=2.000
HOMO ->LUMO	0.64802			

4a in MeCN

HOMO-7 metal d + quinoline pi	HOMO-6 metal d + quinoline pi
HOMO-5 metal d + phenyl pi	HOMO-4 metal d + quinoline pi
HOMO-3 metal d + phenyl pi	HOMO-2 metal d + quinoline pi
HOMO-1 metal d + quinoline pi	HOMO metal d + phenyl pi
LUMO quinoline pi*	LUMO+1 quinoline pi*
LUMO+2 bipy pi*	

Absorption

Excited State 1: Singlet-A	**2.2821 eV**	**543.30 nm**	**f=0.0384**	**<S**2>=0.000**

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HOMO ->LUMO+1	0.70144			
Excited State 2: Singlet-A	2.2907 eV	541.26 nm	f=0.0029	<S**2>=0.000
HOMO ->LUMO	0.70254			
Excited State 3: Singlet-A	2.6945 eV	460.13 nm	f=0.0005	<S**2>=0.000
HOMO ->LUMO+2	0.70274			
Excited State 4: Singlet-A	**2.9549 eV**	**419.59 nm**	**f=0.0509**	**<S**2>=0.000**
HOMO-1 ->LUMO	0.65437			
Excited State 5: Singlet-A	2.9916 eV	414.44 nm	f=0.0155	<S**2>=0.000
HOMO-1 ->LUMO+1	0.65210			
Excited State 6: Singlet-A	**3.1440 eV**	**394.36 nm**	**f=0.1245**	**<S**2>=0.000**
HOMO-2 ->LUMO+1	0.63695			
Excited State 7: Singlet-A	**3.1610 eV**	**392.23 nm**	**f=0.0421**	**<S**2>=0.000**
HOMO-2 ->LUMO	0.59940			
Excited State 8: Singlet-A	**3.2411 eV**	**382.54 nm**	**f=0.1547**	**<S**2>=0.000**
HOMO-3 ->LUMO	0.67342			
Excited State 9: Singlet-A	3.2836 eV	377.58 nm	f=0.0002	<S**2>=0.000
HOMO-3 ->LUMO+1	0.61472			
Excited State 10: Singlet-A	3.3674 eV	368.19 nm	f=0.0103	<S**2>=0.000
HOMO-4 ->LUMO	0.46518			
HOMO-1 ->LUMO+2	-0.39606			
Excited State 11: Singlet-A	**3.3919 eV**	**365.53 nm**	**f=0.1732**	**<S**2>=0.000**
HOMO-4 ->LUMO+1	0.61122			
Excited State 12: Singlet-A	**3.4031 eV**	**364.32 nm**	**f=0.0478**	**<S**2>=0.000**
HOMO-4 ->LUMO	0.44469			
HOMO-1 ->LUMO+2	0.47784			

Emission

Excited State 1: Triplet-A	1.8054 eV	686.75 nm	f=0.0000	<S**2>=2.000
HOMO ->LUMO	0.65116			

3c in MeCN

HOMO-3 metal d + quinoline pi

HOMO-2 metal d + quinoline pi

HOMO-1 metal d + quinoline pi

HOMO metal d + phenyl pi

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LUMO bipy pi* LUMO+1 quinoline pi*

LUMO+2 quinoline pi* LUMO+3 bipy pi*

LUMO+4 bipy pi*

Absorption

Excited State 1: Singlet-A	2.1989 eV	563.85 nm	f=0.0009	<S**2>=0.000
248 -> 249 0.69813				
Excited State 2: Singlet-A	2.3772 eV	521.56 nm	f=0.0007	<S**2>=0.000
248 -> 250 0.70269				
Excited State 3: Singlet-A	**2.3841 eV**	**520.04 nm**	**f=0.0425**	**<S**2>=0.000**
248 -> 251 0.69609				
Excited State 4: Singlet-A	**2.8820 eV**	**430.21 nm**	**f=0.0353**	**<S**2>=0.000**
247 -> 249 0.69544				
Excited State 5: Singlet-A	2.9484 eV	420.52 nm	f=0.0077	<S**2>=0.000
248 -> 252 0.69264				
Excited State 6: Singlet-A	2.9916 eV	414.45 nm	f=0.0014	<S**2>=0.000
246 -> 249 0.63891				
Excited State 7: Singlet-A	**3.0494 eV**	**406.59 nm**	**f=0.0607**	**<S**2>=0.000**
247 -> 250 0.64851				
Excited State 8: Singlet-A	**3.0857 eV**	**401.80 nm**	**f=0.0250**	**<S**2>=0.000**
247 -> 251 0.65933				
Excited State 9: Singlet-A	**3.1882 eV**	**388.89 nm**	**f=0.0685**	**<S**2>=0.000**
245 -> 249 0.58262				
246 -> 250 -0.30898				
Excited State 10: Singlet-A	**3.2292 eV**	**383.94 nm**	**f=0.0925**	**<S**2>=0.000**
246 -> 251 0.54111				
248 -> 253 -0.36947				
Excited State 11: Singlet-A	**3.2350 eV**	**383.25 nm**	**f=0.0392**	**<S**2>=0.000**
246 -> 251 0.34398				
248 -> 253 0.59700				
Excited State 12: Singlet-A	3.2511 eV	381.36 nm	f=0.0118	<S**2>=0.000
245 -> 249 0.31218				
246 -> 250 0.53067				

Emission

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Excited State 1: Triplet-A		1.8827 eV	658.54 nm	f=0.0000	<S**2>=2.000
248 -> 249	0.61056				
248 -> 250	0.31686				

4c in MeCN

HOMO-3 metal d + phenyl pi
HOMO-2 metal d + quinoline pi
HOMO-1 metal d + phenyl pi
HOMO metal d + phenyl pi
LUMO bipy pi*
LUMO+1 quinoline pi*
LUMO+2 quinoline pi*
LUMO+3 bipy pi*

Absorption

Excited State 1: Singlet-A		2.1779 eV	569.27 nm	f=0.0008	<S**2>=0.000
200 ->201	0.69389				
Excited State 2: Singlet-A		2.3165 eV	535.21 nm	f=0.0011	<S**2>=0.000
200 ->202	0.70281				
Excited State 3: Singlet-A		**2.3230 eV**	**533.72 nm**	**f=0.0389**	**<S**2>=0.000**
200 ->203	0.69192				
Excited State 4: Singlet-A		**2.8618 eV**	**433.24 nm**	**f=0.0329**	**<S**2>=0.000**
199 ->201	0.69669				
Excited State 5: Singlet-A		2.9119 eV	425.79 nm	f=0.0069	<S**2>=0.000
200 ->204	0.69444				
Excited State 6: Singlet-A		**2.9733 eV**	**416.99 nm**	**f=0.0176**	**<S**2>=0.000**
198 ->201	0.50681				
199 ->202	-0.40257				
Excited State 7: Singlet-A		**2.9985 eV**	**413.49 nm**	**f=0.0384**	**<S**2>=0.000**
198 ->201	0.41566				
199 ->202	0.53327				
Excited State 8: Singlet-A		**3.0273 eV**	**409.55 nm**	**f=0.0217**	**<S**2>=0.000**
199 ->203	0.66533				
Excited State 9: Singlet-A		**3.1599 eV**	**392.37 nm**	**f=0.0757**	**<S**2>=0.000**
197 ->201	-0.44893				
198 ->202	0.46178				
Excited State 10: Singlet-A		**3.1763 eV**	**390.34 nm**	**f=0.1074**	**<S**2>=0.000**
198 ->203	0.63825				

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Excited State 11: Singlet-A		3.2028 eV	387.11 nm	f=0.0006	<S**2>=0.000
197 ->201	0.47476				
198 ->202	0.40927				
Excited State 12: Singlet-A		3.2207 eV	384.96 nm	f=0.0001	<S**2>=0.000
200 ->205	0.69945				

Emission

Excited State 1: Triplet-A		1.8493 eV	670.43 nm	f=0.0000	<S**2>=2.000
200 ->201	0.53262				
200 ->202	0.42274				