

Supporting information

Theoretical Study on the Electron Transfer and Phosphorescent Properties of Iridium(III) Complexes with 2-Phenylpyridyl and 8-Hydroxyquinolate Ligands

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Table S1. The differences of the bond distances between anion and neutral systems for ligand A (ΔA), B (ΔB) and C (ΔC) in *mer*-AlQ₃ and *mer*-IrQ₃. Bond labels are shown in Figure 4.

	<i>mer</i> -AlQ ₃			<i>mer</i> -IrQ ₃		
	ΔA	ΔB	ΔC	ΔA	ΔB	ΔC
M-N	0.034	-0.043	-0.097	-0.003	-0.016	-0.023
M-O(C)	0.048	0.015	0.000	0.034	0.014	-0.008
1	-0.013	0.001	0.011	-0.007	-0.001	0.014
2	0.006	-0.003	-0.010	0.004	-0.003	-0.013
3	-0.005	0.009	0.018	0.002	0.007	0.015
4	-0.001	0.017	0.031	0.006	0.013	0.028
5	0.001	-0.011	-0.018	-0.004	-0.009	-0.019
6	0.001	0.011	0.018	0.004	0.009	0.020
7	0.002	0.006	0.010	0.003	0.003	0.008
8	-0.000	-0.001	-0.002	-0.000	-0.001	-0.002
9	0.001	0.000	-0.000	0.001	0.002	0.001
10	0.002	0.005	0.007	0.003	0.004	0.006
11	-0.002	-0.005	-0.007	-0.003	-0.004	-0.005
12	0.007	-0.013	0.007	0.007	0.006	0.006

Table S2. The optimized cartesian coordinates and total electronic energies (hartree) for the studied complexes.

1-(ppy)₂IrQ				1-(ppy)IrQ₂			
Energy = -1538.8386176				Energy = -1536.6572962			
Coordinates (Angstroms)				Coordinates (Angstroms)			
	X	Y	Z		X	Y	Z
77	0.189506	-0.043153	-0.106852	77	0.026204	-0.036090	0.000527
8	-1.110947	-0.872090	-1.664520	6	1.247677	1.428246	2.423021
7	0.019975	1.877117	-0.834095	6	1.578013	2.589073	3.124448
7	0.514741	-1.967267	0.591289	6	1.284574	3.853323	2.595172
7	-1.838011	0.150433	0.753605	6	0.657707	3.950456	1.358089
6	-0.578480	2.177347	-2.002066	6	0.323871	2.784288	0.647118
1	-0.965755	1.324569	-2.548725	6	-0.344381	2.790835	-0.655227
6	-0.680454	3.483290	-2.461254	6	-0.732968	3.920152	-1.391173
1	-1.169632	3.685278	-3.407966	6	-1.355158	3.770640	-2.624299
6	-0.141840	4.509296	-1.679115	6	-1.588141	2.486027	-3.125431
1	-0.203471	5.543392	-2.006482	6	-1.188508	1.396066	-2.364641
6	0.479356	4.195414	-0.476889	6	2.612828	-2.995092	1.504487
1	0.908271	4.978306	0.138220	6	3.910977	-3.349853	1.097161
6	0.562554	2.860395	-0.054370	6	4.575355	-2.692652	0.072799
6	1.199810	2.369696	1.167601	6	3.930652	-1.624947	-0.593441
6	1.799686	3.212399	2.118885	6	4.497796	-0.872154	-1.654913
1	1.807366	4.290499	1.976628	6	3.782488	0.152292	-2.234670
6	2.390815	2.673285	3.255694	6	2.484758	0.449068	-1.769910
1	2.855955	3.324062	3.990927	6	2.613478	-1.263403	-0.183536
6	2.383204	1.284895	3.439848	8	-0.811344	-1.541858	-1.337513
1	2.849220	0.857116	4.325140	6	-2.612644	-1.240876	0.184090
6	1.787973	0.444862	2.497623	6	-2.369355	0.390904	1.848603
1	1.802399	-0.628746	2.667180	6	-2.002721	-1.902674	-0.942689
6	1.175288	0.954544	1.339014	6	-3.920208	-1.587196	0.644925
6	-0.291300	-2.619775	1.450594	6	-3.650481	0.103744	2.360476

1	-1.142929	-2.058135	1.813761	6	-2.761529	-2.903597	-1.569721
6	-0.057778	-3.926703	1.852254	6	-4.634293	-2.605777	-0.027376
1	-0.738283	-4.407168	2.546820	6	-4.417106	-0.873172	1.765968
6	1.059129	-4.590369	1.336914	6	-4.046175	-3.238885	-1.111056
1	1.275553	-5.615512	1.623942	7	-1.873277	-0.257249	0.798623
6	1.891200	-3.923018	0.449709	6	0.616082	1.493111	1.170544
1	2.761545	-4.420624	0.038019	7	-0.587207	1.544366	-1.168133
6	1.614674	-2.598765	0.075227	7	1.922088	-0.238551	-0.782172
6	2.410194	-1.780636	-0.835407	6	1.930650	-1.946898	0.876040
6	3.581665	-2.238834	-1.462907	8	0.722511	-1.556550	1.212851
1	3.941948	-3.250606	-1.293726	1	1.475191	0.455064	2.849329
6	4.293802	-1.398437	-2.309506	1	2.068554	2.513170	4.092522
1	5.199584	-1.751075	-2.794971	1	1.544348	4.752951	3.146226
6	3.833191	-0.094053	-2.526262	1	0.428216	4.933404	0.953313
1	4.389001	0.570439	-3.184556	1	-0.542855	4.909385	-0.990317
6	2.670438	0.362809	-1.905378	1	-1.655811	4.646839	-3.191805
1	2.342974	1.381188	-2.095148	1	-2.070363	2.327147	-4.083837
6	1.921620	-0.462888	-1.050452	1	-1.325781	0.366929	-2.679842
6	-2.169439	0.675834	1.927623	1	2.116052	-3.529360	2.308163
1	-1.353259	1.055052	2.534083	1	4.406720	-4.172009	1.607956
6	-3.508487	0.736271	2.369495	1	5.577557	-2.984905	-0.226091
1	-3.729169	1.174643	3.337740	1	5.499257	-1.114242	-2.001973
6	-4.507951	0.237289	1.563942	1	4.197374	0.740517	-3.046703
1	-5.546855	0.270998	1.884105	1	1.895671	1.248528	-2.202975
6	-4.193704	-0.328222	0.299848	1	-1.732363	1.144423	2.294683
6	-5.153622	-0.860030	-0.590866	1	-4.009205	0.658784	3.221176
6	-4.729146	-1.383063	-1.802910	1	-2.323165	-3.420327	-2.418108
1	-5.465656	-1.793470	-2.490403	1	-5.627412	-2.879951	0.315924
6	-3.376920	-1.401927	-2.180521	1	-5.406866	-1.111015	2.148375
1	-3.074655	-1.816502	-3.137537	1	-4.592815	-4.025360	-1.626686
6	-2.374206	-0.888724	-1.339675				
6	-2.811416	-0.346393	-0.072015				

1	-6.204595	-0.850905	-0.316935				
<i>mer</i> -IrQ ₃				<i>mer</i> -AlQ ₃			
Energy = -1534.4726606				Energy = -1672.3646722			
Coordinates (Angstroms)				Coordinates (Angstroms)			
	X	Y	Z		X	Y	Z
7	-2.033466	0.107341	0.535117	13	-0.119739	-0.252836	-0.214937
6	-2.521891	1.034410	1.350850	7	-2.036482	0.022721	0.554584
1	-1.820079	1.765587	1.733988	6	-2.539823	0.883244	1.428101
6	-3.886625	1.065920	1.703931	1	-1.852665	1.607208	1.853397
1	-4.238978	1.842863	2.374403	6	-3.900362	0.866709	1.795618
6	-4.744698	0.115839	1.195154	1	-4.265583	1.593186	2.514259
1	-5.799541	0.125329	1.458283	6	-4.742560	-0.072141	1.236458
6	-4.258037	-0.888798	0.318787	1	-5.795250	-0.100781	1.508239
6	-5.049502	-1.908019	-0.259303	6	-4.241154	-1.010828	0.300738
1	-6.111185	-1.954900	-0.036424	6	-5.004994	-2.019639	-0.335747
6	-4.450743	-2.831478	-1.102375	1	-6.064242	-2.113531	-0.115150
1	-5.059328	-3.615529	-1.546565	6	-4.380148	-2.870699	-1.230227
6	-3.078736	-2.795548	-1.409086	1	-4.965677	-3.646019	-1.718827
1	-2.637408	-3.531411	-2.073596	6	-3.006890	-2.775570	-1.538422
6	-2.252559	-1.807562	-0.862930	1	-2.549717	-3.459879	-2.246010
6	-2.866127	-0.850436	0.010791	6	-2.212394	-1.798958	-0.939776
8	-0.965872	-1.714245	-1.112387	6	-2.854194	-0.912465	-0.008121
7	0.708470	1.510864	0.806561	8	-0.930307	-1.627816	-1.161103
6	1.262253	1.576132	2.012993	7	0.599887	1.473902	0.794401
1	1.298687	0.646418	2.570111	6	1.075504	1.623218	2.023965
6	1.758789	2.794199	2.523952	1	1.108340	0.726941	2.634240
1	2.203949	2.806623	3.513434	6	1.506761	2.878448	2.503167
6	1.671465	3.942127	1.765858	1	1.890383	2.957299	3.515281
1	2.049067	4.886992	2.148773	6	1.433816	3.985195	1.680465
6	1.084826	3.903445	0.472222	1	1.761386	4.959194	2.036766

6	0.941119	5.016315	-0.388239	6	0.930684	3.860266	0.360483
1	1.295303	5.992036	-0.069671	6	0.801866	4.911024	-0.581415
6	0.346424	4.838401	-1.628430	1	1.102209	5.919148	-0.311377
1	0.234913	5.694781	-2.289071	6	0.291696	4.627737	-1.836644
6	-0.123273	3.588145	-2.070875	1	0.191401	5.434376	-2.559017
1	-0.585654	3.481471	-3.047040	6	-0.106283	3.329798	-2.225802
6	-0.005779	2.454107	-1.258657	1	-0.501453	3.147574	-3.220241
6	0.609033	2.636081	0.025896	6	0.004315	2.262799	-1.335567
8	-0.411004	1.253229	-1.615925	6	0.525753	2.553439	-0.030232
7	1.756403	-0.738213	-0.781251	8	-0.320440	1.015534	-1.589492
6	2.370291	-0.347473	-1.890789	7	1.747943	-0.817140	-0.889725
1	1.855021	0.400704	-2.482373	6	2.364634	-0.557599	-2.033327
6	3.613890	-0.896757	-2.268471	1	1.845468	0.105002	-2.717771
1	4.085125	-0.552736	-3.183197	6	3.620711	-1.122303	-2.337526
6	4.205188	-1.858605	-1.477865	1	4.094685	-0.885321	-3.284439
1	5.162470	-2.291442	-1.757773	6	4.225027	-1.968929	-1.429710
6	3.565713	-2.302411	-0.289845	1	5.192929	-2.412933	-1.650988
6	4.075260	-3.287699	0.588692	6	3.586086	-2.272631	-0.200572
1	5.027831	-3.761309	0.371100	6	4.095225	-3.128819	0.807987
6	3.340859	-3.636057	1.711009	1	5.056872	-3.614227	0.669701
1	3.730325	-4.396466	2.383621	6	3.347449	-3.334921	1.953459
6	2.099042	-3.046459	2.015960	1	3.735475	-3.995145	2.725560
1	1.543155	-3.347082	2.898439	6	2.090825	-2.724951	2.165127
6	1.552116	-2.068802	1.180056	1	1.529520	-2.918414	3.074038
6	2.312460	-1.701538	0.021119	6	1.549365	-1.873516	1.204547
8	0.401411	-1.466134	1.412804	6	2.323793	-1.655035	0.014950
77	-0.089277	-0.147527	-0.107893	8	0.395101	-1.246522	1.300575

fac-Ir(ppy)₃

Energy = -1541.0088885

Coordinates (Angstroms)

	X	Y	Z
77	-0.000001	-0.000001	0.026401
6	1.739290	-0.095439	1.063012
6	-0.952392	-1.458570	1.062901
6	-0.787097	1.553999	1.062917
7	1.079137	-1.545415	-1.088965
7	-1.877879	-0.161766	-1.089077
7	0.798947	1.707190	-1.088975
6	0.613223	-2.229191	-2.147512
6	-2.237028	0.583692	-2.147590
6	1.624163	1.645510	-2.147446
6	1.347666	-3.216051	-2.791587
6	-3.458862	0.441128	-2.791742
6	2.111677	2.774942	-2.791531
6	2.624898	-3.508024	-2.303509
6	-4.350365	-0.519032	-2.303779
6	1.725910	4.027079	-2.303547
6	3.107257	-2.811143	-1.204538
6	-3.988091	-1.285287	-1.204843
6	0.881118	4.096450	-1.204654
6	2.320029	-1.819383	-0.591953
6	0.415754	2.918853	-0.592055
6	-2.735619	-1.099457	-0.592178
6	2.707871	-1.022853	0.575418
6	-2.239805	-1.833666	0.575188
6	-0.468225	2.856515	0.575305
6	3.962037	-1.167578	1.198698
6	-2.992281	-2.847453	1.198384
6	-0.970039	4.015024	1.198520
6	4.286015	-0.407777	2.314756
6	-2.496361	-3.507950	2.314472
6	-1.790102	3.915709	2.314530

6	3.347826	0.504728	2.813197
6	-1.237056	-3.151721	2.813028
6	-2.111261	2.646968	2.812988
6	2.105420	0.654197	2.198169
6	-0.486354	-2.150489	2.198086
6	-1.619435	1.496273	2.198025
1	-0.386811	-1.963737	-2.474262
1	-1.507100	1.317039	-2.474249
1	1.894290	0.646705	-2.474124
1	0.927162	-3.740481	-3.643125
1	-3.702731	1.067573	-3.643248
1	2.776173	2.672930	-3.643005
1	3.234482	-4.275101	-2.773314
1	-5.319440	-0.663370	-2.773647
1	2.085495	4.938499	-2.773363
1	4.091953	-3.034467	-0.810742
1	-4.673868	-2.026421	-0.811138
1	0.582168	5.060911	-0.810931
1	1.397279	1.365705	2.611450
1	0.483867	-1.892986	2.611455
1	-1.881551	0.527256	2.611318
1	3.590153	1.102684	3.689549
1	-0.840452	-3.660578	3.689405
1	-2.750321	2.557862	3.689303
1	5.255060	-0.522623	2.792953
1	-3.080387	-4.289751	2.792603
1	-2.175215	4.812354	2.792676
1	4.691455	-1.876920	0.815493
1	-3.971266	-3.124466	0.815089
1	-0.720440	5.001384	0.815302
