PCCP

Electronic Supplementary Information

Photophysical properties on structural isomers of homoleptic Ir-complexes derived from xylenyl-substituted N-heterocyclic carbene ligands

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Table S1 For transitions related to $S_0 \rightarrow T_1$ and $S_0 \rightarrow S_1$. The energies, oscillator strengths, orbital contributions, and assignments of ***f*-Ir(dmpmp)$_3$** and ***m*-Ir(dmpmp)$_3$** evaluated by TD-DFT calculations.

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Table S2 Cartesian Coordinates of ***f*-Ir(dmpmp)$_3$**, ***m*-Ir(dmpmp)$_3$**, ***f*-Ir(pmp)$_3$** and ***m*-Ir(pmp)$_3$**

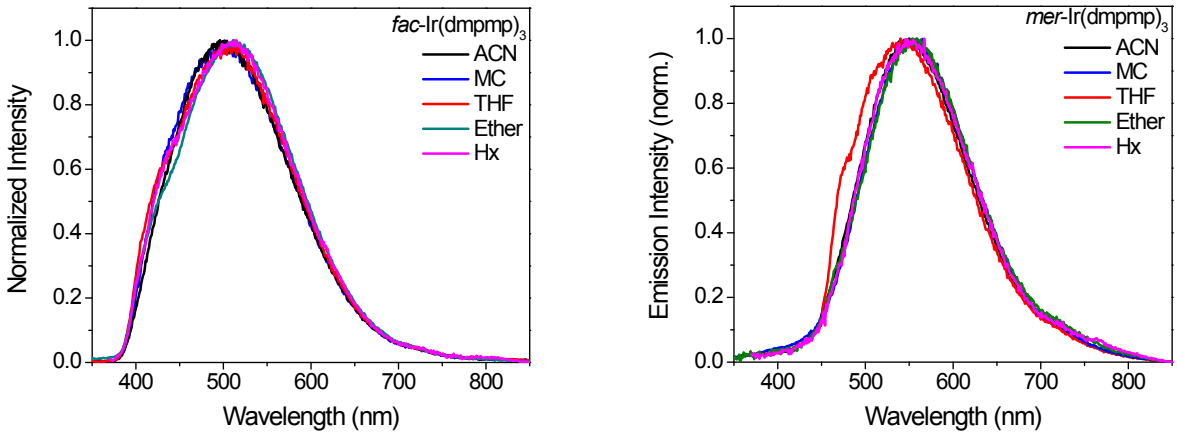


Fig. S1 Phosphorescence emission spectra of **Ir(dmpmp)$_3$** in different solvent polarities.

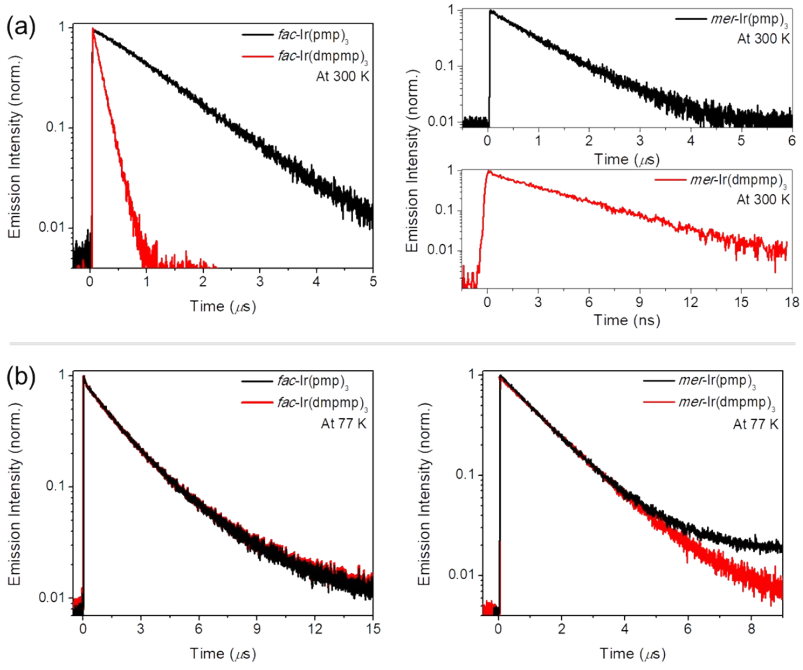


Fig. S2 Phosphorescence emission decay profiles for **Ir(pmp)$_3$** and **Ir(dmpmp)$_3$** measured in (a) CH_2Cl_2 at 300 K, and (b) 2-MeTHF at 77 K.

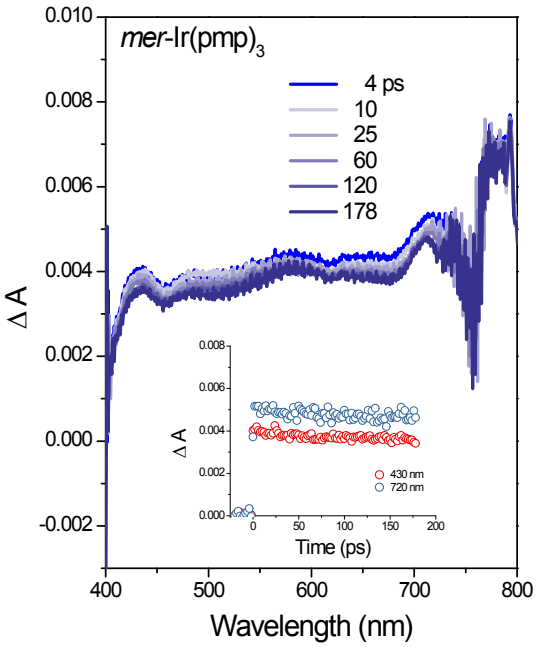


Fig. S3 Femtosecond time-resolved transient absorption spectra of ***mer*-Ir(pmp)$_3$**.

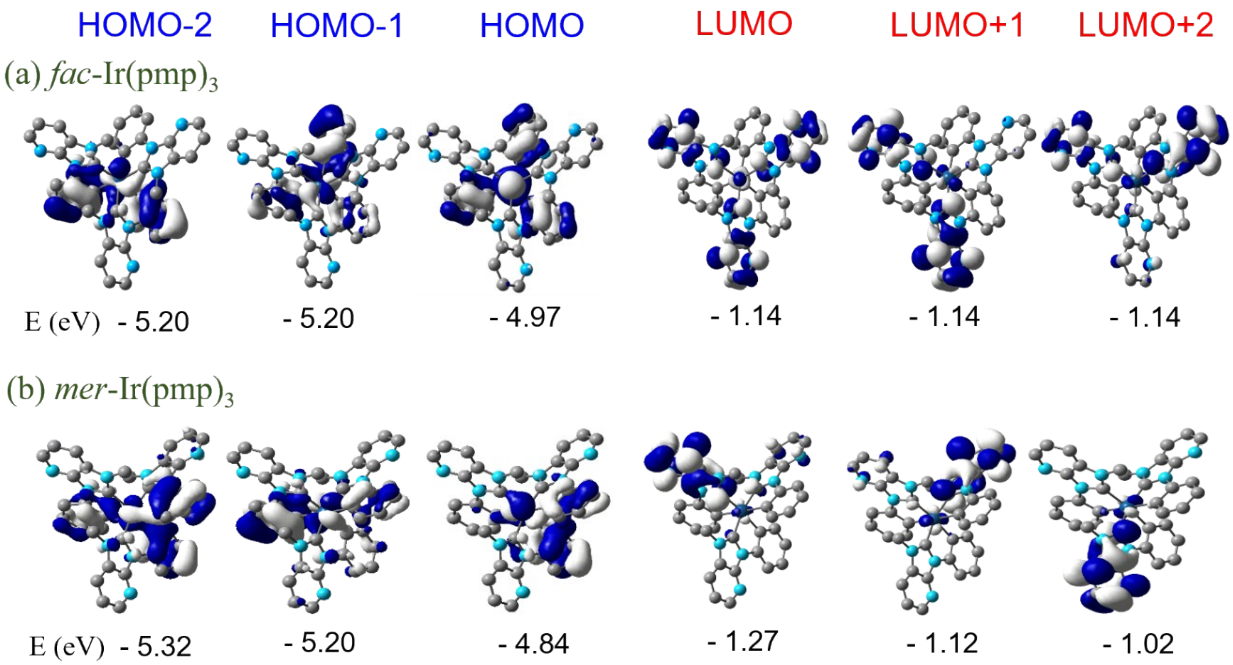


Fig. S4 Frontier molecular orbitals of (a) ***fac*-Ir(pmp)$_3$** and (b) ***mer*-Ir(pmp)$_3$**.

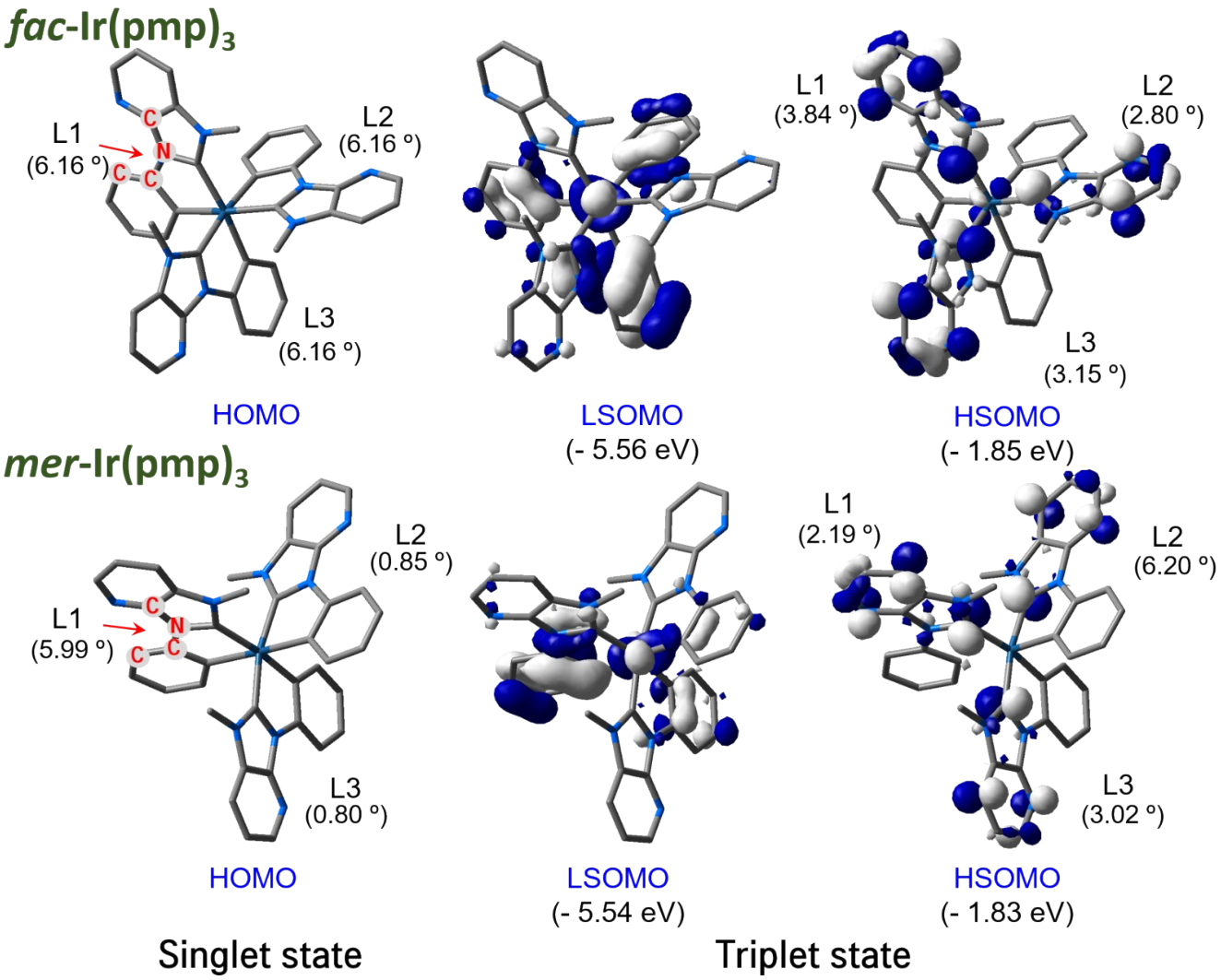
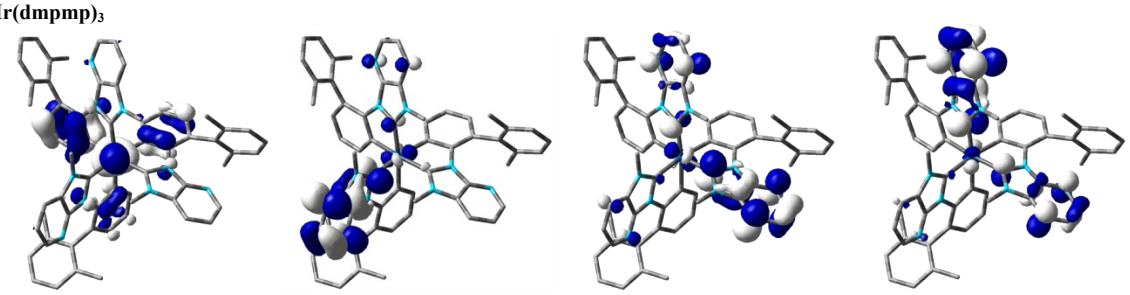


Fig. S5 Frontier molecular orbitals of ***f*-Ir(pmp)$_3$** and ***m*-Ir(pmp)$_3$** for the singlet and triplet manifolds.

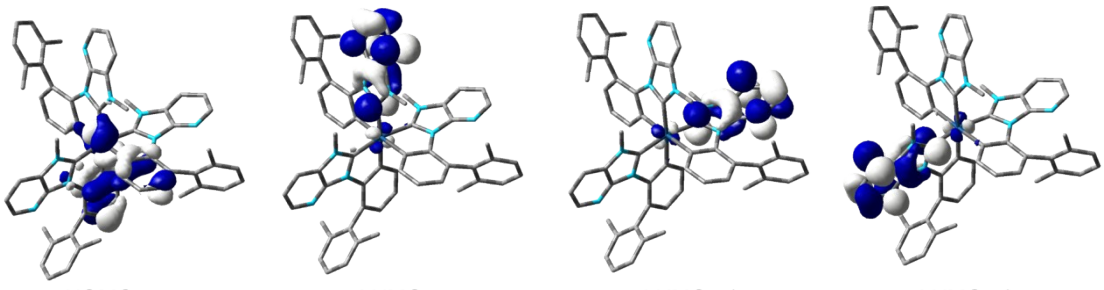
Table S1 For transitions related to $S_0 \rightarrow T_1$ and $S_0 \rightarrow S_1$. The energies (λ_{cal} and E_{cal}), oscillator strengths (f), orbital contributions (>10%), and assignments of ***fac*-Ir(dmpmp)$_3$** and ***mer*-Ir(dmpmp)$_3$** evaluated by TD-DFT calculations

	State	λ_{cal} (E_{cal})	f	Orbital contributions	Assignments
***fac*-Ir(dmpmp)$_3$**	T1	397 nm (3.12 eV)	0	H→L (73%)	MLCT, ILCT, LLCT
	S1	372 nm (3.33 eV)	0.034	H→L (75%), H→L+1 (17%)	MLCT, ILCT, LLCT
	S2	365 nm (3.40 eV)	0.0376	H→L+1 (61%), H→L+2 (17%), H→L (12%)	MLCT, ILCT, LLCT
	S3	361 nm (3.43 eV)	0.0043	H→L+2 (74%), H→L+1 (12%)	MLCT, ILCT, LLCT
***mer*-Ir(dmpmp)$_3$**	T1	415 nm (2.99 eV)	0	H→L (55%), H→L+1 (32%)	MLCT, ILCT, LLCT
	S1	402 nm (3.08 eV)	0.0033	H→L (80%), H→L+1 (15%)	MLCT, ILCT, LLCT
	S2	391 nm (3.17 eV)	0.0016	H→L+1 (51%), H→L (16%)	MLCT, ILCT, LLCT
	S3	377 nm (3.29 eV)	0.0024	H→L+2 (92%)	MLCT, ILCT, LLCT

***fac*-Ir(dmpmp)$_3$**



***mer*-Ir(dmpmp)$_3$**



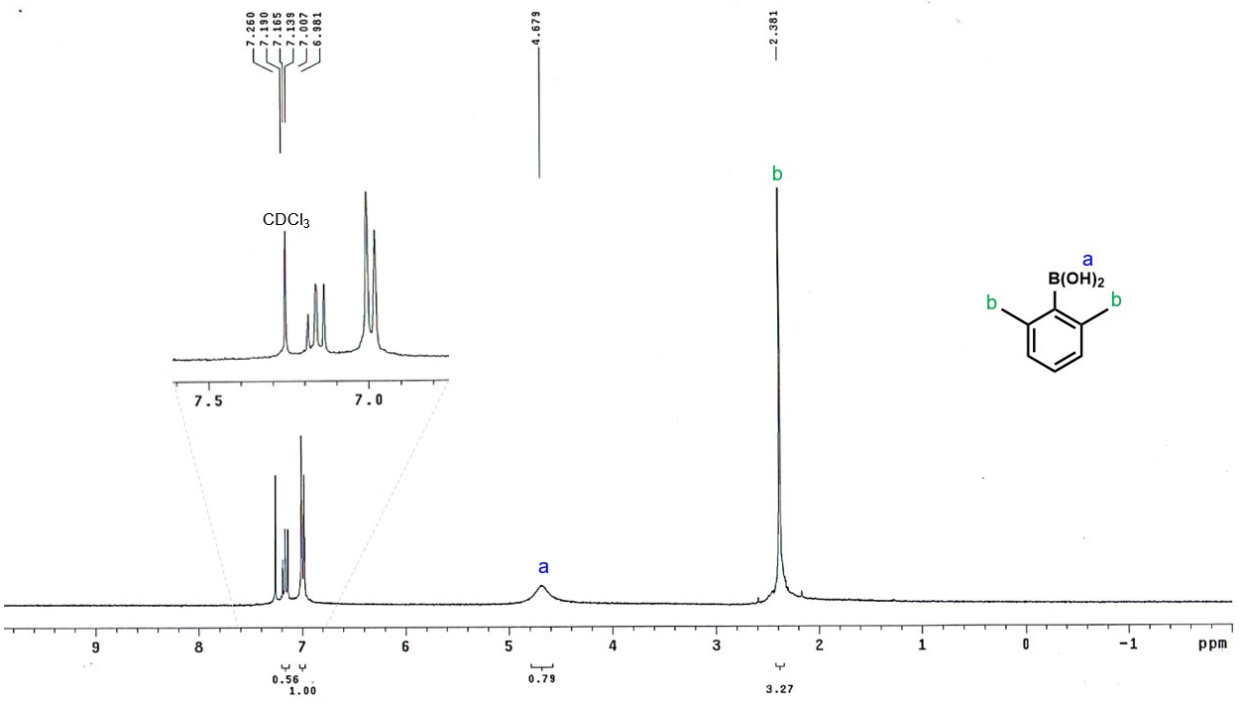


Fig. S6 ^{1}H-NMR spectrum of 2,6-dimethylphenylboronic acid.

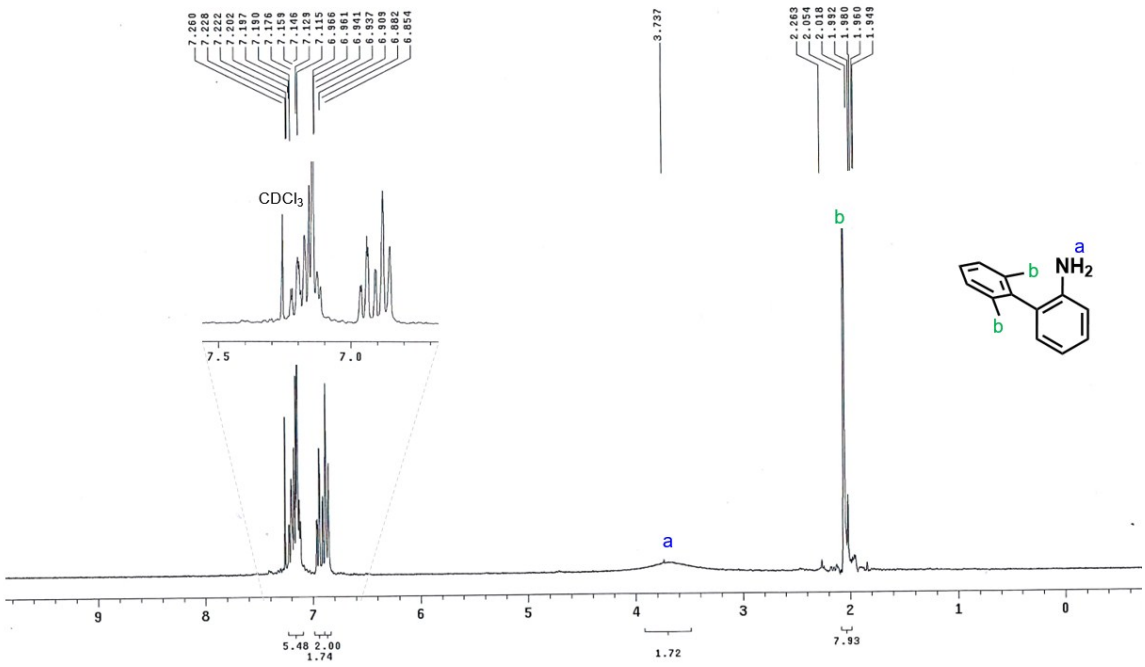


Fig. S7 ^{1}H-NMR spectrum of 2’,6’-Dimethylbiphenyl-2-amine.

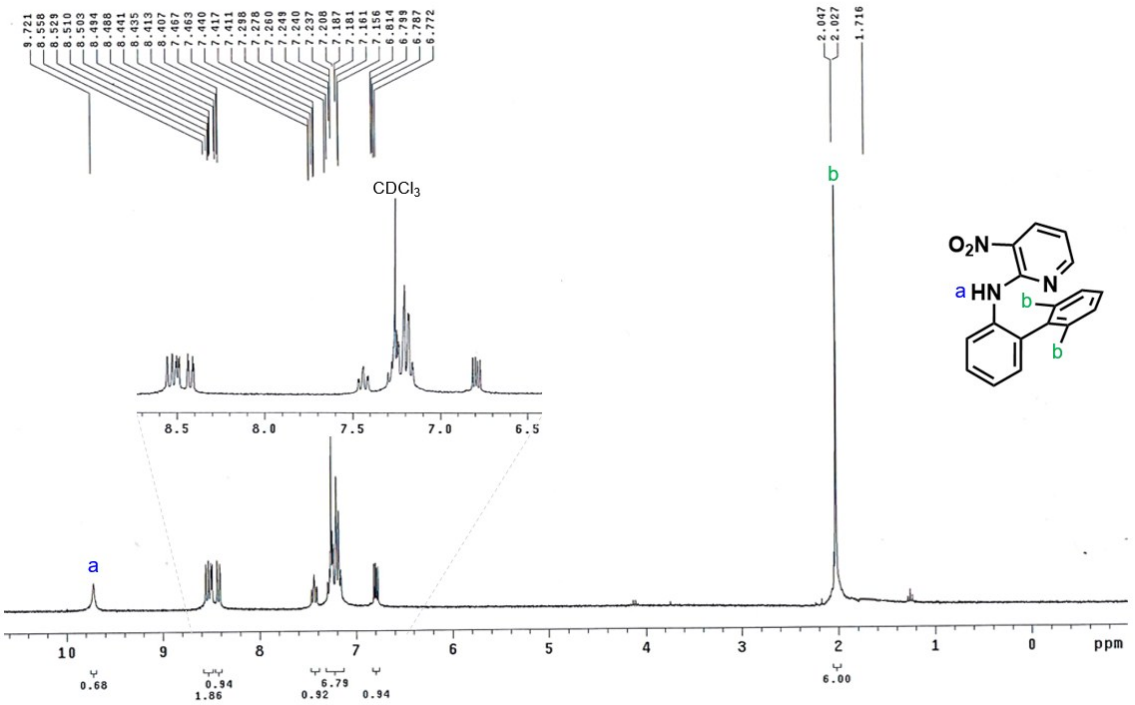


Fig. S8 ^{1}H-NMR spectrum of *N*-(2',6'-dimethylbiphenyl-2-yl)-3-nitropyridin-2-amine.

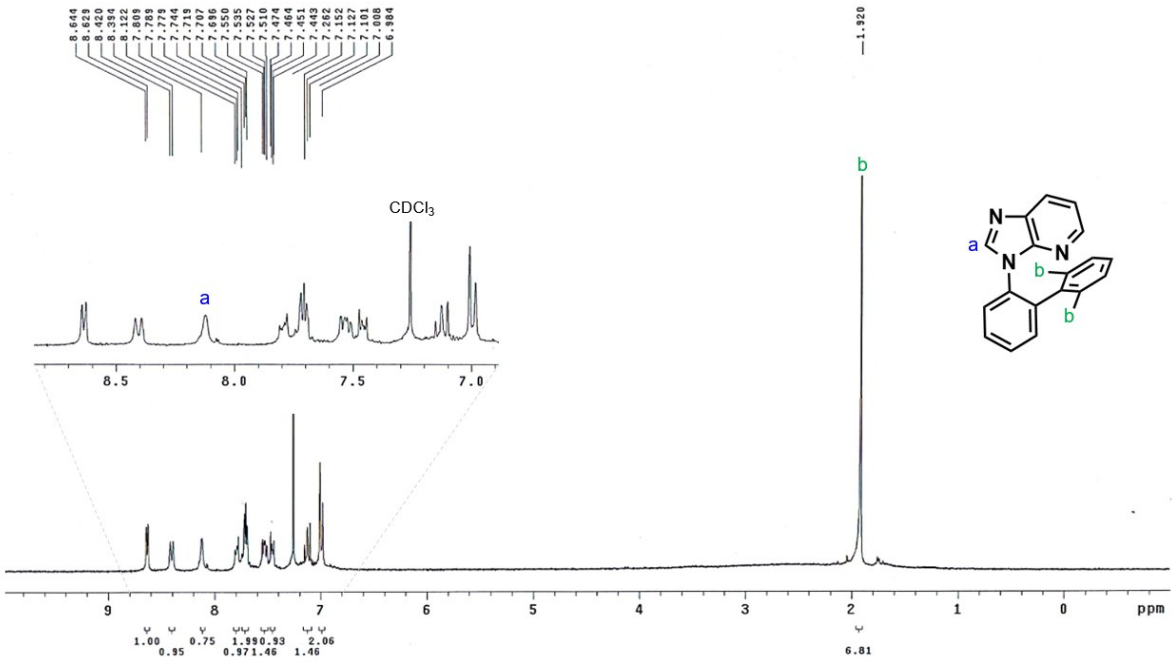


Fig. S9 ^{1}H-NMR spectrum of 3-(2',6'-dimethylbiphenyl-2-yl)-3H-imidazo[4,5-*b*]pyridine.

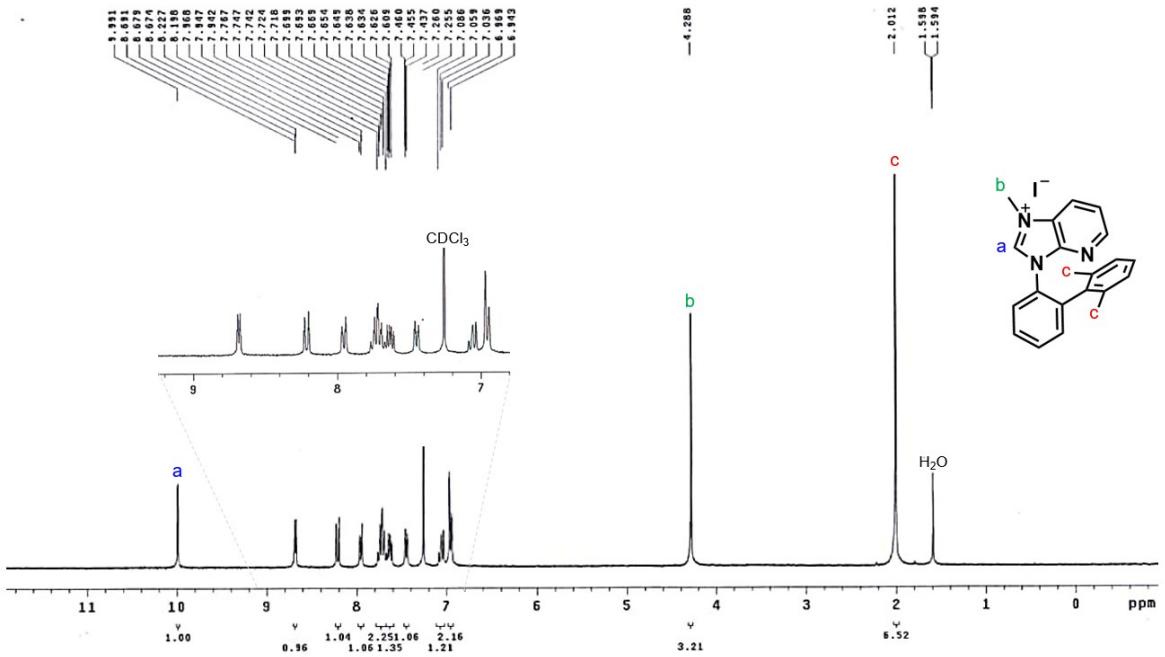


Fig. S10 ^{1}H-NMR spectrum of 3-(2',6'-dimethylbiphenyl-2-yl)-1-methyl-3H-imidazo[4,5-*b*]pyridin-1-ium iodide.

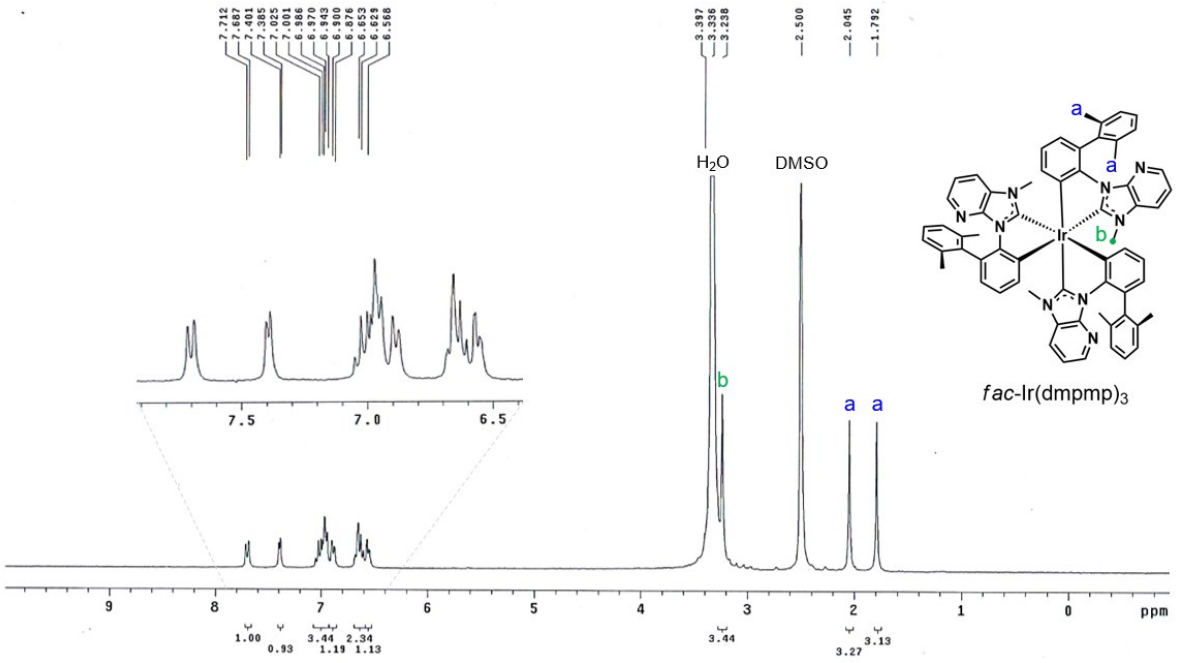


Fig. S11 ^{1}H-NMR spectrum of ***fac*-Ir(dmpmp)$_3$**

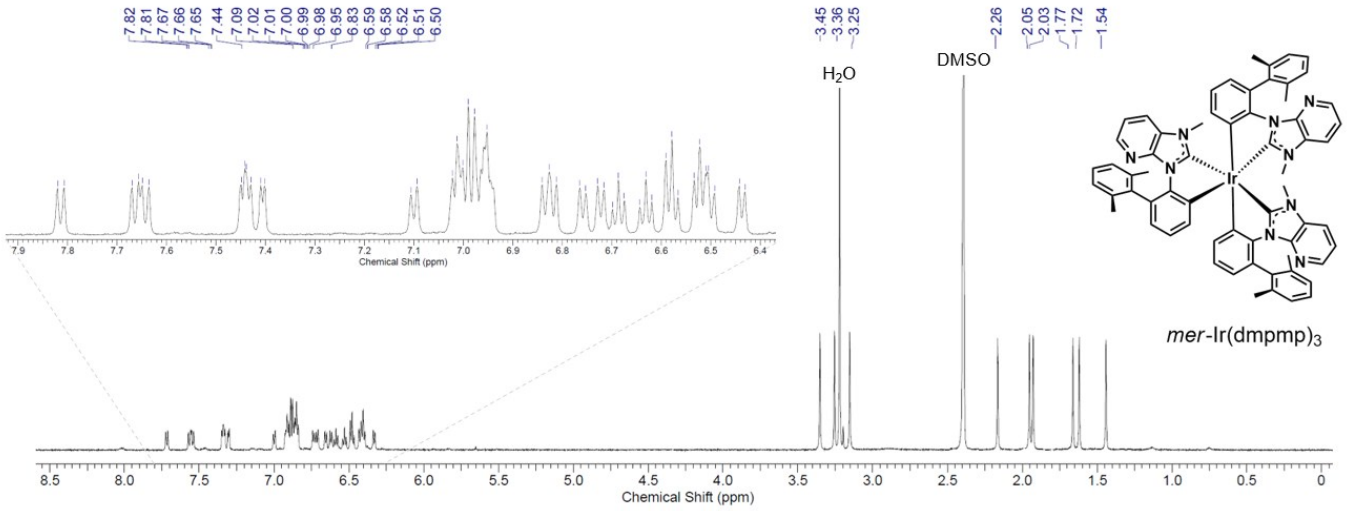


Fig. S12 ^{1}H-NMR spectrum of *mer*-Ir(dmpmp)$_3$.

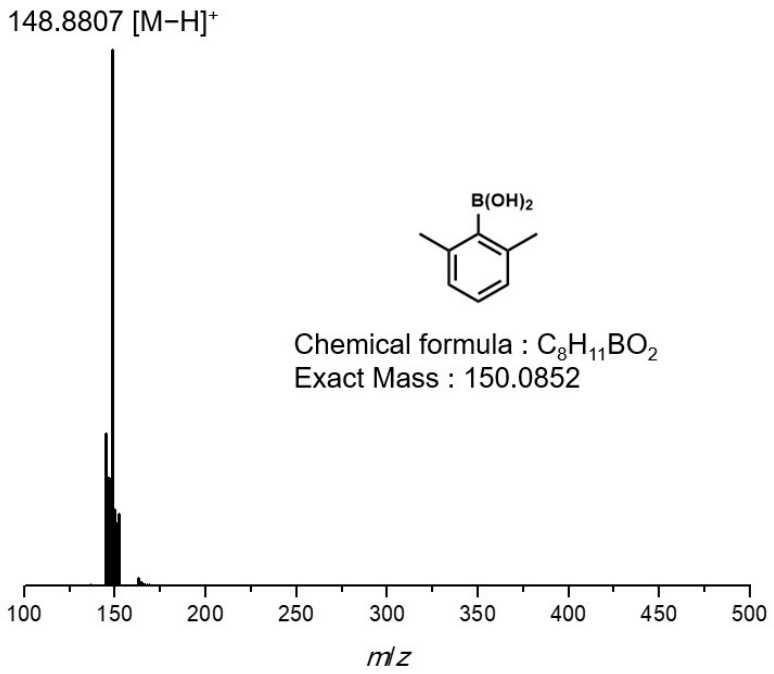


Fig. S13 ESI-Mass spectrum of 2,6-dimethylphenylboronic acid.

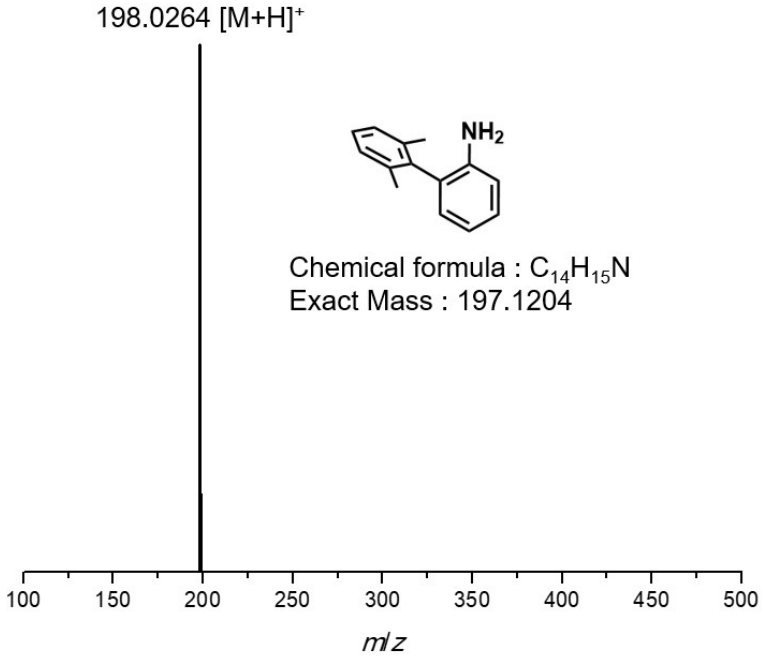


Fig. S14 ESI-Mass spectrum of 2',6'-Dimethylbiphenyl-2-amine.

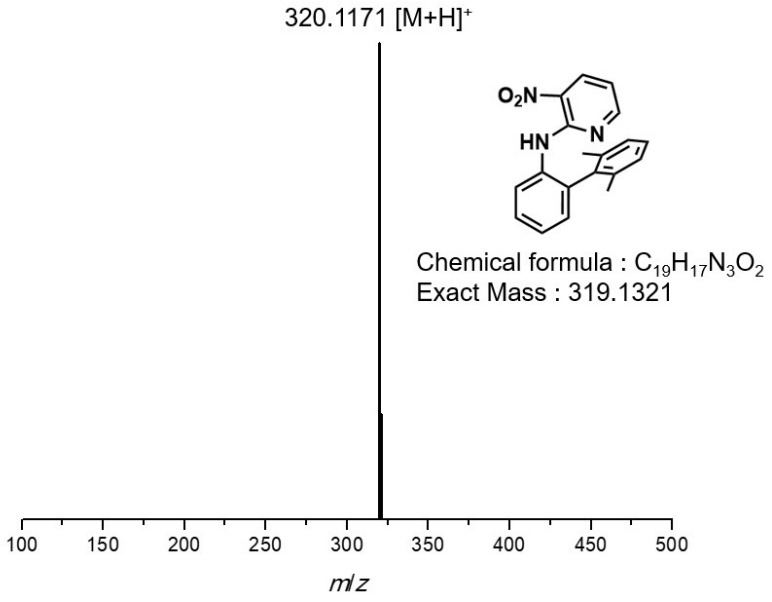


Fig. S15 ESI-Mass spectrum of *N*-(2',6'-dimethylbiphenyl-2-yl)-3-nitropyridin-2-amine.

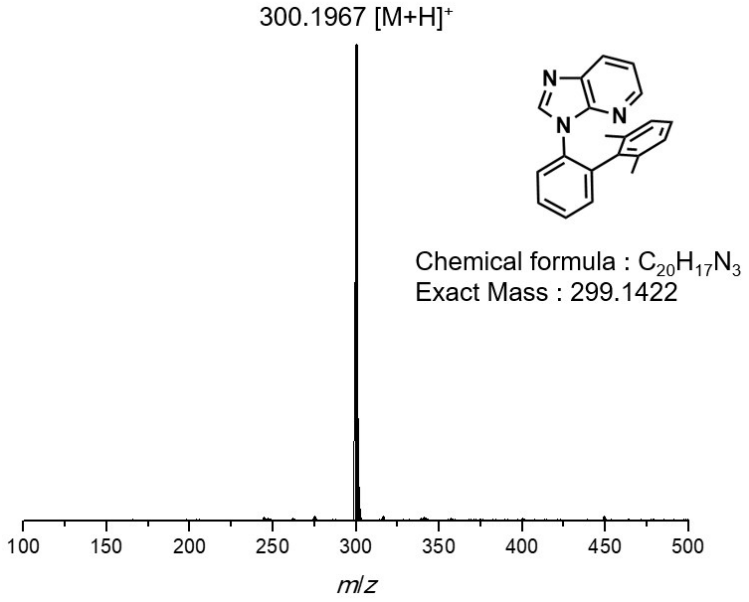


Fig. S16 ESI-Mass spectrum of 3-(2',6'-dimethylbiphenyl-2-yl)-3H-imidazo[4,5-*b*]pyridine.

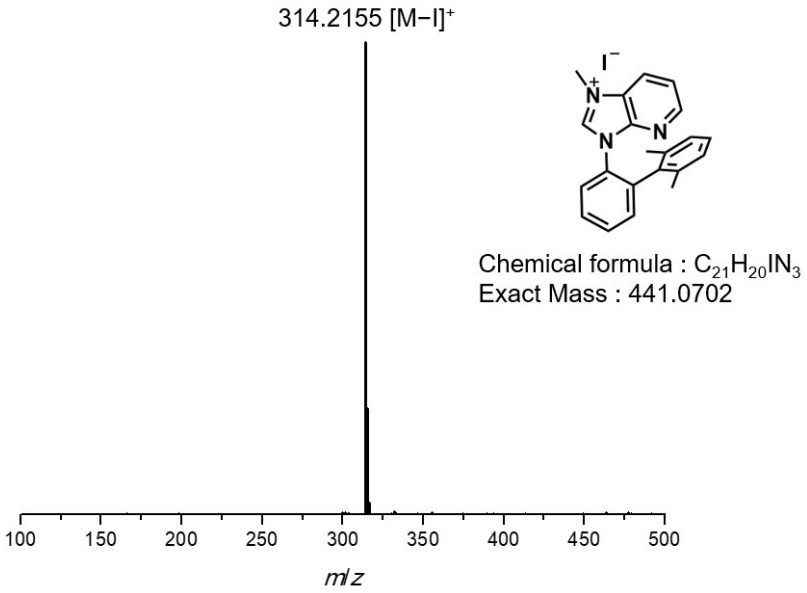


Fig. S17 ESI-Mass spectrum of 3-(2',6'-dimethylbiphenyl-2-yl)-1-methyl-3H-imidazo[4,5-*b*]pyridin-1-ium iodide.

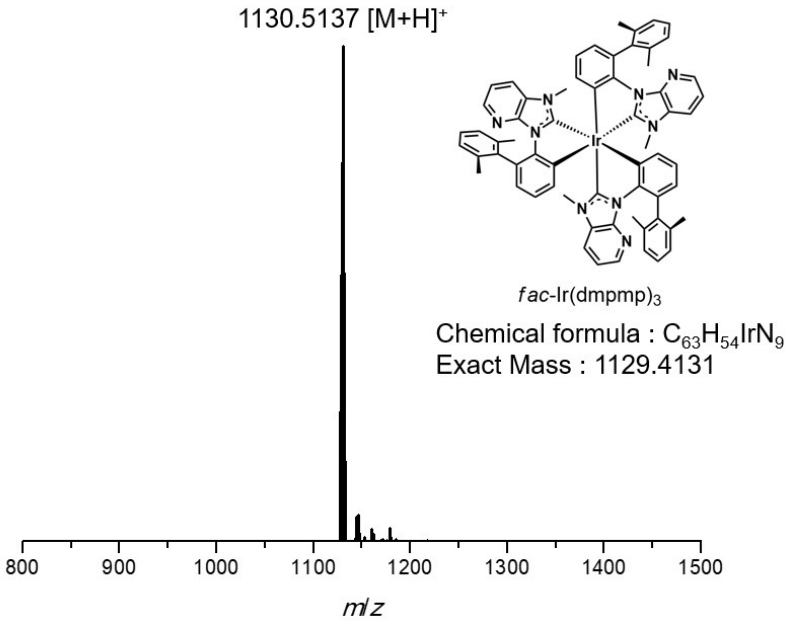


Fig. S18 ESI-Mass spectrum of ***fac*-Ir(dmpmp)$_3$.**

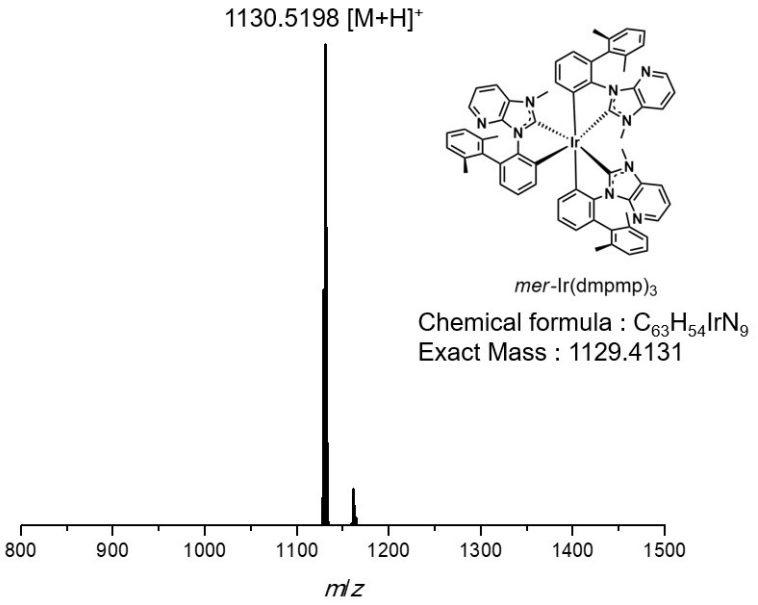


Fig. S19 ESI-Mass spectrum of ***mer*-Ir(dmpmp)$_3$**.

Table S2 Cartesian Coordinates of ***f*-Ir(dmpmp)$_3$**, ***m*-Ir(dmpmp)$_3$**, ***f*-Ir(pmp)$_3$** and ***m*-Ir(pmp)$_3$**

Optimized geometry of singlet ***f*-Ir(dmpmp)$_3$**

Symbol	X	Y	Z
Ir	-0.037298	-0.038519	0.105657
N	0.707811	-2.886641	0.309289
N	-0.796516	-2.553025	1.885358
N	1.897555	2.145637	0.559841
N	2.278865	0.683512	2.166316
N	-2.848506	0.853866	0.30557
N	-1.773754	1.990647	1.855631
C	1.349092	-1.084589	-1.090234
C	2.093733	-0.561669	-2.153491
H	1.913995	0.458681	-2.471499
C	3.062658	-1.320703	-2.810129
H	3.625053	-0.894961	-3.637494
C	2.628458	-3.206478	-1.317235
C	1.593266	-2.437258	-0.739954
C	0.317018	-4.150652	0.76919
C	-0.61533	-3.924705	1.801705
C	-0.044878	-1.909997	0.936413
C	-1.715586	-1.922833	2.814805
H	-1.448615	-2.185871	3.844178
H	-2.741537	-2.246125	2.61861
H	-1.64849	-0.845196	2.680924
C	0.194077	1.723588	-1.037164
C	-0.532889	2.066635	-2.182875
H	-1.353842	1.431973	-2.4986
C	-0.202844	3.185154	-2.947779
H	-0.779209	3.433189	-3.835645
C	1.677993	3.672765	-1.461196
C	1.257795	2.583994	-0.662942
C	2.808252	2.740788	1.442101
C	3.080974	1.780986	2.436836
C	1.511013	0.909193	1.051259
C	2.236448	-0.490164	3.019308
H	2.017335	-0.198545	4.052679
H	3.196241	-1.01468	2.995348
H	1.455439	-1.151981	2.655119
C	-1.684046	-0.709864	-1.038701
C	-1.652383	-1.684357	-2.043819
H	-0.698376	-2.106316	-2.341763
C	-2.817984	-2.125744	-2.669762
H	-2.76957	-2.880554	-3.450833
C	-4.161454	-0.641815	-1.265436
C	-2.95192	-0.169754	-0.70668
C	-1.631218	0.965286	0.955993
C	-0.750765	2.476694	2.76446
H	-1.218657	2.773865	3.707078
H	-0.219878	3.335176	2.341277
H	-0.042122	1.67486	2.95766
C	-1.183551	-5.001522	2.468471
C	-0.789533	-6.269367	2.029537
C	0.109427	-6.386713	0.96224
H	-1.904602	-4.871421	3.268961
H	-1.19089	-7.162628	2.496104
H	0.396846	-7.369071	0.595797
N	0.662121	-5.34571	0.322419
C	3.155598	-4.54184	-0.87285
C	2.953333	-5.688436	-1.672916
C	3.967554	-4.620409	0.277142
C	3.554428	-6.894217	-1.300208
C	4.548264	-5.84713	0.625048
C	4.346188	-6.980533	-0.155936
H	3.39367	-7.776741	-1.914834
H	5.175411	-5.903608	1.511687
H	4.809089	-7.924507	0.11933
C	4.233676	-3.404831	1.136801
H	4.557791	-2.549605	0.535197
H	3.333086	-3.090175	1.677525
H	5.008852	-3.617392	1.879027
C	2.04852	-5.646328	-2.881109
H	1.026969	-5.390632	-2.577725
H	2.362147	-4.894538	-3.611079
H	2.021315	-6.618305	-3.382033
C	-3.006021	2.608213	1.701967
C	-3.687067	1.907651	0.687174
C	-5.572903	-0.307669	-0.869199
C	-6.391043	0.444158	-1.742667
C	-6.122105	-0.858411	0.30625
C	-7.736857	0.638122	-1.418671

C	-7.473654	-0.638553	0.603323
C	-8.281557	0.103513	-0.251915
H	-8.362858	1.22049	-2.090531
H	-7.892892	-1.067519	1.51045
H	-9.330851	0.259624	-0.015926
C	-5.281846	-1.683359	1.254529
H	-5.909866	-2.175673	2.002951
H	-4.711284	-2.451463	0.722445
H	-4.557285	-1.057654	1.789699
C	-5.820395	1.09452	-2.980354
H	-5.358924	0.370307	-3.657859
H	-6.597589	1.630872	-3.532346
H	-5.041482	1.813559	-2.702376
N	-4.85639	2.265119	0.185047
C	4.141454	4.264252	2.437217
H	4.537444	5.27668	2.432233
C	2.916672	4.514454	-1.328826
C	4.157256	3.996663	-1.756005
C	2.818313	5.858939	-0.908734
C	5.287622	4.824209	-1.727405
C	3.965295	6.658026	-0.902273
C	5.198335	6.146722	-1.304093
H	6.243553	4.423199	-2.055503
H	3.888155	7.692029	-0.574277
H	6.081993	6.779456	-1.296283
C	4.288058	2.578513	-2.263862
H	4.034506	1.835425	-1.5004
H	3.616687	2.395155	-3.109797
H	5.311076	2.378441	-2.594811
C	1.512116	6.424576	-0.403828
H	0.69668	6.294257	-1.120978
H	1.210595	5.914014	0.518816
H	1.607127	7.491772	-0.18297
N	3.284541	3.974118	1.447314
C	-4.049821	-1.623403	-2.267906
H	-4.965703	-2.00525	-2.709603
C	0.899509	3.955897	-2.599396
H	1.203974	4.788299	-3.227263
C	3.339585	-2.611443	-2.375916
H	4.141268	-3.183035	-2.834594
C	-3.596565	3.719556	2.288356
H	-3.107045	4.293594	3.068422
C	-5.425628	3.340309	0.748657
H	-6.388331	3.63212	0.336407
C	-4.853794	4.078149	1.792479
H	-5.378906	4.937793	2.194885
C	4.523826	3.362241	3.437749
H	5.229899	3.671402	4.201019
C	3.971978	2.07744	3.459668
H	4.219555	1.361714	4.236817

Optimized geometry of triplet ***f*-Ir(dmpmp)$_3$**

Symbol	X	Y	Z
Ir	-0.041262	0.019438	0.076724
N	1.453169	2.497494	0.438779
N	2.230699	1.094197	2.010454
N	-3.013639	-0.190277	0.532732
N	-2.299121	1.099983	2.163581
N	1.420332	-2.527705	0.279131
N	-0.169249	-2.68416	1.792004
C	-0.293074	1.81192	-1.007309
C	-1.202591	2.078919	-2.03429
H	-1.850017	1.285316	-2.392524
C	-1.286498	3.348013	-2.615246
H	-1.994945	3.535741	-3.418479
C	0.450447	4.18348	-1.115133
C	0.549495	2.874979	-0.595639
C	2.813831	2.707975	0.547652
C	3.28581	1.856714	1.58964
C	1.057846	1.385887	1.261164
C	2.251786	0.219172	3.157474
H	2.096845	0.771085	4.095319
H	3.210436	-0.303566	3.217391
H	1.459484	-0.523039	3.048527
C	-1.497901	-1.055192	-1.060995
C	-1.196369	-1.803011	-2.205637
H	-0.16265	-1.934166	-2.504516
C	-2.209264	-2.34984	-2.993208
H	-1.960859	-2.922554	-3.883209
C	-3.910021	-1.381616	-1.524614
C	-2.85617	-0.919782	-0.702328

C	-4.092018	-0.020298	1.410585	H	1.752061	5.366764	-3.43991
C	-3.63769	0.844521	2.421755	H	3.349156	6.087253	-3.189537
C	-1.891324	0.432867	1.042042	C	0.355234	-3.961108	1.640607
C	-1.489008	1.949802	3.024519	C	1.351585	-3.877476	0.648234
H	-1.503251	1.565065	4.050323	C	4.265331	-3.382997	-0.829527
H	-1.885639	2.969047	3.0181	C	4.435048	-4.491888	-1.688701
H	-0.468355	1.945159	2.627354	C	5.004039	-3.296279	0.367979
C	1.558191	-0.56975	-1.057968	C	5.335621	-5.498559	-1.329281
C	2.162213	0.182346	-2.083032	C	5.89291	-4.327911	0.698428
H	1.69952	1.111235	-2.395481	C	6.062746	-5.423082	-0.142334
C	3.344835	-0.234697	-2.687715	H	5.463416	-6.353575	-1.988586
H	3.804661	0.364966	-3.468233	H	6.46377	-4.257923	1.621176
C	3.40235	-2.229275	-1.25644	H	6.762186	-6.211806	0.121528
C	2.169767	-1.815887	-0.7201	C	4.861729	-2.114365	1.300306
C	0.422652	-1.814213	0.919578	H	5.620898	-2.150515	2.086983
C	-1.282904	-2.376495	2.67377	H	4.961191	-1.160419	0.772957
H	-1.148514	-2.90282	3.622645	H	3.879549	-2.106648	1.787616
H	-2.235023	-2.678701	2.226473	C	3.612818	-4.639042	-2.94671
H	-1.297456	-1.305205	2.860852	H	3.730322	-3.790131	-3.626799
C	4.62786	1.921334	1.961472	H	3.888759	-5.547637	-3.489329
C	5.426526	2.818419	1.229428	H	2.548142	-4.703349	-2.694847
C	4.874603	3.56106	0.18617	N	2.008292	-4.911258	0.152603
H	5.036857	1.316661	2.763535	C	-6.10697	-0.246322	2.392159
H	6.479596	2.929922	1.466958	H	-7.087157	-0.716282	2.377936
H	5.500017	4.236785	-0.392052	C	-5.382774	-1.100425	-1.411267
N	3.574241	3.514458	-0.178317	C	-5.882494	0.157709	-1.807923
C	1.177304	5.391134	-0.599374	C	-6.273885	-2.132681	-1.043754
C	2.141251	6.040489	-1.40507	C	-7.267272	0.372183	-1.80482
C	0.821302	5.942323	0.650669	C	-7.649433	-1.885004	-1.062111
C	2.734577	7.219237	-0.941092	C	-8.149387	-0.638509	-1.435793
C	1.440821	7.121692	1.083847	H	-7.651285	1.342223	-2.110766
C	2.3929	7.760742	0.296073	H	-8.333951	-2.679839	-0.775474
H	3.479337	7.713204	-1.560436	H	-9.221344	-0.460125	-1.447725
H	1.159579	7.544448	2.045515	C	-4.960958	1.26844	-2.258216
H	2.862604	8.678191	0.640798	H	-4.288592	1.603108	-1.46108
C	-0.227835	5.297362	1.5282	H	-4.32355	0.945543	-3.088431
H	-1.12815	5.044532	0.95863	H	-5.535608	2.136885	-2.591869
H	0.142047	4.366435	1.971922	C	-5.764178	-3.471221	-0.56473
H	-0.51427	5.96741	2.344482	H	-5.079956	-3.938529	-1.278687
C	2.578906	5.461032	-2.729612	H	-5.212436	-3.348245	0.375014
H	2.993156	4.460113	-2.572328	H	-6.592183	-4.162247	-0.382276

N	-5.281275	-0.599482	1.39741
C	3.957376	-1.407994	-2.261879
H	4.908636	-1.71013	-2.690281
C	-3.539214	-2.11684	-2.66586
H	-4.331576	-2.480715	-3.31324
C	-0.48203	4.383704	-2.147943
H	-0.58644	5.38328	-2.560442
C	0.054356	-5.190182	2.211875
H	-0.708959	-5.304648	2.974424
C	1.715798	-6.09942	0.702996
H	2.257074	-6.950841	0.298354
C	0.776139	-6.284248	1.724348
H	0.596948	-7.279486	2.116689
C	-5.773211	0.656131	3.411663
H	-6.503419	0.896542	4.176962
C	-4.494753	1.218114	3.449798
H	-4.188311	1.894166	4.241014

Optimized geometry of singlet ***m*-Ir(dmpmp)$_3$**

Symbol	X	Y	Z
Ir	0.074415	0.008613	0.032401
N	-1.262955	-2.601332	-0.292962
N	0.315596	-2.557599	-1.831538
N	2.951864	-0.660631	0.317117
N	1.9288	-1.850078	1.865987
N	-0.876706	2.768421	0.316892
N	0.585827	2.472103	1.940546
C	-1.519698	-0.773183	1.190207
C	-2.174468	-0.146057	2.260602
H	-1.789791	0.795719	2.6443
C	-3.323881	-0.684996	2.840482
H	-3.809912	-0.180531	3.67221
C	-3.285513	-2.528652	1.234973
C	-2.065601	-2.007139	0.750993
C	-1.194599	-3.889359	-0.837994
C	-0.213939	-3.838467	-1.847584
C	-0.272365	-1.81084	-0.850577
C	1.375769	-2.120189	-2.728276
H	1.087715	-2.332813	-3.762085
H	2.311487	-2.641972	-2.501906
H	1.515647	-1.050033	-2.597799
C	1.708349	0.741663	-1.138484
C	1.640034	1.682831	-2.175334
H	0.66601	2.008463	-2.527648
C	2.790511	2.215315	-2.758298
H	2.713032	2.940315	-3.565079
C	4.192277	0.917904	-1.230185
C	3.005257	0.341946	-0.723026
C	3.870923	-1.616686	0.765281
C	3.221736	-2.342838	1.783451
C	1.726803	-0.863239	0.936425
C	0.927713	-2.380096	2.780594
H	1.303685	-2.331345	3.807622
H	0.698659	-3.422422	2.535878
H	0.022321	-1.784341	2.686572
C	-1.347077	0.977676	-1.153458
C	-2.008303	0.443535	-2.266509
H	-1.751285	-0.552744	-2.614577
C	-3.003407	1.151915	-2.93989
H	-3.500344	0.717022	-3.803593
C	-2.772331	3.003096	-1.359938
C	-1.699062	2.297483	-0.772827
C	-0.034321	1.838449	0.89878
C	1.492342	1.876709	2.90517
H	1.057573	1.926881	3.90919
H	2.449148	2.406213	2.903076
H	1.654035	0.837139	2.633896
C	0.080138	-4.978847	-2.583745
C	-0.627049	-6.131881	-2.232147
C	-1.543737	-6.09009	-1.1732
H	0.824706	-4.981125	-3.372913
H	-0.455447	-7.064773	-2.758436
H	-2.07124	-6.99168	-0.871754
N	-1.829854	-4.988079	-0.465423
C	-4.111196	-3.6477	0.664833
C	-4.25153	-4.863122	1.369846
C	-4.855892	-3.422279	-0.512314
C	-5.118328	-5.842244	0.876036
C	-5.708685	-4.430574	-0.981677
C	-5.842667	-5.634207	-0.296726
H	-5.221388	-6.779506	1.417919

H	-6.282485	-4.256078	-1.888548
H	-6.51452	-6.403387	-0.668439
C	-4.773908	-2.110455	-1.259408
H	-4.995117	-1.261028	-0.604973
H	-3.776359	-1.926269	-1.670814
H	-5.484587	-2.092833	-2.090476
C	-3.432167	-5.148205	2.60621
H	-2.366339	-5.1758	2.350622
H	-3.558554	-4.382551	3.377367
H	-3.702417	-6.115967	3.038675
C	0.226139	3.810637	1.974352
C	-0.676031	4.019599	0.913289
C	-3.436526	4.261684	-0.878438
C	-3.294734	5.466114	-1.600707
C	-4.314868	4.194271	0.223428
C	-4.020456	6.59101	-1.197817
C	-5.018532	5.344601	0.603877
C	-4.876104	6.537539	-0.098475
H	-3.907287	7.519844	-1.752016
H	-5.694594	5.293075	1.453983
H	-5.435507	7.419483	0.202524
C	-4.526741	2.904914	0.984962
H	-5.297985	3.02954	1.750529
H	-4.83583	2.09187	0.31973
H	-3.614564	2.561244	1.484353
C	-2.32394	5.574639	-2.752366
H	-2.500344	4.814779	-3.519261
H	-2.387004	6.558903	-3.225548
H	-1.296771	5.435435	-2.395116
N	-1.146579	5.201573	0.555432
C	5.730141	-2.878992	0.935295
H	6.729198	-3.09556	0.565187
C	5.60068	0.754718	-0.730035
C	6.558629	0.075925	-1.517128
C	5.998458	1.396281	0.460697
C	7.889706	0.040016	-1.092439
C	7.340538	1.33518	0.859173
C	8.284948	0.662981	0.090577
H	8.623635	-0.486518	-1.69781
H	7.643039	1.83392	1.776896
H	9.324525	0.630559	0.40552
C	6.156518	-0.663819	-2.770927
H	5.442282	-1.457896	-2.524654
H	5.672151	-0.01217	-3.503969
H	7.026434	-1.124936	-3.247524
C	5.006881	2.150422	1.317106
H	4.367309	2.803374	0.715392
H	4.344885	1.462318	1.856336
H	5.523589	2.763128	2.061784
N	5.083071	-1.88526	0.308777
C	-3.39462	2.398652	-2.468702
H	-4.221776	2.92494	-2.935916
C	4.041648	1.849263	-2.275448
H	4.938691	2.308824	-2.68026
C	-3.88041	-1.843226	2.311672
H	-4.819167	-2.225498	2.701491
C	0.615276	4.877807	2.772308
H	1.302389	4.758711	3.603659
C	-0.766086	6.234715	1.320448
H	-1.158261	7.205145	1.026561
C	0.084061	6.124302	2.427888
H	0.341116	7.009382	2.999964
C	5.195291	-3.624422	1.99396
H	5.786918	-4.410475	2.450917
C	3.893443	-3.369023	2.435102
H	3.432632	-3.950747	3.226708

Optimized geometry of triplet ***m*-Ir(dmpmp)$_3$**

Symbol	X	Y	Z
Ir	0.277213	0.114182	0.044188
N	-1.289878	-2.342516	0.289051
N	-2.096631	-1.014845	1.853371
N	-2.344906	1.629317	-0.342159
N	-2.578343	-0.042502	-1.771678
N	2.992569	1.154288	-0.269109
N	1.837338	2.04072	-1.92172
C	0.367213	-1.53213	-1.205811
C	1.219754	-1.700899	-2.308554
H	1.76797	-0.847808	-2.696868
C	1.397795	-2.952261	-2.893985
H	2.069822	-3.075549	-3.739051

C	-0.13131	-3.958744	-1.258518
C	-0.380346	-2.66205	-0.76505
C	-2.467636	-2.942266	0.75081
C	-2.951794	-2.105145	1.774916
C	-1.116411	-1.111145	0.908368
C	-2.292077	0.078685	2.797707
H	-2.395781	-0.332623	3.806552
H	-3.19068	0.64784	2.538609
H	-1.429049	0.73854	2.75603
C	-0.349925	1.997876	0.881948
C	0.451972	2.79516	1.70763
H	1.42671	2.437644	2.023611
C	0.006124	4.043938	2.152822
H	0.63109	4.641594	2.811813
C	-2.055381	3.794202	0.867811
C	-1.613903	2.503485	0.502432
C	-3.690548	1.282429	-0.332046
C	-3.837542	0.249861	-1.290117
C	-1.595763	0.762761	-1.171613
C	-2.365729	-0.906076	-2.916917
H	-2.900085	-0.516576	-3.793348
H	-2.724525	-1.920959	-2.713815
H	-1.301627	-0.952269	-3.136367
C	1.846827	-0.185551	1.316931
C	1.823005	-0.955501	2.493286
H	0.872762	-1.32317	2.86702
C	2.996148	-1.277873	3.171316
H	2.963956	-1.874054	4.079224
C	4.324307	-0.102411	1.47194
C	3.114595	0.30399	0.881648
C	1.75069	1.174022	-0.879666
C	0.768641	2.351302	-2.861739
H	1.05312	2.030702	-3.869426
H	0.583435	3.429019	-2.865995
H	-0.133696	1.825609	-2.533468
C	-4.120036	-2.445153	2.444116
C	-4.749652	-3.618919	2.014261
C	-4.210232	-4.35291	0.952837
H	-4.533332	-1.830235	3.236137
H	-5.668641	-3.95197	2.484609
H	-4.713994	-5.247668	0.596117
N	-3.078431	-4.025885	0.304822
C	-0.59396	-5.256436	-0.66135
C	-1.510905	-6.078149	-1.353576
C	-0.006904	-5.704493	0.541409
C	-1.834766	-7.33075	-0.823951
C	-0.364488	-6.96207	1.045363
C	-1.270892	-7.773903	0.370928
H	-2.543874	-7.961287	-1.354691
H	0.08916	-7.30744	1.970999
H	-1.532126	-8.750416	0.769693
C	1.019045	-4.87564	1.283056
H	1.845521	-4.577567	0.629479
H	0.593566	-3.951075	1.688081
H	1.437226	-5.440961	2.120391
C	-2.2005	-5.601782	-2.609753
H	-2.852714	-4.753188	-2.372608
H	-1.496646	-5.2668	-3.376998
H	-2.818377	-6.395036	-3.040118
C	3.088955	2.642737	-1.944223
C	3.823012	2.112646	-0.865329
C	5.712646	0.071809	0.927577
C	6.633003	0.924851	1.574432
C	6.123809	-0.722909	-0.163539
C	7.949988	0.980209	1.10897
C	7.449796	-0.632811	-0.607056
C	8.360488	0.210628	0.021795
H	8.658169	1.64012	1.604096
H	7.768367	-1.245061	-1.447025
H	9.388046	0.263022	-0.327915
C	5.175493	-1.683172	-0.847366
H	5.707281	-2.2925	-1.583414
H	4.698396	-2.358837	-0.12989
H	4.365249	-1.164858	-1.37213
C	6.202419	1.823526	2.709017
H	5.735859	1.270146	3.529517
H	7.055103	2.375096	3.114874
H	5.465268	2.551905	2.351982
N	5.022333	2.525367	-0.494445
C	-5.890765	1.250161	0.180737
H	-6.696646	1.649434	0.79165
C	-3.27663	4.484843	0.333673

C	-4.357025	4.79521	1.191439
C	-3.297864	4.923969	-1.008334
C	-5.43911	5.525411	0.688897
C	-4.401858	5.647571	-1.476924
C	-5.469703	5.948687	-0.637586
H	-6.270526	5.757301	1.350005
H	-4.411472	5.985884	-2.510251
H	-6.317864	6.515411	-1.012316
C	-4.395062	4.309866	2.621314
H	-4.41109	3.214978	2.632363
H	-3.524713	4.632835	3.19978
H	-5.292599	4.673889	3.129978
C	-2.144562	4.652982	-1.948284
H	-1.18698	4.930193	-1.494385
H	-2.078956	3.591526	-2.210922
H	-2.261187	5.221778	-2.87554
N	-4.658193	1.759982	0.435832
C	4.221524	-0.879596	2.645238
H	5.144439	-1.197377	3.12145
C	-1.220778	4.53687	1.722068
H	-1.538293	5.534495	2.01173
C	0.751557	-4.061635	-2.351283
H	0.950584	-5.051961	-2.750029
C	3.656147	3.622986	-2.747151
H	3.128678	4.055176	-3.590935
C	5.567754	3.476627	-1.267197
H	6.556677	3.814728	-0.968226
C	4.943115	4.035212	-2.389727
H	5.455354	4.798978	-2.964916
C	-6.155946	0.289545	-0.787399
H	-7.1749	-0.05284	-0.937422
C	-5.105657	-0.25452	-1.556547
H	-5.278782	-1.030221	-2.294539

Optimized geometry of singlet ***f*-Ir(pmp)$_3$**

Symbol	X	Y	Z
Ir	-0.003151	0.015527	0.19521
C	1.421139	1.05274	1.361535
C	1.706711	2.365127	0.931909
C	2.127896	0.622981	2.494155
C	2.620712	3.216401	1.556771
C	3.048935	1.449693	3.14742
H	1.949152	-0.375266	2.881944
C	3.296806	2.742038	2.681733
H	2.787771	4.217501	1.17863
H	3.572772	1.081777	4.026484
H	4.011263	3.384072	3.189284
C	0.833778	3.983932	-0.869827
C	0.100563	1.828057	-0.766127
C	-0.136819	3.796069	-1.876902
C	-0.478574	4.858599	-2.701352
C	1.148516	6.139111	-1.43758
C	0.195359	6.061656	-2.460239
H	-1.226139	4.771543	-3.483125
H	1.670651	7.074808	-1.253233
H	-0.017923	6.939337	-3.060895
C	-1.627804	0.835232	1.273255
C	-1.620907	1.76866	2.319946
C	-2.902088	0.381861	0.874701
C	-2.80411	2.211261	2.922252
H	-0.671236	2.151917	2.680828
C	-4.102694	0.802974	1.450707
C	-4.041969	1.732246	2.490136
H	-2.756856	2.931614	3.735512
H	-5.048849	0.408475	1.101044
H	-4.960416	2.075131	2.958279
C	-3.84851	-1.352754	-0.775976
C	-1.617868	-0.890045	-0.701524
C	-3.191143	-2.185429	-1.706575
C	-3.931693	-3.089043	-2.455482
C	-5.865084	-2.217104	-1.278445
C	-5.311764	-3.091805	-2.221469
H	-3.474969	-3.760659	-3.17516
H	-6.937494	-2.221309	-1.099378
H	-5.958709	-3.771436	-2.765665
C	0.083279	-1.693117	1.438536
C	-0.732367	-2.049394	2.522396
C	1.106266	-2.611204	1.12361
C	-0.535435	-3.237514	3.235408
H	-1.533076	-1.381143	2.824501
C	1.33	-3.806511	1.810314

C	0.4904	-4.115411	2.881416
H	-1.186155	-3.475812	4.073446
H	2.139104	-4.465283	1.51973
H	0.643109	-5.037657	3.434957
C	3.086773	-2.729513	-0.517208
C	1.589724	-1.012083	-0.597974
C	3.494861	-1.832052	-1.526762
C	4.648485	-2.098107	-2.250599
C	4.82991	-4.1023	-0.896418
C	5.32559	-3.275463	-1.911787
H	5.01327	-1.435063	-3.028408
H	5.357752	-5.016469	-0.636004
H	6.23714	-3.55227	-2.430498
C	2.652317	0.345851	-2.430301
H	2.924631	0.022318	-3.439443
H	3.404378	1.051988	-2.063942
H	1.683793	0.839814	-2.458662
C	-0.814547	-2.544946	-2.415036
H	-0.57712	-3.520342	-1.978459
H	0.081094	-1.927657	-2.415835
H	-1.159858	-2.685041	-3.443568
C	-1.589221	1.898356	-2.627548
H	-1.554677	0.816134	-2.523603
H	-1.416589	2.170273	-3.673459
H	-2.577661	2.255957	-2.321509
N	-0.549273	2.472457	-1.791826
N	0.950048	2.76268	-0.215388
N	1.483634	5.116137	-0.633944
N	-2.856326	-0.57838	-0.184842
N	-1.840888	-1.865581	-1.643669
N	-5.155382	-1.341291	-0.548016
N	3.715689	-3.850716	-0.189498
N	1.923191	-2.195009	0.024909
N	2.555037	-0.809763	-1.555709

Optimized geometry of triplet ***f*-Ir(pmp)$_3$**

Symbol	X	Y	Z
Ir	-0.008323	-0.016026	0.405547
C	-1.401516	1.029472	1.499977
C	-2.758111	0.864347	1.075465
C	-1.198501	1.890932	2.602069
C	-3.840796	1.481533	1.706235
C	-2.263713	2.509807	3.246467
H	-0.190249	2.050682	2.967128
C	-3.582337	2.305182	2.799582
H	-4.845902	1.311949	1.34039
H	-2.07855	3.149373	4.105341
H	-4.410626	2.79045	3.307507
C	-4.08338	-0.413347	-0.692756
C	-1.786915	-0.53997	-0.601897
C	-3.648751	-1.29244	-1.693134
C	-4.595577	-1.920261	-2.532036
C	-6.260425	-0.673316	-1.249223
C	-5.940327	-1.565179	-2.268837
H	-4.322756	-2.622022	-3.311726
H	-7.30003	-0.415316	-1.063075
H	-6.739878	-1.995187	-2.864296
C	-0.221555	-1.803335	1.457639
C	-1.08887	-2.109861	2.51992
C	0.622999	-2.850157	1.039694
C	-1.086497	-3.365521	3.134555
H	-1.760218	-1.341662	2.888256
C	0.64332	-4.117096	1.62647
C	-0.225226	-4.365854	2.689803
H	-1.755657	-3.560396	3.968542
H	1.317483	-4.881869	1.262003
H	-0.223608	-5.341296	3.167274
C	2.471389	-3.245021	-0.725225
C	1.390916	-1.259745	-0.592539
C	3.002433	-2.391307	-1.694902
C	4.031245	-2.84141	-2.527734
C	3.823348	-4.926725	-1.310327
C	4.433404	-4.150063	-2.313288
H	4.48903	-2.217074	-3.287316
H	4.14277	-5.952372	-1.148142
H	5.224307	-4.583815	-2.915758
C	1.618243	0.671273	1.517606
C	2.282974	0.058641	2.595781
C	2.121606	1.94284	1.107866
C	3.348614	0.683058	3.248247
H	1.938555	-0.907918	2.948107

C	3.197592	2.581444	1.746421
C	3.80299	1.941345	2.822388
H	3.823613	0.195527	4.095871
H	3.534183	3.54851	1.395134
H	4.632187	2.423205	3.332658
C	1.641042	3.722078	-0.673295
C	0.411705	1.791946	-0.582322
C	0.662884	3.760666	-1.689264
C	0.576737	4.889863	-2.531768
C	2.457612	5.750588	-1.239794
C	1.523499	5.896119	-2.265791
H	-0.165569	4.985333	-3.3157
H	3.181065	6.539714	-1.051047
H	1.530903	6.804024	-2.861071
C	-1.193284	2.267617	-2.451495
H	-0.966709	2.534103	-3.488317
H	-2.082932	2.820645	-2.130163
H	-1.397225	1.198766	-2.383207
C	2.619316	-0.008533	-2.397791
H	3.54016	0.461563	-2.036891
H	1.810646	0.704811	-2.336645
H	2.75075	-0.306328	-3.436477
C	-1.451978	-2.212186	-2.459105
H	-0.421238	-1.889026	-2.435767
H	-1.812244	-2.1655	-3.485926
H	-1.511101	-3.24895	-2.106811
N	-2.257159	-1.339934	-1.616253
N	-2.924277	0.02918	-0.047082
N	-5.346179	-0.069598	-0.425983
N	1.476232	-2.507351	-0.069856
N	2.305705	-1.188069	-1.584868
N	2.84353	-4.491803	-0.505492
N	2.544424	4.66491	-0.416384
N	1.464269	2.500536	-0.013122
N	-0.053248	2.576343	-1.607951

Optimized geometry of singlet ***m*-Ir(pmp)$_3$**

Symbol	X	Y	Z
Ir	-0.088011	-0.204887	-0.055476
N	2.451999	-1.545133	0.534506
N	2.772776	-0.617162	-1.429316
N	0.363078	2.693013	-0.404077
N	1.15904	2.275857	1.599365
N	-2.85774	-1.12982	-0.091503
N	-2.929094	0.759155	1.021701
C	0.387624	-1.330462	1.680074
C	-0.399856	-1.643614	2.801098
H	-1.416781	-1.261342	2.862365
C	0.076457	-2.436666	3.851583
H	-0.568995	-2.654887	4.699401
C	1.685393	-1.88456	1.692683
C	3.745509	-1.883808	0.152789
C	3.946447	-1.285509	-1.107671
C	1.848567	-0.764667	-0.429357
C	2.594074	0.116389	-2.674857
H	2.848434	-0.530909	-3.519622
H	3.241569	0.999337	-2.693073
H	1.554462	0.423645	-2.755893
C	-0.51655	0.970657	-1.789555
C	-1.108554	0.595136	-3.007224
H	-1.355623	-0.450336	-3.17141
C	-1.38221	1.523453	-4.018642
H	-1.836769	1.189757	-4.948673
C	-0.23558	2.347756	-1.659272
C	0.887882	3.893722	0.063999
C	1.400185	3.619629	1.349083
C	0.524497	1.689219	0.531253
C	1.561686	1.60793	2.829379
H	1.150939	2.140074	3.69362
H	2.653291	1.588847	2.911636
H	1.181521	0.588973	2.812181
C	-0.811096	-1.972398	-0.928924
C	-0.125014	-2.973979	-1.6328
H	0.950208	-2.894378	-1.771872
C	-0.778281	-4.08962	-2.168288
H	-0.205813	-4.84232	-2.705324
C	-2.200766	-2.176888	-0.805982
C	-2.077026	-0.098827	0.375024
C	-2.559083	2.009192	1.662583
H	-3.157594	2.142031	2.567768
H	-2.723603	2.860201	0.993531

H	-1.508119	1.962875	1.936206
C	5.164911	-1.445758	-1.75322
C	6.118528	-2.212852	-1.075588
C	5.816504	-2.762735	0.17708
H	5.370302	-1.005401	-2.723359
H	7.095592	-2.385727	-1.513893
H	6.560861	-3.357327	0.70111
N	4.641179	-2.611249	0.808491
C	-4.236085	0.294141	0.944815
C	-4.192665	-0.924198	0.235414
N	-5.240882	-1.688657	-0.041336
C	1.503231	6.056618	0.174293
H	1.539198	7.031164	-0.306525
N	0.922308	5.076636	-0.537252
C	-2.156319	-4.243071	-2.014957
H	-2.66521	-5.109378	-2.427731
C	-1.077657	2.874119	-3.839791
H	-1.29012	3.596482	-4.622958
C	1.372222	-2.953452	3.813545
H	1.744236	-3.571458	4.625702
C	-5.45579	0.773846	1.400927
H	-5.548181	1.709692	1.942285
C	-6.416508	-1.219313	0.406471
H	-7.28557	-1.834207	0.185633
C	-6.571292	-0.02118	1.114878
H	-7.560397	0.28638	1.436854
C	2.04381	5.890409	1.455734
H	2.495915	6.737844	1.959814
C	1.999717	4.637789	2.077834
H	2.412138	4.476841	3.068532
C	-2.887219	-3.27578	-1.323691
H	-3.957912	-3.366957	-1.188825
C	-0.49787	3.303181	-2.644465
H	-0.252428	4.34543	-2.481195
C	2.196321	-2.679535	2.720219
H	3.20379	-3.073038	2.662526

Optimized geometry of triplet ***m*-Ir(pmp)$_3$**

Symbol	X	Y	Z
Ir	0.030158	-0.30384	0.087857
N	-2.62143	-1.346441	-0.559803
N	-2.876191	-0.50913	1.449952
N	-0.055663	2.680342	0.500203
N	-0.992066	2.443895	-1.465363
N	2.746972	-1.380342	0.014423
N	2.942927	0.538103	-1.024087
C	-0.572187	-1.09756	-1.744209
C	0.175263	-1.302284	-2.918335
H	1.195329	-0.931084	-2.969526
C	-0.356177	-1.976776	-4.018522
H	0.251797	-2.135036	-4.905219
C	-1.906018	-1.589205	-1.756716
C	-3.954595	-1.572712	-0.214873
C	-4.109538	-1.032782	1.075351
C	-1.953516	-0.694037	0.460756
C	-2.643686	0.152208	2.725646
H	-2.923313	-0.516115	3.546249
H	-3.243412	1.065656	2.791308
H	-1.588316	0.404279	2.803104
C	0.604938	0.831324	1.831679
C	1.15045	0.338029	3.027356
H	1.266587	-0.73266	3.162788
C	1.534375	1.195325	4.066058
H	1.943889	0.777634	4.982569
C	0.491913	2.230254	1.731409
C	-0.363198	3.967467	0.061623
C	-0.966268	3.806177	-1.197973
C	-0.428579	1.730181	-0.429945
C	-1.612067	1.918163	-2.670516
H	-1.177422	2.40166	-3.551684
H	-2.689376	2.116377	-2.659213
H	-1.441035	0.848074	-2.72937
C	0.655647	-2.057539	0.911548
C	-0.09329	-3.0159	1.632088
H	-1.147033	-2.833107	1.817378
C	0.479375	-4.190633	2.108946
H	-0.127131	-4.911711	2.649757
C	2.038921	-2.364969	0.729225
C	2.035857	-0.267912	-0.396917
C	2.666549	1.8406	-1.607927
H	3.260241	1.959331	-2.5183

H	2.913647	2.646287	-0.909473
H	1.608643	1.893925	-1.856604
C	-5.353592	-1.096956	1.702298
C	-6.36862	-1.719082	0.95433
C	-6.106539	-2.221244	-0.320492
H	-5.532258	-0.69397	2.692686
H	-7.368592	-1.810919	1.365562
H	-6.900761	-2.697685	-0.889461
N	-4.901318	-2.164128	-0.935247
C	4.212367	-0.034159	-0.996645
C	4.092355	-1.271513	-0.337389
N	5.072687	-2.13788	-0.110771
C	-0.58967	6.208233	-0.002563
H	-0.433966	7.16645	0.486996
N	-0.154739	5.124398	0.687364
C	1.841087	-4.447678	1.892338
H	2.288016	-5.363182	2.269225
C	1.394388	2.576119	3.927796
H	1.693202	3.242953	4.731635
C	-1.671627	-2.452819	-3.980237
H	-2.088896	-2.971243	-4.838731
C	5.460573	0.373854	-1.464889
H	5.619713	1.323128	-1.963482
C	6.28056	-1.736984	-0.573252
H	7.102321	-2.426352	-0.397678
C	6.512281	-0.530702	-1.233374
H	7.517485	-0.291125	-1.564378
C	-1.203465	6.159208	-1.252163
H	-1.521927	7.083489	-1.723546
C	-1.415344	4.926591	-1.900633
H	-1.897785	4.85887	-2.868782
C	2.635486	-3.534742	1.1967
H	3.688736	-3.714467	1.019567
C	0.869092	3.110194	2.750442
H	0.74974	4.177697	2.613024
C	-2.461316	-2.2653	-2.843729
H	-3.481677	-2.625829	-2.793838