

Supporting Information

Quantitative calculations of the non-radiative rate of phosphorescent iridium(III) complexes

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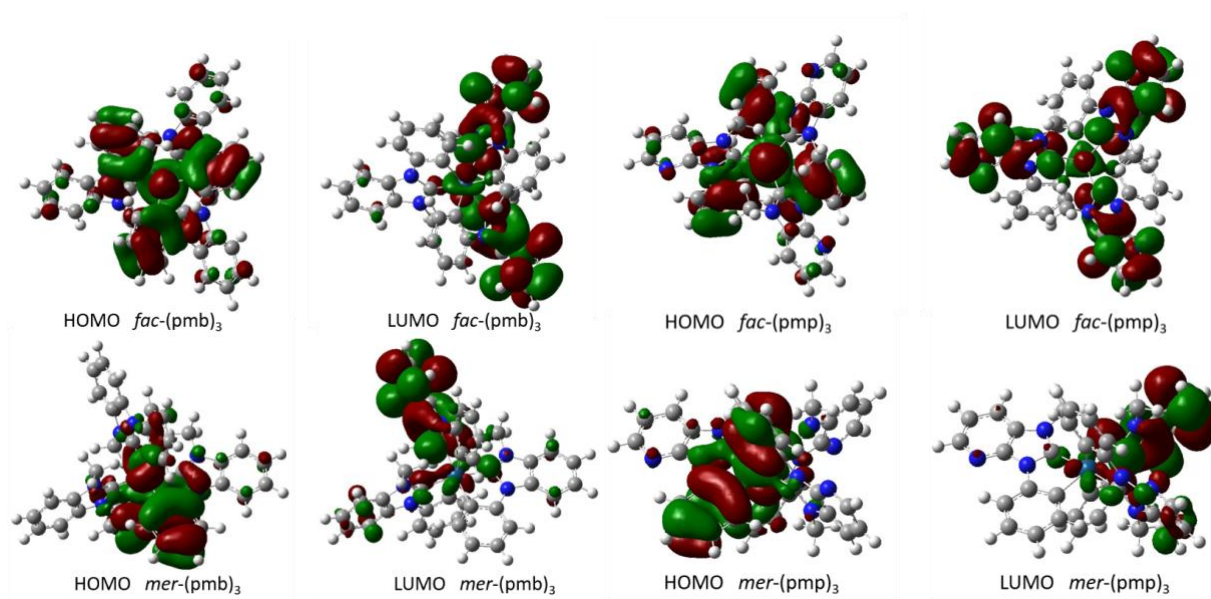
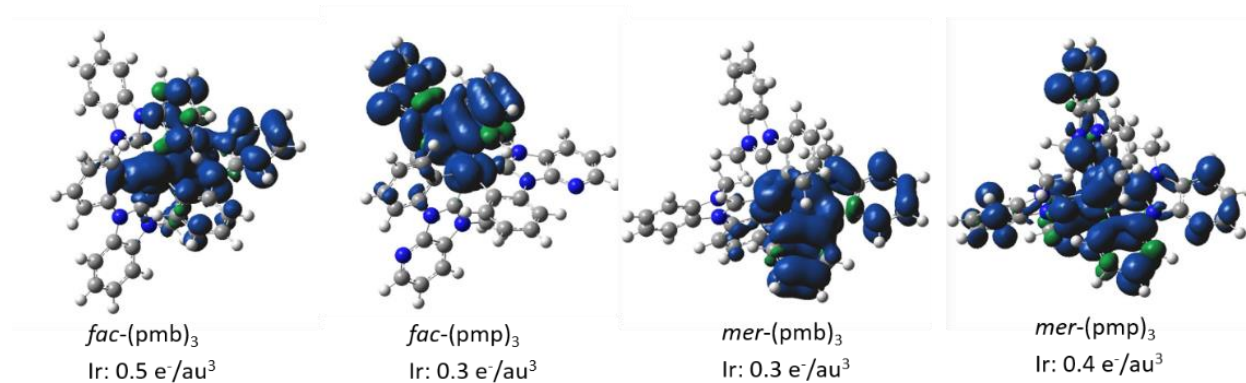


Figure S1: Frontier molecular orbitals (HOMO and LUMO) of the four investigated complexes in their optimized ground state geometries.

Triplet spin density of the optimized ³MLCT state and Mulliken spin density on Ir atom



Triplet spin density of the optimized ³MC state and Mulliken spin density on Ir atom

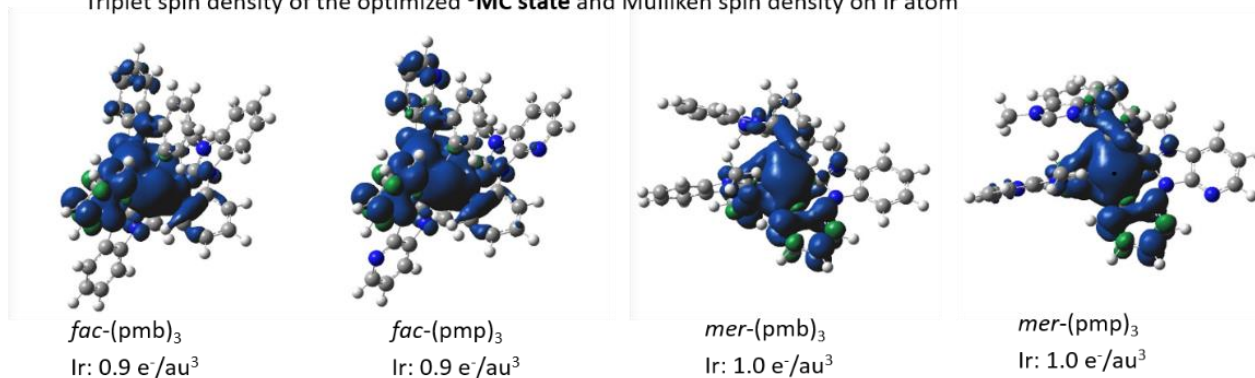


Figure S2: Triplet spin density of the optimized ³MLCT state and ³MC state.

Table S1. Cartesian coordinates of the optimized singlet ground-state geometry of the four complexes studied in this work.

<i>fac</i> -Ir(pmb) ₃			
82			
Ir	0.00314	0.00000	0.29215
C	0.51098	1.69562	1.43554
C	1.07688	4.19020	2.68632
C	1.40928	1.79819	2.50782
C	-0.10922	2.90081	1.03797
C	0.17275	4.13714	1.62397
C	1.68480	3.01825	3.13443
H	1.90535	0.90075	2.86507
H	-0.26978	5.05517	1.26066
H	2.38308	3.05342	3.96712
H	1.30156	5.14526	3.15256
C	-0.72838	-1.71048	-0.59445
C	-1.16510	-3.70406	-1.59794
N	-0.33546	-2.58508	-1.56956
N	-1.85039	-2.27119	-0.02212
C	-2.14057	-3.51260	-0.59925
C	-1.11377	1.48379	-0.60484
C	-2.63608	2.84850	-1.60132
N	-1.03902	2.73821	-0.03818
N	-2.07471	1.57353	-1.57387
C	-1.97890	3.60335	-0.60949
C	-1.71490	-0.40273	1.44424
C	-4.14863	-1.15727	2.71450
C	-2.44950	-1.54514	1.05644
C	-2.24714	0.32903	2.51599
C	-3.43745	-0.04052	3.15140
C	-3.65597	-1.91883	1.65328
H	-1.71659	1.20981	2.86553
H	-3.81338	0.55081	3.98279
H	-4.22912	-2.76581	1.30033
H	-5.08417	-1.43988	3.18874
C	1.84672	0.21870	-0.60251
C	3.78808	0.83839	-1.61165
N	2.40363	0.99269	-1.58266
N	2.89590	-0.46671	-0.02829
C	4.11435	-0.09521	-0.60781
C	1.21542	-1.27846	1.44768
C	3.09266	-3.00155	2.71839
C	2.57083	-1.34404	1.05502
C	0.85328	-2.10057	2.52479
C	1.77191	-2.94239	3.16094
C	3.50060	-2.19908	1.65135
H	-0.17331	-2.08178	2.87792
H	1.45164	-3.55967	3.99676
H	4.51866	-2.27449	1.29288
H	3.80752	-3.66809	3.19243
C	0.82769	-2.43558	-2.42478
H	1.62290	-3.12597	-2.12509
H	1.18955	-1.41415	-2.33688
H	0.55318	-2.63795	-3.46484
C	1.68803	1.91696	-2.44307
H	0.62262	1.72410	-2.34352
H	1.99120	1.76731	-3.48414
H	1.89416	2.95363	-2.15727
C	-2.53103	0.48556	-2.41933
H	-3.51812	0.13355	-2.10217
H	-1.81888	-0.33221	-2.34229
H	-2.58934	0.82194	-3.45920
C	-3.65246	3.37920	-2.39146
H	-4.15315	2.78096	-3.14538
C	-2.36061	4.92800	-0.37729
H	-1.91182	5.52906	0.40038
C	-4.01429	4.70749	-2.16395
H	-4.80413	5.15627	-2.75811
C	-3.37976	5.46275	-1.16812
H	-3.68998	6.48918	-0.99833
C	5.45252	-0.42633	-0.37535
H	5.75013	-1.10575	0.41038
C	4.75436	1.44015	-2.41357
H	4.48534	2.16231	-3.17726
C	6.42382	0.17609	-1.17782
H	7.46791	-0.06833	-1.00817
C	6.08566	1.09003	-2.18533

H	6.86825	1.53959	-2.78843
C	-3.10304	-4.50032	-0.37000
H	-3.84496	-4.41240	0.41060
C	-1.12826	-4.84425	-2.39629
H	-0.36477	-4.97822	-3.15535
C	-3.06872	-5.64481	-1.16947
H	-3.80780	-6.42225	-1.00220
C	-2.10329	-5.81663	-2.17103
H	-2.10642	-6.72069	-2.77182

mer-Ir(pmb)₃

82			
Ir	0.12201	-0.20198	0.07106
C	2.10777	0.03496	-0.34117
C	4.23222	0.54941	-0.95128
N	2.96248	-0.92915	0.14473
C	4.28578	-0.64943	-0.21391
N	2.89244	0.92609	-1.01367
C	-0.63312	1.63714	-0.53670
C	-1.73343	3.45287	-1.35349
N	-1.32322	2.14538	-1.60217
N	-0.57947	2.65955	0.39065
C	-1.26935	3.78839	-0.06646
C	0.44856	1.02669	1.78808
C	1.01767	3.01173	3.75600
C	0.08841	2.38410	1.62727
C	1.08860	0.71252	2.99869
C	1.35831	1.67732	3.97572
C	0.38229	3.37573	2.56702
H	1.38791	-0.31612	3.18084
H	1.85013	1.38865	4.90165
H	0.16401	4.41976	2.38259
H	1.24858	3.77263	4.49609
C	-1.78252	-0.88928	0.40481
C	-3.87534	-1.49662	1.03417
N	-2.74092	-0.76036	1.36555
N	-2.31311	-1.73743	-0.54694
C	-3.61207	-2.12592	-0.19801
C	-0.23228	-1.39189	-1.64195
C	-0.97095	-3.19556	-3.72491
C	-1.47730	-2.06158	-1.66249
C	0.61680	-1.66845	-2.72657
C	0.26200	-2.54655	-3.75636
C	-1.85127	-2.95556	-2.66763
H	1.59136	-1.18769	-2.77212
H	0.95264	-2.73054	-4.57591
H	-2.79368	-3.48512	-2.64156
H	-1.25281	-3.89074	-4.51037
C	-1.63576	1.43601	-2.83331
H	-2.71638	1.28223	-2.92150
H	-1.13233	0.47216	-2.81647
H	-1.29124	2.01710	-3.69491
C	-2.64419	0.02399	2.58720
H	-1.63704	0.42406	2.66997
H	-2.85328	-0.61426	3.45125
H	-3.36849	0.84528	2.56893
C	-4.59604	-2.92114	-0.79448
H	-4.44927	-3.40695	-1.74812
C	-5.08705	-1.64297	1.70507
H	-5.26954	-1.14803	2.65290
C	-5.81184	-3.06969	-0.12462
H	-6.58515	-3.68452	-0.57478
C	-6.05753	-2.44611	1.10691
H	-7.01506	-2.58566	1.59881
C	-1.58016	5.03654	0.48236
H	-1.28429	5.31412	1.48396
C	-2.47343	4.33800	-2.13395
H	-2.82281	4.06151	-3.12305
C	-2.32440	5.92472	-0.29675
H	-2.57524	6.89795	0.11382
C	-2.75912	5.58912	-1.58701
H	-3.33401	6.30679	-2.16388
C	5.51647	-1.27905	-0.00428
H	5.60765	-2.20548	0.54357
C	5.36988	1.15515	-1.47829
H	5.30892	2.08382	-2.03568
C	6.59319	0.52217	-1.25815
H	7.50327	0.96361	-1.65201

C	6.65883	-0.67627	-0.53427
H	7.62166	-1.15292	-0.37806
C	2.44493	2.12470	-1.69882
H	2.73104	3.02204	-1.14018
H	1.36373	2.08753	-1.79393
H	2.89274	2.16691	-2.69622
C	2.36481	-1.99522	0.88728
C	1.03264	-3.96254	2.29727
C	0.95961	-1.88799	0.98481
C	3.09643	-3.03107	1.46998
C	2.41965	-4.02361	2.18104
C	0.32534	-2.90979	1.70755
H	4.17349	-3.08453	1.39296
H	2.98035	-4.83441	2.63698
H	-0.75542	-2.89181	1.81996
H	0.49837	-4.73318	2.84762

fac-Ir(pmp)₃
79

Ir	0.00101	-0.00030	0.27604
C	0.51404	1.68843	1.43842
C	0.98062	4.16626	2.76443
C	1.38871	1.78488	2.53067
C	-0.10795	2.89383	1.05324
C	0.10121	4.12338	1.68162
C	1.61973	2.99934	3.18671
H	1.89347	0.89122	2.88484
H	-0.41469	5.01169	1.33828
H	2.30081	3.03181	4.03381
H	1.15967	5.10895	3.27385
C	-0.73466	-1.70528	-0.60813
C	-1.20690	-3.67954	-1.62921
N	-0.34674	-2.58968	-1.58602
N	-1.87101	-2.24363	-0.04572
C	-2.19390	-3.45607	-0.64547
C	-1.10828	1.48709	-0.61178
C	-2.58507	2.88212	-1.63005
N	-1.00476	2.74103	-0.05116
N	-2.07084	1.59228	-1.58741
C	-1.89501	3.62610	-0.64924
C	-1.71910	-0.39894	1.43949
C	-4.09860	-1.23018	2.76689
C	-2.45118	-1.54212	1.05804
C	-2.24112	0.31451	2.52843
C	-3.40884	-0.09081	3.18487
C	-3.62062	-1.97432	1.68726
H	-1.72047	1.20051	2.87930
H	-3.77889	0.48598	4.02918
H	-4.13071	-2.86713	1.34687
H	-5.00468	-1.54504	3.27692
C	1.84359	0.21470	-0.61093
C	3.78857	0.79171	-1.63464
N	2.41432	0.98999	-1.59206
N	2.87930	-0.49649	-0.04584
C	4.09003	-0.17048	-0.64722
C	1.20763	-1.28529	1.44235
C	3.12039	-2.92429	2.77323
C	2.56350	-1.34704	1.06034
C	0.85269	-2.09205	2.53341
C	1.78896	-2.89755	3.19167
C	3.52400	-2.14055	1.69127
H	-0.17487	-2.08580	2.88418
H	1.47550	-3.50494	4.03744
H	4.55191	-2.13600	1.34992
H	3.84721	-3.54937	3.28435
C	0.84203	-2.46730	-2.41141
H	1.64599	-3.11010	-2.03864
H	1.17288	-1.43150	-2.38405
H	0.60622	-2.74750	-3.44244
C	1.71318	1.95295	-2.42332
H	0.65033	1.72347	-2.39330
H	2.07222	1.88102	-3.45441
H	1.86997	2.97321	-2.05857
C	-2.56418	0.50090	-2.40929
H	-3.51683	0.12162	-2.02576
H	-1.83002	-0.30166	-2.39418
H	-2.70294	0.84752	-3.43769
C	-3.55972	3.50445	-2.39719

H	-4.12836	2.97638	-3.15574
N	-2.08627	4.91261	-0.38812
C	-3.77592	4.86112	-2.12910
H	-4.52290	5.41747	-2.68505
C	-3.02940	5.50795	-1.13654
H	-3.19979	6.56191	-0.93111
N	5.30069	-0.64481	-0.38433
C	4.81308	1.32057	-2.40685
H	4.63780	2.07153	-3.17031
C	6.28627	-0.12977	-1.13773
H	7.28492	-0.50667	-0.93111
C	6.09707	0.83309	-2.13676
H	6.95126	1.19902	-2.69625
N	-3.21182	-4.26563	-0.38396
C	-1.26006	-4.83273	-2.39913
H	-0.52009	-5.05889	-3.15996
C	-3.25734	-5.37828	-1.13507
H	-4.08453	-6.05326	-0.92962
C	-2.32621	-5.69904	-2.13067
H	-2.43588	-6.62268	-2.68872

mer-Ir(pmp)₃

79			
H	1.83406	1.18919	4.94971
H	1.28789	3.59598	4.62394
C	1.38014	1.52303	4.01942
C	1.07585	2.87374	3.84054
H	-2.85031	-0.52875	3.51894
H	1.35388	-0.45067	3.17193
C	1.10704	0.59485	3.00772
H	-1.55536	0.42458	2.75548
H	-5.37107	-1.00470	2.72228
C	0.49688	3.30303	2.64489
H	0.20523	-4.84198	2.70559
H	0.25166	4.34533	2.48159
C	-2.59504	0.11776	2.67387
H	2.66468	-5.10906	2.42855
H	-3.24213	1.00103	2.69098
C	0.77780	-4.08933	2.16860
C	2.15587	-4.24279	2.01558
H	-7.09586	-2.38561	1.51293
C	-5.16535	-1.44536	1.75236
C	0.51584	0.97060	1.78973
C	0.23512	2.34775	1.65943
H	-0.95060	-2.89412	1.77171
C	0.12465	-2.97373	1.63287
H	3.95765	-3.36675	1.18978
C	2.88693	-3.27556	1.32439
C	-6.11872	-2.21280	1.07478
N	-2.77319	-0.61665	1.42877
C	-3.94673	-1.28518	1.10706
C	0.81089	-1.97223	0.92904
N	-0.92189	5.07685	0.53690
C	2.20059	-2.17673	0.80641
H	-1.53843	7.03147	0.30594
N	-0.36287	2.69318	0.40393
C	-1.84869	-0.76438	0.42905
C	-1.50249	6.05689	-0.17482
C	-0.88742	3.89392	-0.06431
C	-5.81632	-2.76311	-0.17762
N	2.85771	-1.12973	0.09199
N	5.24083	-1.68866	0.04226
Ir	0.08804	-0.20469	0.05536
H	7.28555	-1.83431	-0.18437
C	-3.74542	-1.88391	-0.15315
C	4.19265	-0.92428	-0.23485
H	-6.56050	-3.35794	-0.70163
C	6.41652	-1.21945	-0.40547
C	2.07708	-0.09876	-0.37483
C	-0.52413	1.68940	-0.53143
N	-2.45188	-1.54526	-0.53468
N	-4.64087	-2.61170	-0.80877
H	2.72402	2.86010	-0.99477
C	4.23624	0.29390	-0.94454
N	2.92928	0.75902	-1.02157
C	6.57146	-0.02150	-1.11413
C	-2.04277	5.89072	-1.45639

C	-1.39944	3.61986	-1.34953
H	7.56062	0.28596	-1.43603
C	5.45601	0.77350	-1.40051
N	-1.15834	2.27607	-1.59973
H	-2.49463	6.73820	-1.96062
C	2.55937	2.00867	-1.66325
C	-0.38733	-1.33078	-1.67995
C	-1.68503	-1.88505	-1.69259
C	-1.99870	4.63807	-2.07844
H	5.54848	1.70921	-1.94210
H	1.50839	1.96231	-1.93679
H	3.15785	2.14087	-2.56855
H	-3.20303	-3.07415	-2.66228
H	1.41727	-1.26183	-2.86197
C	-2.19562	-2.68051	-2.71992
C	0.40039	-1.64423	-2.80073
H	-2.41086	4.47714	-3.06925
C	-1.56098	1.60796	-2.82964
H	-1.18139	0.58879	-2.81196
H	-2.65258	1.58943	-2.91217
H	-1.14973	2.13955	-3.69397
C	-1.37127	-2.95474	-3.81298
C	-0.07558	-2.43777	-3.85100
H	-1.74307	-3.57312	-4.62495
H	0.57006	-2.65618	-4.69861

Table S2. Cartesian coordinates of the optimized ³MLCT state geometry denoted in Figure 4

fac-Ir(pmb)3

82

Ir	-0.02373	-0.09559	0.26439
C	0.61502	1.50684	1.36407
C	1.41688	3.92563	2.62222
C	1.52422	1.51735	2.44019
C	0.09818	2.77413	0.97491
C	0.49889	3.96903	1.56902
C	1.92105	2.70107	3.06299
H	1.92280	0.57238	2.79362
H	0.13295	4.92796	1.22838
H	2.62677	2.67084	3.88860
H	1.73057	4.85251	3.09367
C	-0.84533	-1.87852	-0.60155
C	-1.31231	-3.92522	-1.46242
N	-0.47976	-2.80957	-1.52602
N	-1.94797	-2.39859	0.03680
C	-2.25365	-3.67631	-0.44700
C	-1.07010	1.44924	-0.61902
C	-2.43165	2.94425	-1.64832
N	-0.84769	2.70229	-0.08860
N	-2.02889	1.61141	-1.57093
C	-1.67924	3.65498	-0.69206
C	-1.77492	-0.47606	1.42051
C	-4.22634	-1.10857	2.70641
C	-2.52560	-1.61671	1.08174
C	-2.29747	0.33016	2.44343
C	-3.49495	0.01422	3.09261
C	-3.74589	-1.93068	1.68655
H	-1.75475	1.21945	2.74946
H	-3.86088	0.65275	3.89282
H	-4.34038	-2.77440	1.36209
H	-5.17122	-1.34600	3.18653
C	1.65881	-0.08781	-1.00530
C	3.53605	1.15851	-1.52060
N	2.21130	0.94836	-1.80966
N	2.80905	-0.56576	-0.26938
C	3.92263	0.20824	-0.53302
C	1.23529	-1.44365	1.27873
C	3.22120	-3.16462	2.36163
C	2.56699	-1.45934	0.79093
C	0.94688	-2.32196	2.33030
C	1.92357	-3.16182	2.88039
C	3.55022	-2.31743	1.30421
H	-0.05824	-2.34104	2.74338
H	1.67064	-3.81752	3.70989

H	4.54155	-2.35260	0.86557
H	3.97457	-3.83331	2.76903
C	0.63928	-2.71744	-2.45210
H	1.32968	-3.54973	-2.28441
H	1.15206	-1.76966	-2.25812
H	0.27623	-2.75517	-3.48484
C	1.47245	1.69190	-2.79903
H	0.58296	1.12388	-3.07516
H	2.08547	1.83624	-3.69578
H	1.16033	2.67842	-2.43086
C	-2.60901	0.54980	-2.37383
H	-3.66280	0.40563	-2.11515
H	-2.06060	-0.36742	-2.17121
H	-2.53299	0.79679	-3.43769
C	-3.37898	3.56152	-2.46042
H	-3.95171	2.99746	-3.18893
C	-1.88329	5.02733	-0.52534
H	-1.34633	5.60710	0.21178
C	-3.56879	4.93382	-2.29349
H	-4.29918	5.45134	-2.90732
C	-2.83342	5.64914	-1.33851
H	-3.00562	6.71450	-1.22133
C	5.22085	0.21422	-0.01234
H	5.51530	-0.47101	0.77157
C	4.44561	2.09524	-2.01835
H	4.14818	2.82890	-2.75992
C	6.13155	1.14750	-0.52822
H	7.14814	1.15848	-0.14697
C	5.75522	2.06210	-1.51722
H	6.48621	2.76901	-1.89887
C	-3.19755	-4.65303	-0.11434
H	-3.90365	-4.52214	0.69312
C	-1.30087	-5.11019	-2.19500
H	-0.56863	-5.28335	-2.97627
C	-3.18531	-5.84346	-0.84283
H	-3.90925	-6.61456	-0.59810
C	-2.25987	-6.06961	-1.87255
H	-2.28282	-7.00779	-2.41805

mer-Ir(pmb)3

82			
Ir	0.04929	-0.33503	-0.00117
C	1.99586	-0.31115	-0.74148
C	4.22842	0.21464	-0.95143
N	2.82319	-1.35910	-0.16806
C	4.18454	-1.05579	-0.32175
N	2.93605	0.64135	-1.16129
C	-0.47154	1.65180	-0.50145
C	-1.28269	3.65772	-1.18695
N	-1.17496	2.29889	-1.47409
N	-0.10620	2.62059	0.40596
C	-0.60821	3.87309	0.02986
C	0.81062	0.79888	1.63698
C	1.95053	2.60114	3.53082
C	0.66069	2.19955	1.53913
C	1.53792	0.34704	2.75227
C	2.08980	1.22333	3.69198
C	1.23336	3.09904	2.44191
H	1.67589	-0.72147	2.89290
H	2.64075	0.82869	4.54220
H	1.16523	4.16942	2.30109
H	2.39858	3.29131	4.23973
C	-1.90612	-0.71624	0.54132
C	-4.01034	-0.92646	1.35834
N	-2.72106	-0.45664	1.59969
N	-2.68217	-1.38632	-0.38166
C	-3.99747	-1.51985	0.08041
C	-0.70597	-1.33354	-1.71237
C	-1.95582	-2.89458	-3.73192
C	-2.04141	-1.78435	-1.59940
C	-0.03554	-1.68693	-2.89262
C	-0.64407	-2.44824	-3.89508
C	-2.66417	-2.56799	-2.57263
H	0.99546	-1.36215	-3.01431
H	-0.09232	-2.70488	-4.79629
H	-3.66694	-2.95280	-2.44340
H	-2.43281	-3.50139	-4.49629
C	-1.76070	1.69865	-2.66339

H	-2.85259	1.77354	-2.62868
H	-1.46677	0.65327	-2.70912
H	-1.39924	2.21922	-3.55582
C	-2.33302	0.22355	2.82596
H	-1.26153	0.40895	2.79438
H	-2.57149	-0.40493	3.68952
H	-2.86815	1.17435	2.91921
C	-5.17699	-2.05047	-0.45143
H	-5.22108	-2.48586	-1.43946
C	-5.16085	-0.86263	2.14058
H	-5.15032	-0.40141	3.12234
C	-6.33228	-1.98551	0.32964
H	-7.25667	-2.39236	-0.06860
C	-6.32869	-1.40719	1.60711
H	-7.24663	-1.37658	2.18559
C	-0.59321	5.15030	0.60023
H	-0.12660	5.35157	1.55375
C	-1.92034	4.68425	-1.88014
H	-2.43395	4.49838	-2.81735
C	-1.23367	6.18042	-0.09041
H	-1.23113	7.17803	0.33772
C	-1.88134	5.95815	-1.31449
H	-2.36640	6.78505	-1.82357
C	5.36006	-1.71436	0.02939
H	5.35543	-2.66407	0.54528
C	5.44649	0.82451	-1.26345
H	5.48293	1.79895	-1.73771
C	6.62465	0.14014	-0.92237
H	7.58368	0.59392	-1.15660
C	6.58810	-1.09729	-0.28410
H	7.51321	-1.59933	-0.01977
C	2.61158	1.86039	-1.86345
H	2.75183	2.74489	-1.22908
H	1.57088	1.81386	-2.18123
H	3.24423	1.96567	-2.75267
C	2.17253	-2.34825	0.50465
C	0.67059	-4.22482	1.94145
C	0.75653	-2.07814	0.74820
C	2.78153	-3.56012	0.92649
C	2.03266	-4.47518	1.63541
C	0.06397	-3.06031	1.49133
H	3.80258	-3.79236	0.65826
H	2.49125	-5.40811	1.95220
H	-0.98709	-2.90179	1.71342
H	0.10457	-4.95707	2.50983

fac-Ir(pmp)₃

79			
Ir	0.06240	0.01570	0.29326
C	0.51963	1.69069	1.40363
C	0.84661	4.16544	2.79437
C	1.39160	1.80618	2.50518
C	-0.16917	2.90830	1.02044
C	-0.01539	4.13222	1.71752
C	1.55485	3.00372	3.19050
H	1.92900	0.92530	2.84047
H	-0.57393	5.00167	1.39476
H	2.22223	3.05267	4.04688
H	0.98399	5.09255	3.34391
C	-0.67556	-1.70252	-0.60085
C	-1.18343	-3.65846	-1.63074
N	-0.28834	-2.59789	-1.56407
N	-1.84048	-2.19937	-0.06694
C	-2.18719	-3.40294	-0.67346
C	-0.96804	1.50075	-0.77246
C	-2.67697	2.84167	-1.54649
N	-0.98631	2.77562	-0.07217
N	-2.07579	1.61028	-1.62972
C	-1.98808	3.60427	-0.56936
C	-1.68963	-0.32526	1.38059
C	-4.13645	-1.07154	2.64011
C	-2.43464	-1.46470	1.00307
C	-2.23615	0.42259	2.43728
C	-3.43533	0.06224	3.05729
C	-3.63551	-1.85350	1.59903
H	-1.70608	1.29986	2.79637
H	-3.82072	0.66563	3.87541
H	-4.15423	-2.74152	1.25957

H	-5.06703	-1.35346	3.12423
C	1.94207	0.20535	-0.61954
C	3.89324	0.69442	-1.66234
N	2.52685	0.93727	-1.61753
N	2.95554	-0.51459	-0.02872
C	4.17418	-0.23934	-0.64344
C	1.26757	-1.26241	1.47411
C	3.16117	-2.89906	2.83123
C	2.62422	-1.33742	1.09630
C	0.90021	-2.05845	2.56945
C	1.82717	-2.86170	3.24211
C	3.57562	-2.13052	1.74289
H	-0.13062	-2.04275	2.91176
H	1.50623	-3.45847	4.09258
H	4.60514	-2.13939	1.40678
H	3.88167	-3.52222	3.35338
C	0.91566	-2.50627	-2.37209
H	1.69887	-3.16587	-1.98500
H	1.26921	-1.47815	-2.34813
H	0.68736	-2.78517	-3.40486
C	1.83893	1.87694	-2.49137
H	0.78057	1.86666	-2.21816
H	1.96469	1.58257	-3.53877
H	2.24299	2.88448	-2.35215
C	-2.51663	0.57567	-2.53720
H	-3.48378	0.16149	-2.22763
H	-1.77606	-0.22294	-2.53951
H	-2.61722	0.97376	-3.55434
C	-3.75512	3.42822	-2.22192
H	-4.33606	2.89848	-2.96753
N	-2.25202	4.85358	-0.21479
C	-4.04454	4.75967	-1.85335
H	-4.86400	5.28502	-2.33506
C	-3.30033	5.41729	-0.88084
H	-3.53394	6.44260	-0.60839
N	5.37485	-0.73240	-0.36612
C	4.92628	1.16772	-2.46040
H	4.76258	1.89017	-3.25334
C	6.36823	-0.27023	-1.14168
H	7.35839	-0.66376	-0.92537
C	6.19781	0.65940	-2.17672
H	7.05845	0.98072	-2.75347
N	-3.23689	-4.17849	-0.43665
C	-1.25556	-4.80878	-2.40414
H	-0.50575	-5.05851	-3.14765
C	-3.30061	-5.28842	-1.18996
H	-4.15447	-5.93570	-1.00596
C	-2.35584	-5.63893	-2.16294
H	-2.48255	-6.55784	-2.72513

mer-Ir(pmp)₃

79			
H	1.94388	0.77765	4.98257
H	1.69318	3.24296	4.73164
C	1.53437	1.19534	4.06606
C	1.39437	2.57613	3.92780
H	-2.92331	-0.51612	3.54625
H	1.26660	-0.73265	3.16278
C	1.15045	0.33804	3.02735
H	-1.58832	0.40427	2.80310
H	-5.53226	-0.69399	2.69268
C	0.86907	3.11020	2.75044
H	-0.12712	-4.91171	2.64975
H	0.74971	4.17770	2.61303
C	-2.64369	0.15220	2.72565
H	2.28803	-5.36318	2.26922
H	-3.24341	1.06565	2.79131
C	0.47939	-4.19063	2.10894
C	1.84110	-4.44767	1.89234
H	-7.36858	-1.81095	1.36556
C	-5.35359	-1.09698	1.70230
C	0.60494	0.83133	1.83168
C	0.49190	2.23026	1.73141
H	-1.14702	-2.83311	1.81737
C	-0.09328	-3.01590	1.63209
H	3.68875	-3.71446	1.01957
C	2.63550	-3.53473	1.19670
C	-6.36861	-1.71911	0.95433

N	-2.87619	-0.50914	1.44995
C	-4.10953	-1.03280	1.07535
C	0.65565	-2.05754	0.91155
N	-0.15477	5.12440	0.68737
C	2.03893	-2.36496	0.72923
H	-0.43401	7.16645	0.48700
N	-0.05568	2.68034	0.50020
C	-1.95351	-0.69404	0.46076
C	-0.58971	6.20823	-0.00256
C	-0.36322	3.96747	0.06162
C	-6.10653	-2.22127	-0.32049
N	2.74698	-1.38033	0.01443
N	5.07270	-2.13786	-0.11077
Ir	0.03016	-0.30384	0.08786
H	7.10233	-2.42633	-0.39767
C	-3.95459	-1.57273	-0.21487
C	4.09236	-1.27150	-0.33739
H	-6.90075	-2.69771	-0.88946
C	6.28057	-1.73696	-0.57325
C	2.03586	-0.26791	-0.39692
C	-0.42858	1.73018	-0.42995
N	-2.62142	-1.34645	-0.55980
N	-4.90131	-2.16415	-0.93525
H	2.91365	2.64630	-0.90948
C	4.21237	-0.03415	-0.99664
N	2.94293	0.53811	-1.02408
C	6.51229	-0.53068	-1.23337
C	-1.20350	6.15920	-1.25217
C	-0.96628	3.80617	-1.19798
H	7.51749	-0.29110	-1.56437
C	5.46058	0.37387	-1.46488
N	-0.99207	2.44389	-1.46537
H	-1.52196	7.08348	-1.72355
C	2.66655	1.84061	-1.60793
C	-0.57218	-1.09756	-1.74421
C	-1.90601	-1.58921	-1.75672
C	-1.41536	4.92659	-1.90064
H	5.61971	1.32315	-1.96348
H	1.60864	1.89393	-1.85659
H	3.26023	1.95934	-2.51831
H	-3.48166	-2.62584	-2.79384
H	1.19533	-0.93108	-2.96952
C	-2.46130	-2.26531	-2.84373
C	0.17527	-1.30228	-2.91833
H	-1.89780	4.85886	-2.86879
C	-1.61207	1.91816	-2.67052
H	-1.44104	0.84807	-2.72937
H	-2.68937	2.11638	-2.65923
H	-1.17741	2.40165	-3.55169
C	-1.67162	-2.45283	-3.98023
C	-0.35617	-1.97678	-4.01852
H	-2.08888	-2.97126	-4.83873
H	0.25181	-2.13504	-4.90522

Table S3. Cartesian coordinates of the optimized ^3MC state geometry denoted in Figure 4

fac-Ir(pmb)₃

82

Ir	-0.54061	-0.38333	0.65550
C	0.32767	1.20482	1.68259
C	1.43119	3.55248	2.84189
C	1.01811	1.16876	2.90294
C	0.22420	2.47149	1.06634
C	0.76039	3.63495	1.61952
C	1.56126	2.32077	3.48246
H	1.13606	0.21543	3.41238
H	0.67378	4.59660	1.13203
H	2.08666	2.25569	4.43212
H	1.85119	4.45201	3.28261
C	-1.41968	-2.04986	-0.20252
C	-2.03017	-3.98112	-1.21927
N	-1.20965	-2.85534	-1.27876
N	-2.40114	-2.66588	0.54796
C	-2.79541	-3.87342	-0.03998
C	-0.93648	1.17521	-0.57318
C	-1.59783	2.72796	-2.09049
N	-0.48307	2.42457	-0.17264
N	-1.63168	1.38698	-1.73933

C	-0.86335	3.40248	-1.08954
C	-1.90814	-0.92012	2.09775
C	-4.04536	-1.72909	3.77261
C	-2.73881	-2.02733	1.77434
C	-2.18846	-0.25095	3.30193
C	-3.23623	-0.65162	4.13462
C	-3.80319	-2.42162	2.58227
H	-1.57726	0.59882	3.58529
H	-3.42693	-0.11623	5.06093
H	-4.46062	-3.23288	2.29752
H	-4.87258	-2.03383	4.40712
C	1.87049	0.11495	-1.81877
C	3.29933	1.90348	-1.58235
N	2.32401	1.28567	-2.36617
N	2.58459	0.00072	-0.65266
C	3.47111	1.07000	-0.46572
C	1.24888	-1.46863	0.83596
C	3.62349	-2.96974	1.31321
C	2.47436	-1.12321	0.23620
C	1.25844	-2.60880	1.66461
C	2.42111	-3.34064	1.91496
C	3.64049	-1.86579	0.46518
H	0.33653	-2.91995	2.14751
H	2.38175	-4.20269	2.57619
H	4.55840	-1.57259	-0.03666
H	4.53257	-3.53756	1.48852
C	-0.21307	-2.63308	-2.31861
H	0.50222	-3.46167	-2.32453
H	0.32646	-1.69963	-2.12728
H	-0.70303	-2.58577	-3.29768
C	1.85639	1.80893	-3.63594
H	1.14522	1.09330	-4.04755
H	2.69043	1.93095	-4.33617
H	1.36108	2.77702	-3.50467
C	-2.31850	0.37681	-2.51856
H	-3.33980	0.70596	-2.73420
H	-2.35376	-0.54072	-1.93726
H	-1.79630	0.19042	-3.46334
C	-2.14057	3.39117	-3.19020
H	-2.69834	2.85628	-3.95151
C	-0.66556	4.78397	-1.18581
H	-0.11051	5.33971	-0.44406
C	-1.93544	4.76887	-3.27546
H	-2.34245	5.31929	-4.11792
C	-1.20963	5.44879	-2.28722
H	-1.06354	6.52093	-2.37579
C	4.37064	1.39764	0.54833
H	4.48674	0.76458	1.42031
C	4.03114	3.08093	-1.73607
H	3.89843	3.72371	-2.60049
C	5.10207	2.57641	0.39779
H	5.80968	2.86268	1.17005
C	4.93982	3.40313	-0.72664
H	5.52823	4.31206	-0.80979
C	-3.69100	-4.88717	0.30908
H	-4.26947	-4.85694	1.22203
C	-2.14738	-5.06714	-2.08289
H	-1.54972	-5.13578	-2.98552
C	-3.80813	-5.97781	-0.55559
H	-4.49837	-6.77624	-0.30131
C	-3.05530	-6.06797	-1.73489
H	-3.17419	-6.93092	-2.38253

mer-Ir(pmb)3

82			
Ir	0.58458	-0.52873	0.24219
C	2.58373	-0.48674	-0.12860
C	4.75165	-0.14128	-0.66426
N	3.35768	-1.43560	0.50839
C	4.71184	-1.25024	0.20642
N	3.43814	0.29119	-0.84032
C	-0.31498	2.32532	-1.52389
C	-2.56353	2.80698	-1.58776
N	-1.42180	2.47195	-2.31507
N	-0.78404	2.57832	-0.25788
C	-2.15023	2.88342	-0.24618
C	0.74109	1.33468	1.24044
C	0.96181	3.70671	2.81672

C	0.05240	2.51824	0.90739
C	1.57373	1.40787	2.37804
C	1.67555	2.55874	3.16276
C	0.16081	3.68378	1.67778
H	2.14171	0.52913	2.67200
H	2.31821	2.55740	4.03983
H	-0.37607	4.57513	1.36472
H	1.04137	4.61235	3.41100
C	-1.41676	-0.71304	0.52906
C	-3.59104	-0.85523	1.15390
N	-2.28777	-0.59527	1.57101
N	-2.17863	-1.06332	-0.56823
C	-3.53192	-1.15552	-0.22313
C	-0.06617	-0.99768	-1.66501
C	-1.24498	-1.84422	-4.10577
C	-1.45979	-1.25580	-1.77930
C	0.69973	-1.17919	-2.83010
C	0.12681	-1.59305	-4.03421
C	-2.04568	-1.67999	-2.97155
H	1.76965	-0.99751	-2.79556
H	0.75028	-1.72570	-4.91477
H	-3.10261	-1.90270	-3.03558
H	-1.69708	-2.17793	-5.03526
C	-1.40188	2.26844	-3.75232
H	-2.03770	1.42238	-4.03292
H	-0.37482	2.04725	-4.03897
H	-1.74527	3.16693	-4.27724
C	-1.93033	-0.21874	2.92858
H	-0.84992	-0.10204	2.98242
H	-2.25386	-0.99210	3.63261
H	-2.40722	0.72970	3.19529
C	-4.70427	-1.44899	-0.92288
H	-4.70649	-1.66760	-1.98147
C	-4.78916	-0.84810	1.86244
H	-4.81609	-0.61318	2.92120
C	-5.90775	-1.44321	-0.21333
H	-6.82848	-1.66968	-0.74209
C	-5.95417	-1.15113	1.15627
H	-6.90781	-1.15642	1.67480
C	-3.05219	3.19888	0.77032
H	-2.73065	3.26358	1.80416
C	-3.88662	3.04777	-1.95682
H	-4.20609	2.98823	-2.99236
C	-4.37749	3.43953	0.40136
H	-5.10496	3.68927	1.16797
C	-4.78855	3.36700	-0.93951
H	-5.82700	3.56162	-1.19010
C	5.89714	-1.88556	0.58428
H	5.91181	-2.72585	1.26427
C	5.94562	0.35145	-1.18402
H	5.95750	1.20649	-1.85127
C	7.12384	-0.29464	-0.80839
H	8.07460	0.06043	-1.19346
C	7.09550	-1.39203	0.06343
H	8.02685	-1.87316	0.34575
C	3.06393	1.45191	-1.64017
H	3.56412	2.34305	-1.24756
H	1.98012	1.60182	-1.60107
H	3.37665	1.29994	-2.67874
C	2.65260	-2.36178	1.32857
C	1.09357	-4.07252	2.86444
C	1.25665	-2.10643	1.41115
C	3.25500	-3.43688	1.97894
C	2.46689	-4.29191	2.75515
C	0.50364	-2.99771	2.19440
H	4.31421	-3.63665	1.88454
H	2.93264	-5.13092	3.26376
H	-0.57060	-2.85723	2.27507
H	0.48186	-4.74247	3.46310
fac-Ir(pmp)3			
79			
Ir	-0.52052	-0.31555	0.57950
C	0.35684	1.30669	1.55706
C	1.44548	3.71884	2.60372
C	1.08574	1.32406	2.75587
C	0.21454	2.55453	0.91404
C	0.73578	3.75366	1.40123

C	1.62118	2.50812	3.27613
H	1.24507	0.39274	3.29343
H	0.58511	4.67989	0.86014
H	2.18041	2.48323	4.20819
H	1.86027	4.63794	3.00806
C	-1.40486	-1.97966	-0.25583
C	-2.06432	-3.89343	-1.26902
N	-1.21488	-2.79472	-1.33609
N	-2.38896	-2.57362	0.50545
C	-2.82324	-3.75567	-0.08596
C	-0.96800	1.20424	-0.67925
C	-1.73507	2.74268	-2.16517
N	-0.52940	2.46626	-0.29862
N	-1.72189	1.40307	-1.82345
C	-0.97033	3.42782	-1.19087
C	-1.86385	-0.83422	2.04355
C	-3.90265	-1.72138	3.80109
C	-2.68904	-1.95194	1.74991
C	-2.11414	-0.17533	3.26049
C	-3.11860	-0.61240	4.12803
C	-3.69445	-2.40555	2.59934
H	-1.51143	0.68554	3.52821
H	-3.28890	-0.08608	5.06357
H	-4.29018	-3.26960	2.32997
H	-4.68158	-2.05959	4.47845
C	1.90130	0.16014	-1.60299
C	3.47664	1.81503	-1.39581
N	2.40358	1.32451	-2.12893
N	2.68667	-0.07927	-0.50190
C	3.66856	0.90414	-0.33988
C	1.20497	-1.48700	0.88263
C	3.47191	-3.08110	1.53169
C	2.48521	-1.19493	0.37712
C	1.10245	-2.63068	1.69972
C	2.21281	-3.40824	2.03410
C	3.60191	-1.97763	0.69408
H	0.13619	-2.90489	2.11165
H	2.08860	-4.26914	2.68628
H	4.56999	-1.70763	0.28687
H	4.34270	-3.68075	1.77992
C	-0.20895	-2.58730	-2.37088
H	0.47984	-3.43768	-2.38998
H	0.35512	-1.67535	-2.14883
H	-0.69160	-2.50113	-3.35091
C	1.88735	1.94902	-3.33249
H	1.07649	1.32533	-3.70762
H	2.66805	2.02369	-4.09787
H	1.50419	2.95244	-3.11886
C	-2.42849	0.38103	-2.56881
H	-3.45215	0.71146	-2.77063
H	-2.46014	-0.52364	-1.96730
H	-1.92856	0.16866	-3.52068
C	-2.31303	3.45966	-3.20500
H	-2.90754	2.98434	-3.97823
N	-0.74089	4.73546	-1.17742
C	-2.08125	4.84226	-3.19943
H	-2.49926	5.47041	-3.97887
C	-1.30641	5.42038	-2.18868
H	-1.12703	6.49279	-2.18948
N	4.60477	0.98960	0.59412
C	4.31762	2.91547	-1.50578
H	4.21440	3.65034	-2.29789
C	5.40995	2.05782	0.48424
H	6.18302	2.14803	1.24386
C	5.30869	3.02552	-0.52519
H	6.00423	3.85806	-0.53875
N	-3.75046	-4.60206	0.33896
C	-2.27369	-4.99744	-2.08352
H	-1.71497	-5.15529	-3.00009
C	-3.94619	-5.66767	-0.45674
H	-4.70247	-6.37368	-0.12293
C	-3.24894	-5.90258	-1.64822
H	-3.46975	-6.79122	-2.22976
mer-Ir(pmp) ₃			
79			
H	2.20900	2.19787	4.36430
H	0.52230	4.04287	4.27189

C	1.46053	2.22070	3.57589
C	0.52058	3.25100	3.52867
H	-2.64491	-1.59142	3.40230
H	2.18349	0.42038	2.68688
C	1.44482	1.21334	2.61064
H	-1.09185	-0.82074	2.98532
H	-5.07217	-1.59622	2.42992
C	-0.42218	3.24986	2.50506
H	0.49901	-5.26699	2.64070
H	-1.16788	4.03633	2.43677
C	-2.16442	-0.81712	2.79766
H	2.97018	-5.50473	2.50025
H	-2.57493	0.16830	3.03774
C	1.09726	-4.47259	2.20161
C	2.48528	-4.60908	2.12299
H	-6.91918	-2.03896	0.77615
C	-4.88605	-1.59599	1.36124
C	0.48998	1.16587	1.56807
C	-0.43591	2.22900	1.54768
H	-0.60878	-3.24496	1.77731
C	0.47294	-3.32137	1.71444
H	4.33810	-3.68258	1.47844
C	3.26065	-3.59563	1.55296
C	-5.90928	-1.83681	0.43542
N	-2.38525	-1.08983	1.38427
C	-3.62840	-1.35302	0.82834
C	1.20930	-2.26974	1.14104
N	-0.15352	3.20487	-1.33477
C	2.61392	-2.45722	1.07759
H	0.61291	3.96144	-3.09620
N	-1.46643	2.32634	0.54275
C	-1.45897	-0.89468	0.39965
C	-0.29778	3.63544	-2.59897
C	-1.27833	2.80995	-0.75303
C	-5.63624	-1.81440	-0.93684
N	3.30668	-1.36838	0.48097
N	5.70064	-1.87309	0.56306
Ir	0.52622	-0.50772	0.27907
H	7.76062	-1.95451	0.47363
C	-3.46390	-1.35133	-0.57527
C	4.65698	-1.10876	0.27431
H	-6.43353	-2.00027	-1.65236
C	6.89306	-1.34086	0.24411
C	2.53616	-0.31384	0.03780
C	-2.78896	2.05569	0.80956
N	-2.12244	-1.06820	-0.79809
N	-4.42290	-1.56905	-1.46483
H	3.52785	2.71267	-0.35822
C	4.71512	0.17104	-0.31953
N	3.40676	0.62178	-0.44448
C	7.06418	-0.08252	-0.34581
C	-1.51833	3.68463	-3.28513
C	-2.55681	2.82442	-1.34487
H	8.06504	0.27069	-0.56972
C	5.95116	0.71275	-0.64315
N	-3.42868	2.36040	-0.36886
H	-1.54109	4.04394	-4.30847
C	3.03894	1.93626	-0.95458
C	0.00773	-0.57751	-1.72729
C	-1.34942	-0.91091	-1.97841
C	-2.69505	3.27060	-2.65341
H	6.05353	1.69237	-1.09813
H	1.95923	2.06574	-0.88415
H	3.35270	2.03505	-1.99888
H	-2.92100	-1.33644	-3.38556
H	1.87285	-0.17728	-2.73949
C	-1.87676	-1.07708	-3.25697
C	0.82174	-0.42111	-2.86391
H	-3.65428	3.29775	-3.16048
C	-4.85965	2.19815	-0.55666
H	-5.27427	1.85241	0.38973
H	-5.32643	3.15007	-0.83327
H	-5.06863	1.45707	-1.33527
C	-1.02817	-0.90404	-4.35362
C	0.31644	-0.57894	-4.15650
H	-1.42028	-1.02990	-5.35874
H	0.97406	-0.45137	-5.01279

Table S4. Cartesian coordinates of the optimized transition state geometry
fac-Ir(pmb)₃

82			
Ir	-0.33005	-0.02292	0.38378
C	1.40664	0.11929	1.53500
C	3.88093	0.55967	2.86912
C	1.86507	-0.74338	2.54178
C	2.23728	1.22751	1.24554
C	3.46710	1.44532	1.87312
C	3.07501	-0.52717	3.21058
H	1.26352	-1.60799	2.80914
H	4.11536	2.26354	1.58622
H	3.39391	-1.21460	3.99018
H	4.83308	0.71971	3.36697
C	-2.14263	-0.15563	-0.60517
C	-4.02434	-0.61471	-1.78421
N	-2.63048	-0.67753	-1.76104
N	-3.24252	0.26098	0.11732
C	-4.42908	-0.01971	-0.57206
C	0.57224	1.60220	-0.43305
C	1.10123	3.68108	-1.20441
N	1.70945	2.06751	0.22855
N	0.23829	2.60359	-1.33038
C	2.04360	3.34918	-0.20335
C	-1.61092	0.63981	1.81842
C	-3.57025	1.79993	3.50828
C	-2.97340	0.76757	1.42024
C	-1.29024	1.09838	3.11178
C	-2.25307	1.66338	3.94971
C	-3.93818	1.35560	2.23341
H	-0.26593	1.00801	3.45695
H	-1.97578	2.00537	4.94311
H	-4.95676	1.49758	1.89624
H	-4.31972	2.25604	4.14867
C	1.30016	-1.17889	-1.38124
C	3.53252	-1.66423	-1.57259
N	2.50706	-0.78113	-1.90054
N	1.58606	-2.35876	-0.72861
C	2.94372	-2.68357	-0.80032
C	-0.41054	-2.14291	0.60010
C	-0.49420	-4.96618	0.91975
C	0.56436	-2.98488	0.03342
C	-1.43403	-2.77227	1.32808
C	-1.46740	-4.15988	1.50797
C	0.51996	-4.37654	0.16530
H	-2.21144	-2.16882	1.78696
H	-2.26205	-4.60634	2.10051
H	1.25357	-4.99520	-0.34138
H	-0.52837	-6.04618	1.03066
C	-1.82111	-1.28920	-2.80559
H	-2.10831	-2.33768	-2.93185
H	-0.77166	-1.23144	-2.50149
H	-1.97140	-0.76384	-3.75521
C	2.69340	0.38496	-2.74117
H	1.72455	0.85642	-2.89331
H	3.11024	0.09552	-3.71245
H	3.36992	1.10397	-2.26723
C	-0.90780	2.60108	-2.21466
H	-1.69589	3.26799	-1.84471
H	-1.29978	1.58890	-2.27293
H	-0.60930	2.93201	-3.21480
C	1.12942	4.90649	-1.86934
H	0.39519	5.15317	-2.62888
C	3.02726	4.27253	0.16367
H	3.73458	4.07062	0.95558
C	2.13235	5.81203	-1.51074
H	2.18582	6.77416	-2.01084
C	3.05808	5.49949	-0.50815
H	3.81743	6.22643	-0.23670
C	3.72007	-3.71780	-0.27501
H	3.28972	-4.48463	0.35678
C	4.89177	-1.66673	-1.87957
H	5.33875	-0.87999	-2.47852
C	5.08525	-3.71744	-0.57642
H	5.71213	-4.51116	-0.18133
C	5.66150	-2.71711	-1.37172
H	6.72467	-2.75238	-1.58942
C	-5.78753	0.14527	-0.29267

H	-6.13843	0.56693	0.63900
C	-4.93801	-1.03502	-2.74660
H	-4.60936	-1.49274	-3.67357
C	-6.70597	-0.27774	-1.25652
H	-7.76647	-0.15901	-1.05725
C	-6.29302	-0.85359	-2.46601
H	-7.03621	-1.16942	-3.19130

mer-Ir(pmb)3

82

Ir	-0.22045	-0.29177	-0.03404
C	-2.17342	0.05566	0.60704
C	-4.29680	0.85357	0.89655
N	-3.11037	-0.88209	0.11150
C	-4.42373	-0.41524	0.28647
N	-2.94483	1.11575	1.04494
C	0.76826	1.51883	0.67101
C	2.26097	3.09900	1.34874
N	1.64170	1.89338	1.65974
N	0.81794	2.53840	-0.26205
C	1.74735	3.51736	0.10533
C	-0.63328	1.16380	-1.55021
C	-1.18494	3.32794	-3.31203
C	-0.04435	2.43568	-1.38834
C	-1.50174	1.02181	-2.64496
C	-1.76079	2.07562	-3.52823
C	-0.32695	3.51802	-2.22858
H	-1.98090	0.06309	-2.81973
H	-2.42408	1.92024	-4.37540
H	0.07168	4.50469	-2.02934
H	-1.40816	4.16089	-3.97257
C	1.66389	-0.92950	-0.55120
C	3.70743	-1.50044	-1.34917
N	2.54032	-0.77668	-1.58089
N	2.27704	-1.78674	0.34668
C	3.55094	-2.15272	-0.10963
C	0.30379	-1.43175	1.64022
C	1.24107	-3.17966	3.66343
C	1.55743	-2.08679	1.54087
C	-0.44627	-1.68132	2.79907
C	0.00604	-2.54420	3.80107
C	2.02359	-2.95775	2.52728
H	-1.40988	-1.19031	2.90778
H	-0.60483	-2.72791	4.68112
H	2.96655	-3.47790	2.43173
H	1.60233	-3.85398	4.43457
C	1.89785	1.18645	2.90399
H	2.90734	0.76133	2.90864
H	1.17314	0.38517	3.01502
H	1.80505	1.88232	3.74390
C	2.31612	0.01117	-2.78354
H	1.29299	0.37999	-2.77224
H	2.47191	-0.61453	-3.66784
H	3.00970	0.85750	-2.81969
C	4.58403	-2.95034	0.39142
H	4.51559	-3.46172	1.34061
C	4.86449	-1.62081	-2.11636
H	4.96736	-1.10721	-3.06606
C	5.74656	-3.07221	-0.37588
H	6.55875	-3.68671	-0.00006
C	5.88786	-2.42321	-1.60898
H	6.80556	-2.54176	-2.17645
C	2.22492	4.68494	-0.49772
H	1.89227	5.00416	-1.47550
C	3.21754	3.84066	2.04401
H	3.60419	3.50961	3.00164
C	3.18850	5.42721	0.19611
H	3.57144	6.33852	-0.25285
C	3.66977	5.02058	1.44637
H	4.41456	5.62411	1.95610
C	-5.68189	-0.92904	-0.02004
H	-5.81157	-1.87909	-0.51899
C	-5.41467	1.60945	1.25587
H	-5.31173	2.57455	1.73959
C	-6.67717	1.07673	0.95664
H	-7.56640	1.64123	1.22193
C	-6.80907	-0.15926	0.32473
H	-7.79772	-0.54463	0.09572

C	-2.43484	2.28859	1.72078
H	-2.89951	3.19069	1.30968
H	-1.35822	2.33703	1.56416
H	-2.63975	2.24755	2.79829
C	-2.59690	-1.93502	-0.62768
C	-1.39371	-3.90015	-2.21625
C	-1.18595	-1.81513	-0.93173
C	-3.34955	-3.04864	-1.04087
C	-2.74668	-4.01301	-1.83808
C	-0.63954	-2.82903	-1.75318
H	-4.37355	-3.18332	-0.71955
H	-3.32850	-4.87142	-2.16301
H	0.41172	-2.77595	-2.01989
H	-0.94207	-4.66156	-2.84520

fac-Ir(pmp)₃

79			
Ir	-0.43777	-0.00681	0.41808
C	1.27402	-0.06230	1.61432
C	3.70133	0.17511	3.08122
C	1.63845	-1.00445	2.58821
C	2.18951	0.99347	1.41571
C	3.38722	1.13649	2.11866
C	2.83052	-0.89159	3.31321
H	0.97922	-1.84595	2.78419
H	4.04297	1.97609	1.92255
H	3.07953	-1.64026	4.06133
H	4.62569	0.26318	3.64527
C	-2.21205	0.01045	-0.63188
C	-4.04789	-0.23717	-1.93429
N	-2.66066	-0.32159	-1.87896
N	-3.33356	0.30771	0.11264
C	-4.48596	0.16898	-0.65474
C	0.57843	1.61315	-0.25274
C	1.36440	3.62355	-0.97362
N	1.76298	1.91065	0.41397
N	0.35857	2.68457	-1.10750
C	2.27167	3.12778	-0.00673
C	-1.77114	0.42651	1.90566
C	-3.83310	1.17576	3.70091
C	-3.12330	0.57736	1.49423
C	-1.50160	0.67234	3.26520
C	-2.51709	1.04165	4.15054
C	-4.15060	0.94436	2.35824
H	-0.48465	0.56712	3.62727
H	-2.28153	1.22340	5.19581
H	-5.16638	1.03860	1.99317
H	-4.62068	1.46153	4.39229
C	1.44026	-1.01008	-1.67504
C	3.68365	-1.45821	-1.57251
N	2.69970	-0.58807	-2.02187
N	1.64858	-2.18226	-0.98808
C	3.00718	-2.49742	-0.90330
C	-0.45828	-2.11742	0.24177
C	-0.49501	-4.96051	0.22963
C	0.56933	-2.87174	-0.35420
C	-1.52441	-2.84680	0.80082
C	-1.54057	-4.24410	0.81106
C	0.55896	-4.27076	-0.36437
H	-2.34706	-2.31536	1.26913
H	-2.37261	-4.76776	1.27524
H	1.38153	-4.80685	-0.82286
H	-0.50020	-6.04659	0.22865
C	-1.81080	-0.77977	-2.97128
H	-2.09258	-1.79789	-3.25727
H	-0.77062	-0.77434	-2.62923
H	-1.92697	-0.12177	-3.83965
C	2.96518	0.60694	-2.80019
H	2.00897	1.07496	-3.03030
H	3.47872	0.35608	-3.73524
H	3.58442	1.31035	-2.23395
C	-0.78885	2.86622	-1.97307
H	-1.42590	3.68079	-1.60981
H	-1.36363	1.94448	-1.98416
H	-0.46078	3.10208	-2.99113
C	1.61495	4.84954	-1.57706
H	0.94780	5.28041	-2.31630
N	3.38467	3.73679	0.38371

C	2.78674	5.50483	-1.16993
H	3.05199	6.46650	-1.59627
C	3.62013	4.92236	-0.21102
H	4.52845	5.43261	0.10007
N	3.57916	-3.54815	-0.33250
C	5.06880	-1.49748	-1.66615
H	5.64039	-0.72348	-2.16821
C	4.91928	-3.57575	-0.42233
H	5.40678	-4.42943	0.04273
C	5.68992	-2.59801	-1.06450
H	6.76955	-2.70129	-1.09181
N	-5.74685	0.36773	-0.29818
C	-4.98572	-0.46259	-2.93188
H	-4.70500	-0.78106	-3.93042
C	-6.64783	0.14753	-1.27125
H	-7.68779	0.30422	-0.99606
C	-6.32308	-0.25868	-2.57136
H	-7.11537	-0.41501	-3.29550

mer-Ir(pmp)₃

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H	1.73986	-0.36223	4.97959
H	1.31181	2.07399	5.33772
C	1.31722	0.24620	4.18367
C	1.08473	1.60622	4.38408
H	-2.89780	-2.10373	3.24980
H	1.20120	-1.40264	2.82084
C	1.01164	-0.34120	2.95206
H	-1.41502	-1.17126	2.90464
H	-5.49919	-1.38980	2.68300
C	0.56278	2.37117	3.34392
H	-0.14563	-5.81279	1.24209
H	0.39747	3.43395	3.47212
C	-2.49946	-1.17445	2.82964
H	2.28058	-6.11956	0.79890
H	-2.89360	-0.32572	3.39767
C	0.46155	-4.96541	0.93392
C	1.82449	-5.14047	0.68432
H	-7.52870	-1.38148	1.19021
C	-5.41058	-1.26952	1.60837
C	0.46337	0.39411	1.88235
C	0.27546	1.77125	2.11093
H	-1.18781	-3.59409	0.98307
C	-0.12506	-3.70511	0.78675
H	3.67121	-4.17433	0.07975
C	2.61282	-4.05853	0.28040
C	-6.53485	-1.26298	0.77187
N	-2.87325	-1.06248	1.42879
C	-4.18482	-1.11004	0.97776
C	0.62520	-2.58376	0.38968
N	0.98345	4.70207	1.41650
C	2.00034	-2.81599	0.14076
H	1.81130	6.59446	1.41473
N	-0.20652	2.58425	1.03744
C	-2.01191	-0.87086	0.38044
C	1.16740	5.91516	0.86082
C	0.18961	3.88891	0.73074
C	-6.38299	-1.10228	-0.60903
N	2.70093	-1.65010	-0.27543
N	5.04952	-2.26880	-0.57981
Ir	-0.02038	-0.63775	0.06914
H	7.07702	-2.42388	-0.92893
C	-4.14516	-0.95528	-0.42517
C	4.03490	-1.41582	-0.58968
H	-7.25771	-1.09698	-1.25460
C	6.23287	-1.73887	-0.93249
C	1.95842	-0.49763	-0.40931
C	-1.04347	2.06226	0.07061
N	-2.80115	-0.81860	-0.75324
N	-5.19831	-0.94772	-1.22934
H	2.80246	2.49811	-0.24713
C	4.11390	-0.04975	-0.93530
N	2.82904	0.46903	-0.82192
C	6.42337	-0.39796	-1.28888
C	0.58944	6.32834	-0.34346
C	-0.43036	4.19835	-0.49951
H	7.41584	-0.05243	-1.55737
C	5.34092	0.48927	-1.29525

N	-1.15168	3.07236	-0.86282
H	0.78470	7.32890	-0.71509
C	2.47480	1.85796	-1.07142
C	-0.74213	-0.39838	-1.86367
C	-2.14198	-0.59937	-1.98805
C	-0.23566	5.45298	-1.06400
H	5.46095	1.53411	-1.56188
H	1.39256	1.91478	-1.16794
H	2.94161	2.19382	-2.00176
H	-3.87907	-0.77348	-3.24825
H	1.03189	-0.01690	-3.03496
C	-2.80972	-0.60203	-3.21344
C	-0.04271	-0.17603	-3.06308
H	-0.69204	5.74247	-2.00504
C	-1.99116	3.00001	-2.04724
H	-2.51131	2.04471	-2.04093
H	-2.72227	3.81609	-2.04547
H	-1.38700	3.06376	-2.95795
C	-2.07073	-0.37422	-4.37704
C	-0.69028	-0.16433	-4.30098
H	-2.57481	-0.36847	-5.33910
H	-0.11679	0.00535	-5.20901