Supporting Information

Influence of halogen atoms on a homologous series of bis-cyclometalated iridium(III) complexes

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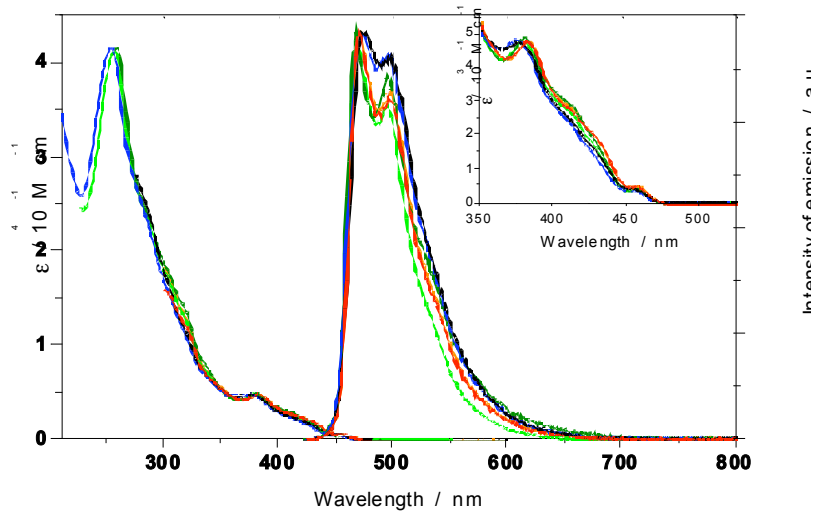

Figure S1. Absorption (left) and emission (right) spectra of **FIrPic** at 298 K in different solvents: dimethyl sulfoxide (black), acetonitrile (blue), chloroform (olive), dichloromethane (green), 1,2-dichlorobenzene (orange) and toluene (red). The absorption spectral window between 350 and 525 nm is magnified in the inset for the sake of clarity. Emission spectra (λ_{exc} = 407 nm) are corrected for the detector response.

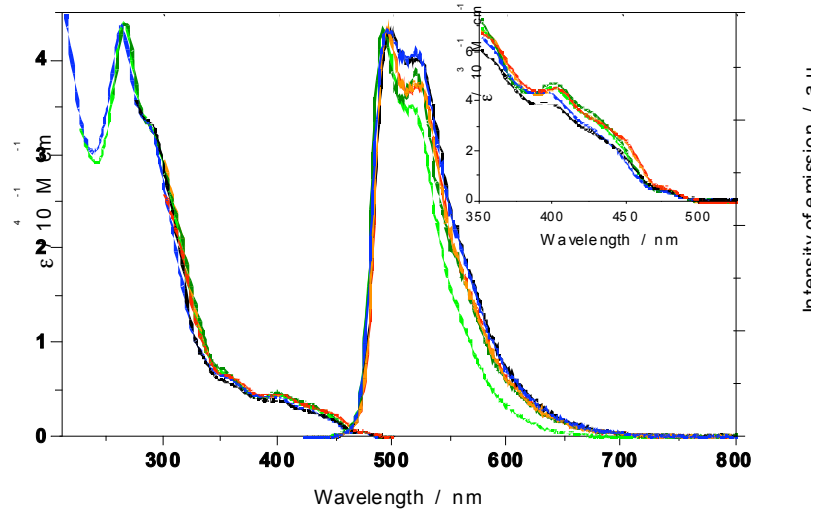

Figure S2. Absorption (left) and emission (right) spectra of **ClIrPic** at 298 K in different solvents: dimethyl sulfoxide (black), acetonitrile (blue), chloroform (olive), dichloromethane (green), 1,2-dichlorobenzene (orange) and toluene (red). The absorption spectral window between 350 and 525 nm is magnified in the inset for the sake of clarity. Emission spectra (λ_{exc} = 407 nm) are corrected for the detector response.

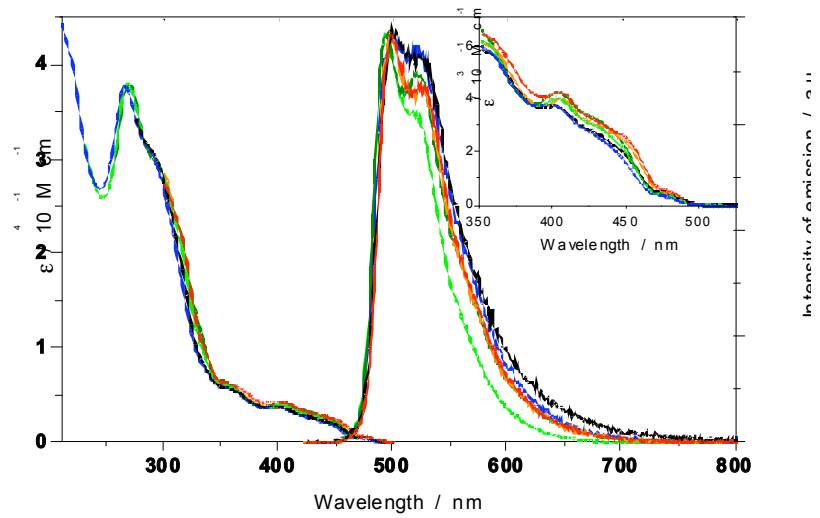

Figure S3. Absorption (left) and emission (right) spectra of **BrIrPic** at 298 K in different solvents: dimethyl sulfoxide (black), acetonitrile (blue), chloroform (olive), dichloromethane (green), 1,2-dichlorobenzene (orange) and toluene (red). The absorption spectral window between 350 and 525 nm is magnified in the inset for the sake of clarity. Emission spectra (λ_{exc} = 407 nm) are corrected for the detector response.

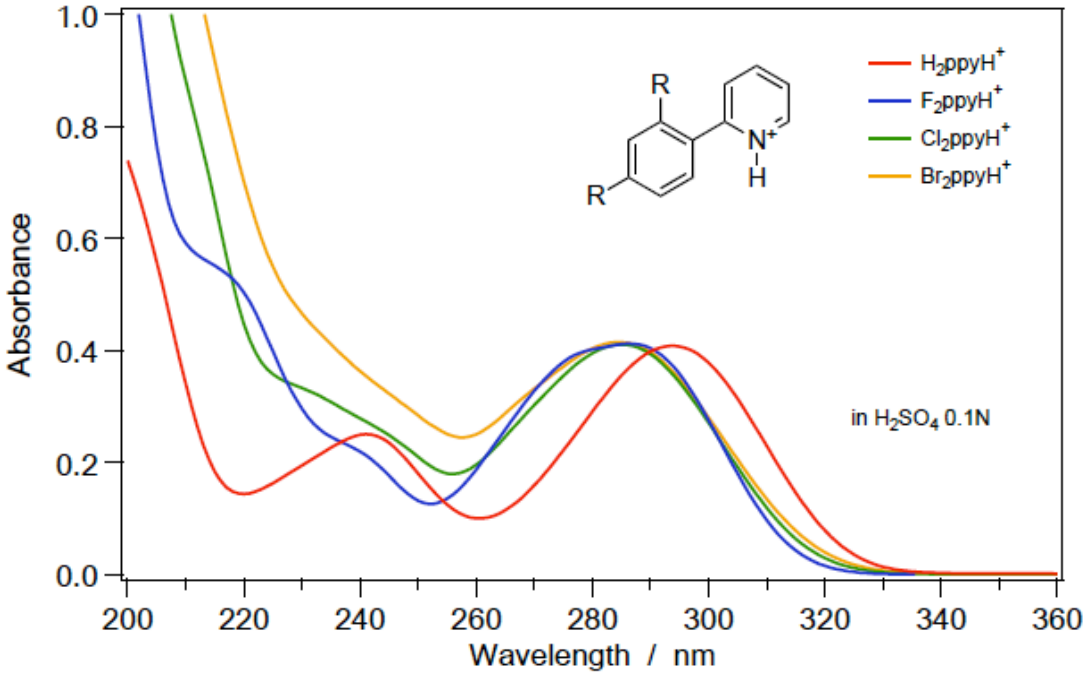

Figure S4. Normalized absorption spectra of the protonated forms of the 2-(2,4-di-X-phenyl)pyridines (X = H, F, Cl, Br) in 0.1 N H_2SO_4 at room temperature.

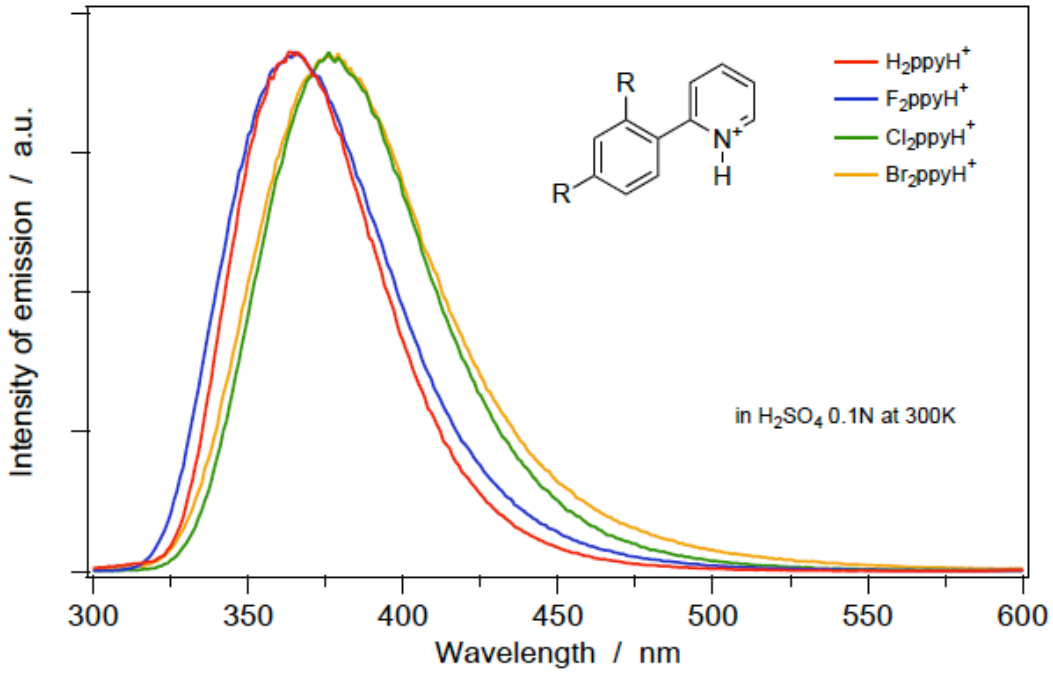

Figure S5. Normalized fluorescence spectra of the protonated forms of the 2-(2,4-di-X-phenyl)pyridines (X = H, F, Cl, Br) in 0.1 N H_2SO_4 at room-temperature (λ_{exc} = 285 nm).

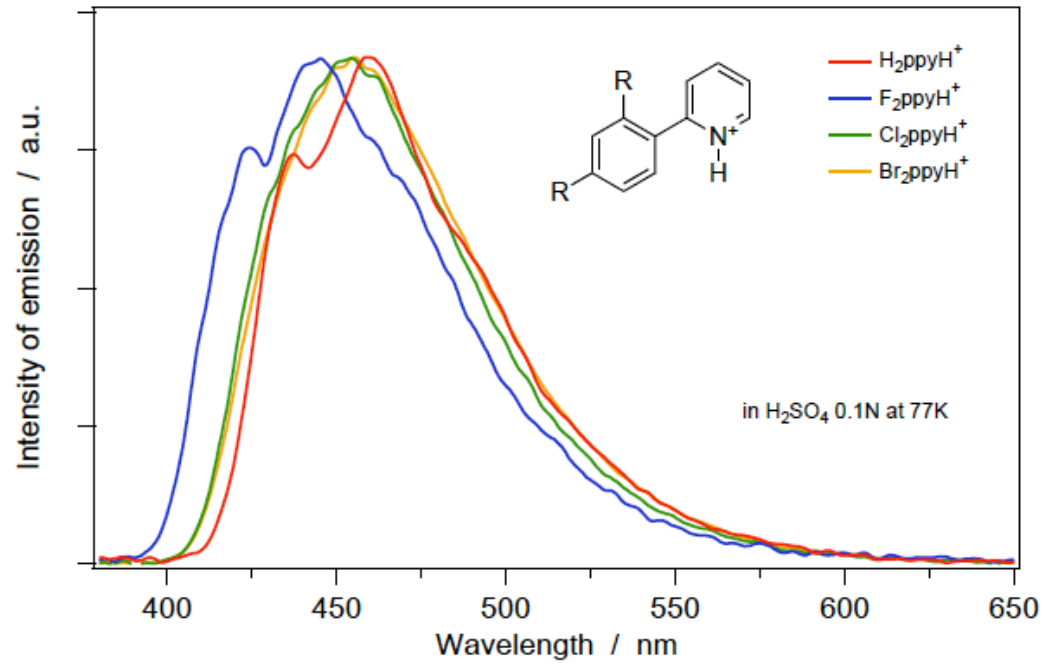

Figure S6. Normalized phosphorescence spectra of the protonated forms of the 2-(2,4-di-X-phenyl)pyridines (X = H, F, Cl, Br) in 0.1 N H_2SO_4 at 77 K (λ_{exc} = 285 nm, 10 μs delay).

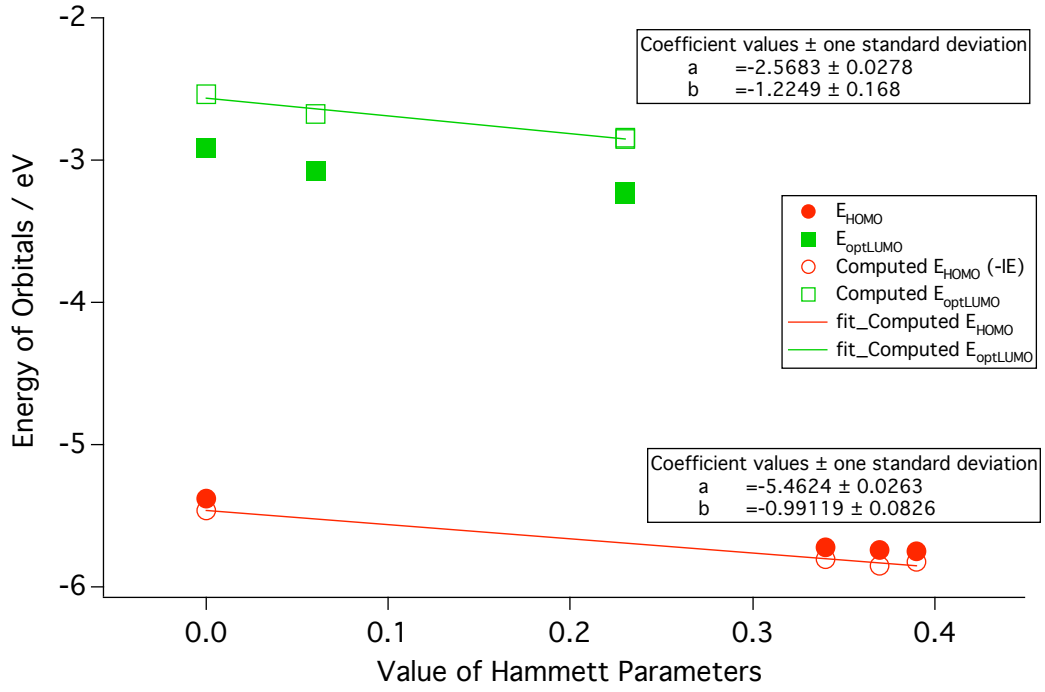

Figure S7. Correlation between the orbital energy levels (experimental and computed) and Hammett parameters. $E_{optLUMO}$ is correlated with the values σp and E_{HOMO} (-IE) with the values σm. Fits are of the form y=a+bx.

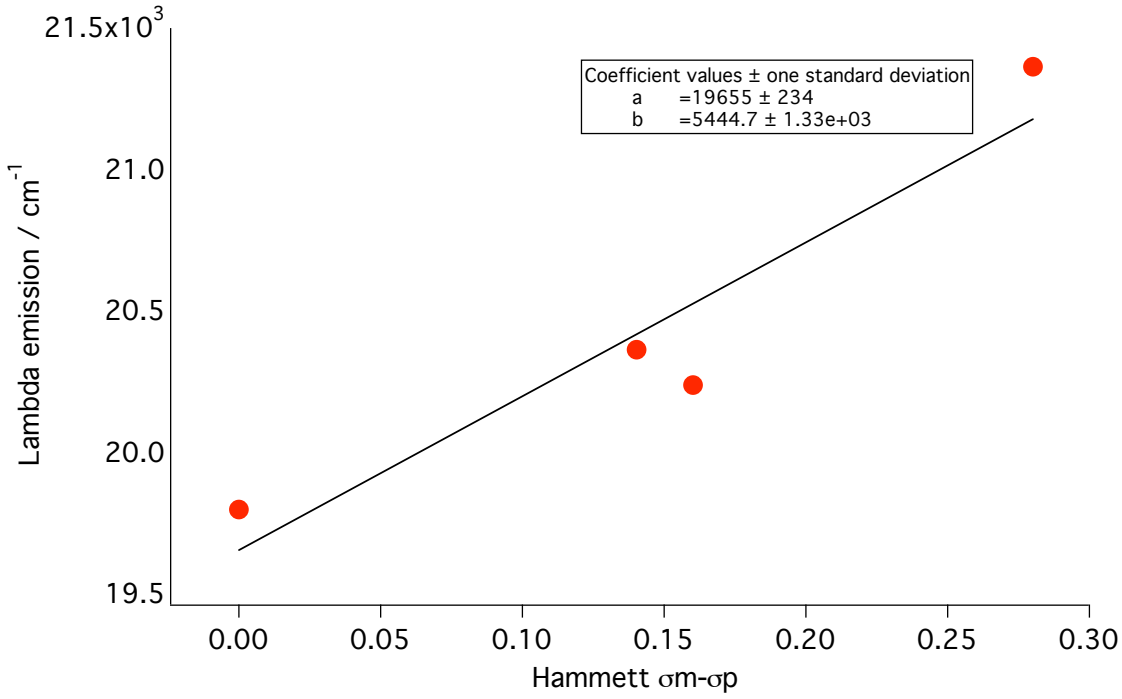

Figure S8. Correlation between emission maxima and the value (σm-σp). Fit is of the form y=a+bx.

Details of the calculations. Full geometry optimizations of the iridium compounds in their singlet ground state were performed with DFT using the M06 functional,[1] with the relativistic effective core pseudo-potential LANL2DZ[2] for the iridium and the 6-311G*[3] basis set for the remaining atoms. Remarkably, the use of more flexible basis sets including diffuse functions showed no significant changes in the main geometrical features of the optimized compounds. Tests were also been performed using LANL2DZ for bromine atoms. No symmetry constraints were applied during the geometry optimizations, which were carried out with the Gaussian 09 package.[4] The nature of the stationary points located was further checked by computations of harmonic vibrational frequencies at the same theory level.

Other *xc*-functionals have been used to test both geometries and vertical excitations. Interestingly, CAM-B3LYP[5] provides ground state geometries as good as M06 (Table 1), whereas LR-TDDFT first vertical excitations computed with this functional are energetically overestimated. Note that the performance of M06 functional for excitations within LR-TDDFT has been recently assessed.[6]

At each respective ground state (singlet) geometry, LR-TDDFT calculations were performed using the same basis sets and *xc*-functional. To fully characterize the experimental data, the first 140 vertical excitations (singlet and triplet) were considered. To take into account condensed-phase effects in the context of vertical excitations, we used a self-consistent reaction-field (SCRF) model in which the solvent is implicitly represented by a dielectric continuum characterized by its relative static dielectric permittivity ε. The solute, which is placed in a cavity created in the continuum after spending some cavitation energy, polarizes the continuum, which in turn creates an electric field inside the cavity. Within the different approaches that can be followed to calculate the electrostatic potential created by the polarized continuum in the cavity, we have employed the integral equation formalism of the polarizable continuum model (IEFPCM).[7] As the solvent molecules have no time to geometrically rearrange within the time of a vertical excitation, non-equilibrium solvation[8] has been used for LR-TDDFT absorption spectra. A relative permittivity of 8.93 (35.69) was employed to simulate dichloromethane (acetonitrile), the solvents used in the experimental work. Spin-orbit coupling (SOC) LR-TDDFT was performed with the ADF2009 package using the ZORA methodology. Full electron basis sets have been used for all the atoms (Iridium: TZP, all other atoms: DZP).

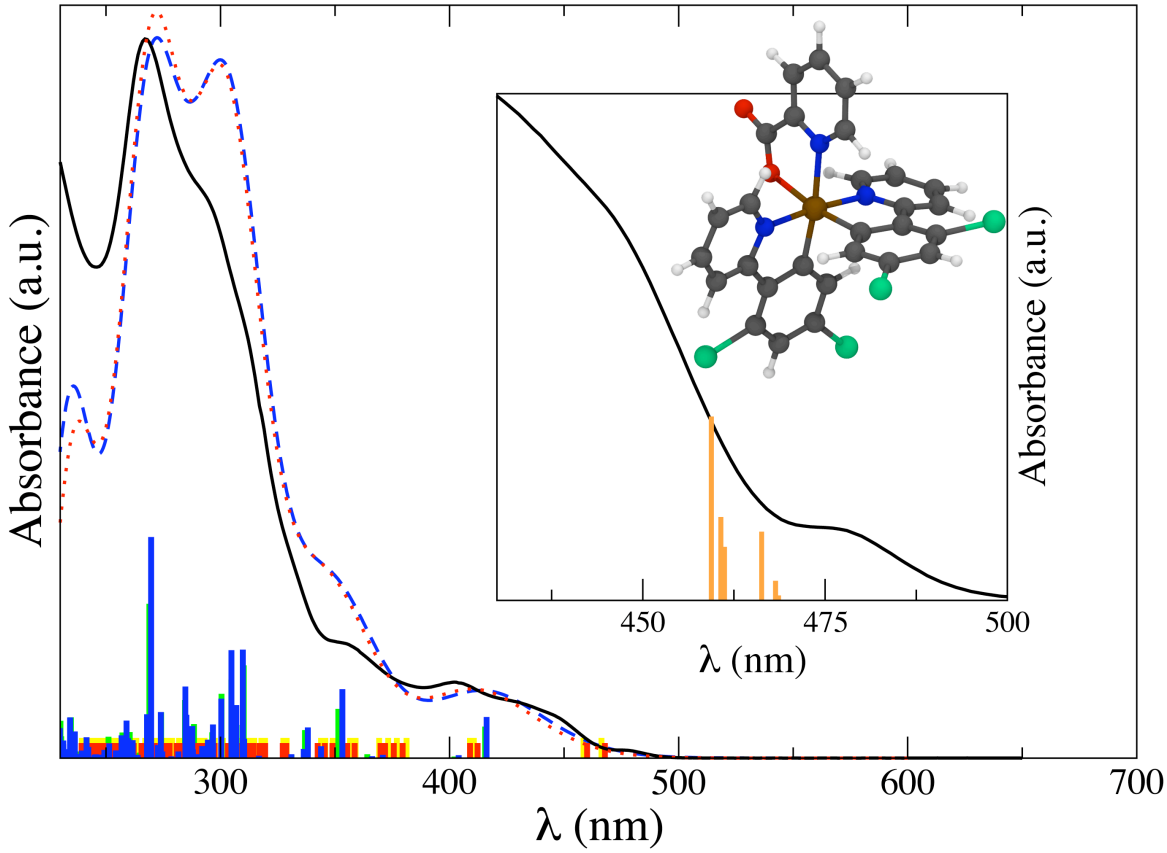

Figure S9: Absorption spectrum of **BrIrPic** : experimental results (black lines), LR-TDDFT/M06 convoluted absorption spectrum (dashed blue line), LR-TDDFT/M06 convoluted absorption spectrum with effective core potentials on bromine atoms (dashed blue line singlet (triplet) vertical excitation energies are represented by blue (red) bars. Vertical excitations for singlet (triplet) vertical excitations, computed for a solvated optimized geometry, are shown with green (yellow) bars. Inset presents a zoom on the low energy tail of the absorption spectrum, on which SOC/LR-TDDDT first vertical excitations are superimposed.

Figure S9 presents the absorption spectrum of **BrIrPic** computed in different conditions. The dotted red line represents the convoluted spectrum obtained with M06, using an effective core potential (ECP) for bromine. Only minor changes are observed for some oscillator strengths. Concerning the effect of the solvent (dichloromethane) on the ground state geometry, we perform additional tests on **BrIrPic**. With a geometry fully optimized in an implicit solvent, the vertical excitations obtained are represented by green (yellow) bars for the singlet (triplet) excited states. It can be observed that the geometrical changes due to the implicit solvent do not modified strongly the absorption spectrum of **BrIrPic** and only minor deviations are

observed. Same behavior is observed when the basis set is increased or the integration grid refined.

To gain insights in the phosphorescence of the different iridium compounds, we optimized the geometry of the first triplet state using unrestricted DFT (U-DFT) with the same basis set as described before. As suggested from a very recent work,[9] we used the *xc*-functional M05-2X for this task, presenting great emission results for a series of iridium-based compounds (see computational details for more information and discussion about the functional). At the minimum energy structure, we computed the difference in energy between the triplet (T_1) and singlet (S_0) with the inclusion of implicit solvent (non-equilibrium solvation for S_0) and obtained an estimation of the first phosphorescence band. Perturbative spin-orbit calculations[10] based on LR-TDDFT/M06 have been performed on the triplet structures of **ClIrPic** and **BrIrPic** and indicate that the first excited state as a dominant triplet character. Conformers for which the populated π* orbital (and the resulting distortion) is located on the second *ppy* ligand were computed for **ClIrPic** and **BrIrPic** and are almost degenerate (1 kJ/mol) with the presented structures. For those structures, theoretical bands are computed at 2.37 eV (**ClIrpIc**) and 2.27 eV (**BrIrPic**) and the same trend in ligand distortion is observed due to the halogen substituents.

To validate the methodology, we compared the absorption spectra obtained at U-DFT T_1 geometry with LR-TDDFT/M05-2X with those obtained from a full LR-TDDFT optimization on the T_1 electronic state of **FIrPic**. The transition to the first triplet differs only by ~ 0.05 eV. Furthermore, the U-DFT and LR-TDDFT geometries for T_1 are in very good agreement.

We have further tested the effect of the solvent on T_1 geometry optimization. The resulting geometries for the three compounds differ only by an energy of ~1.5 kJ/mol in average.

It is important to note here that this method considers that each electronic state is well represented by a single determinant and neglects spin-orbit coupling.

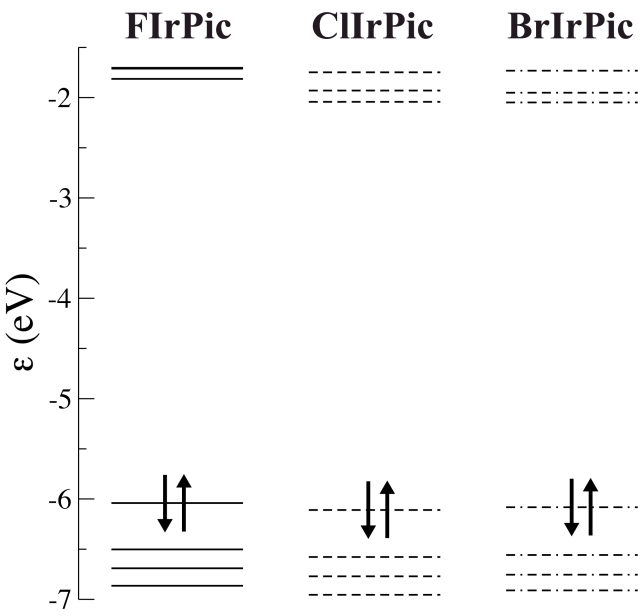

Figure S10. Kohn-Sham molecular orbital energies close to the HOMO/LUMO gap (DFT/M06).

Table S1: Comparison between optimized ground state (S_0) and optimized first triplet state (T_1). Notations follow Fig. 1 and Table 1 in text. Distances are given in Ångström.

	S_0(FIrPic) M05-2X	**T_1(FIrPic) M05-2X**	**S_0(ClIrPic) M05-2X**	**T_1(ClIrPic) M05-2X**	**S_0(BrIrPic) M05-2X**	**T_1(BrIrPic) M05-2X**
Bond distance						
Ir-N(1)	2.05	2.03	2.04	2.04	2.04	2.04
Ir-N(2)	2.06	2.07	2.06	2.06	2.05	2.05
Ir-N(3)	2.18	2.20	2.19	2.20	2.19	2.20
Ir-C(7)	1.99	1.97	1.99	1.96	1.99	1.96
Ir-C(12)	1.99	1.99	2.00	1.99	2.00	1.99
Ir-O(1)	2.17	2.17	2.18	2.17	2.17	2.17
Bond angle						
C(7)-Ir-C(12)	88.89	89.47	89.08	90.22	90.32	90.78
C(7)-Ir-N(1)	80.81	82.29	80.30	81.98	80.34	82.04
C(12)-Ir-N(1)	94.92	95.05	95.32	96.16	95.64	96.15
C(7)-Ir-N(3)	97.69	97.04	96.46	96.53	96.70	96.76
C(12)-Ir-O(1)	97.45	97.59	98.44	97.14	96.92	96.30
N(1)-Ir-N(2)	175.15	175.51	175.20	176.12	175.21	175.74

FIrPic - DFT/M06 Ground state

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Ir	-0.180720	-0.316864	-0.247182
F	-1.353358	4.403854	1.739250
F	1.064160	1.661941	4.606992
F	3.547889	2.693984	-2.709989
F	5.025098	-1.072898	-0.428376
O	-0.590747	-1.695970	-1.889873
O	-2.083589	-3.183413	-2.654499
N	-1.159781	1.258885	-1.126903
N	0.960760	-1.794290	0.634749
N	-2.133294	-1.169846	0.249489
C	-1.597365	1.221358	-2.391751
H	-1.410423	0.287513	-2.918253
C	-2.216524	2.303785	-2.980157
H	-2.552521	2.240463	-4.010054
C	-2.383449	3.455947	-2.223703
H	-2.863790	4.331401	-2.653999
C	-1.928695	3.496779	-0.919499
H	-2.043318	4.393545	-0.325533
C	-1.302172	2.378562	-0.367455
C	-0.718963	2.253517	0.961133
C	-0.066195	1.019145	1.236287
C	0.537214	0.837722	2.480064
H	1.061657	-0.081755	2.733596
C	0.484879	1.846787	3.420086
C	-0.150201	3.055254	3.187757
H	-0.180666	3.836928	3.939114
C	-0.739145	3.231136	1.955418
C	1.648884	0.257720	-0.841663
C	2.698888	-0.595889	-0.416729
C	4.003352	-0.289009	-0.804706
C	4.313472	0.807701	-1.575787

H	5.338147	1.018924	-1.862041
C	3.265874	1.623928	-1.965472
C	1.955104	1.374882	-1.614363
H	1.190407	2.067688	-1.960625
C	2.301069	-1.728035	0.402651
C	3.140933	-2.696749	0.958182
H	4.205968	-2.644026	0.774981
C	2.611747	-3.708037	1.732917
H	3.268978	-4.458698	2.164638
C	1.241736	-3.760020	1.952601
H	0.785771	-4.541393	2.552015
C	0.455722	-2.783601	1.381702
H	-0.622716	-2.772894	1.517249
C	-2.886695	-0.870498	1.313055
H	-2.477625	-0.129086	1.998160
C	-4.111529	-1.472721	1.533051
H	-4.694010	-1.205154	2.409826
C	-4.570326	-2.411020	0.617537
H	-5.530547	-2.899725	0.765257
C	-3.789146	-2.711986	-0.484306
H	-4.080117	-3.431322	-1.244106
C	-2.570275	-2.072094	-0.641704
C	-1.680359	-2.368561	-1.849220

FIrPic - U-DFT/M05-2X First Triplet State

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Ir	-0.152765	-0.324852	-0.245300
F	-1.515325	4.388807	1.706546
F	0.959935	1.702562	4.620543
F	3.433414	2.845966	-2.703468
F	5.071266	-0.851125	-0.391390
O	-0.507585	-1.717305	-1.875569
O	-1.943561	-3.266788	-2.634509

N	-1.192276	1.167426	-1.152867
N	1.041858	-1.763427	0.643895
N	-2.083673	-1.246314	0.256682
C	-1.642845	1.135185	-2.387484
H	-1.425848	0.229417	-2.937937
C	-2.338922	2.199787	-2.967393
H	-2.681500	2.114999	-3.986034
C	-2.567932	3.370601	-2.197505
H	-3.098392	4.207638	-2.627680
C	-2.108526	3.435190	-0.920140
H	-2.264514	4.318060	-0.325176
C	-1.392726	2.322264	-0.343719
C	-0.829526	2.225130	0.914023
C	-0.109392	0.965578	1.236378
C	0.480377	0.826052	2.480184
H	1.030070	-0.068351	2.739307
C	0.389811	1.844908	3.413850
C	-0.288874	3.056775	3.158604
H	-0.337546	3.831190	3.909849
C	-0.869717	3.228197	1.950415
C	1.637613	0.323036	-0.837404
C	2.721626	-0.477706	-0.405489
C	4.010942	-0.111116	-0.782028
C	4.279092	0.997163	-1.553631
H	5.289242	1.254953	-1.831197
C	3.194360	1.757664	-1.953021
C	1.892252	1.450274	-1.614174
H	1.098165	2.094455	-1.963403
C	2.371510	-1.642414	0.408631
C	3.254290	-2.589529	0.934456
H	4.309029	-2.496903	0.748178
C	2.763277	-3.640981	1.685629
H	3.445536	-4.375467	2.090784
C	1.396951	-3.748841	1.910366

H	0.974705	-4.557163	2.487405
C	0.573429	-2.784479	1.365916
H	-0.497303	-2.812176	1.501046
C	-2.853110	-0.960286	1.309591
H	-2.470246	-0.207887	1.986253
C	-4.063171	-1.598590	1.523033
H	-4.660615	-1.342152	2.385549
C	-4.480934	-2.561618	0.611232
H	-5.420576	-3.077326	0.753804
C	-3.679977	-2.847652	-0.482806
H	-3.940218	-3.577723	-1.234064
C	-2.482384	-2.164183	-0.630588
C	-1.571304	-2.431888	-1.835596

ClIrPic - DFT/M06 Ground state

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Ir	-0.219091	-0.570039	-0.350554
Cl	-2.889227	4.207202	1.157262
Cl	-0.014444	1.726806	4.880357
Cl	3.365708	3.233663	-2.675779
Cl	5.438176	-0.506840	0.466525
O	-0.205244	-2.118419	-1.890767
O	-1.372436	-3.847168	-2.711053
N	-1.255131	0.774291	-1.496395
N	0.967179	-1.804810	0.790674
N	-2.102094	-1.643603	-0.046780
C	-1.423553	0.586223	-2.810715
H	-1.026713	-0.350601	-3.196925
C	-2.027753	1.532662	-3.610957
H	-2.142447	1.350122	-4.674502
C	-2.451707	2.711167	-3.017242
H	-2.911697	3.495150	-3.613517
C	-2.281069	2.901068	-1.658313

H	-2.596253	3.830310	-1.206352
C	-1.682220	1.910592	-0.878654
C	-1.366350	1.944754	0.553589
C	-0.550712	0.863441	1.001679
C	-0.130360	0.819685	2.329903
H	0.512547	0.015768	2.682534
C	-0.538955	1.795342	3.217682
C	-1.374402	2.828648	2.826948
H	-1.709920	3.575540	3.538664
C	-1.780103	2.888839	1.505679
C	1.591302	0.227067	-0.705501
C	1.814346	1.348456	-1.500926
H	0.990907	1.861971	-1.992783
C	3.095301	1.830396	-1.674862
C	4.182740	1.231578	-1.063576
H	5.184371	1.625990	-1.197007
C	3.968516	0.122674	-0.266577
C	2.686786	-0.417641	-0.066427
C	2.312280	-1.580597	0.741485
C	3.155303	-2.451943	1.435187
H	4.224350	-2.310563	1.396140
C	2.637435	-3.501666	2.166879
H	3.310216	-4.168966	2.699457
C	1.266439	-3.695761	2.212688
H	0.815809	-4.506690	2.775583
C	0.471768	-2.824204	1.502299
H	-0.609743	-2.928540	1.490790
C	-3.031601	-1.369204	0.874696
H	-2.822160	-0.524488	1.529821
C	-4.186906	-2.119499	0.991400
H	-4.918667	-1.868467	1.753413
C	-4.383416	-3.184142	0.121482
H	-5.282077	-3.792426	0.190289
C	-3.421198	-3.458399	-0.834708

H	-3.507684	-4.271425	-1.549583
C	-2.285927	-2.666625	-0.894852
C	-1.198089	-2.927955	-1.937193

ClIrPic - U-DFT/M05-2X First Triplet State

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Ir	0.143748	0.589640	-0.253287
Cl	3.788154	-3.467693	0.957133
Cl	-0.260443	-2.772807	4.378770
Cl	-3.194174	-3.098386	-3.038208
Cl	-5.496344	0.206321	0.412416
O	0.008607	2.277936	-1.611492
O	1.069520	4.145209	-2.263465
N	1.267623	-0.504852	-1.557740
N	-1.100991	1.620572	1.021022
N	1.975315	1.732728	0.150848
C	1.427603	-0.209974	-2.835191
H	0.916185	0.682116	-3.171633
C	2.180532	-1.003618	-3.696971
H	2.276133	-0.723554	-4.733846
C	2.771578	-2.172885	-3.186232
H	3.325474	-2.831638	-3.839989
C	2.629647	-2.489743	-1.863086
H	3.048826	-3.402221	-1.477452
C	1.878472	-1.635494	-0.995590
C	1.612780	-1.806794	0.358705
C	0.553035	-0.913545	0.933341
C	-0.010560	-1.244879	2.143731
H	-0.830124	-0.660583	2.538283
C	0.474221	-2.328554	2.879809
C	1.641476	-3.033498	2.470863
H	2.086151	-3.756754	3.139663
C	2.225079	-2.757895	1.280522

C	-1.603931	-0.246704	-0.722696
C	-1.755466	-1.287162	-1.634743
H	-0.899197	-1.707326	-2.141046
C	-3.011525	-1.798845	-1.895407
C	-4.137931	-1.309246	-1.257368
H	-5.113610	-1.722647	-1.458521
C	-3.991387	-0.280870	-0.342399
C	-2.738399	0.281955	-0.054621
C	-2.430074	1.371513	0.893532
C	-3.327879	2.143150	1.633930
H	-4.383885	1.991622	1.532484
C	-2.864025	3.120030	2.497115
H	-3.570871	3.711484	3.062004
C	-1.501156	3.333368	2.627325
H	-1.097124	4.081819	3.291654
C	-0.655955	2.559744	1.858249
H	0.415468	2.684206	1.895536
C	2.944696	1.410600	1.011157
H	2.787844	0.508393	1.587802
C	4.077776	2.192230	1.158653
H	4.843689	1.899556	1.861373
C	4.200942	3.342265	0.387213
H	5.074382	3.972760	0.481309
C	3.192419	3.667654	-0.505964
H	3.221398	4.541594	-1.138955
C	2.089508	2.832700	-0.601614
C	0.958484	3.140860	-1.591712

BrIrPic - DFT/M06 Ground state

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Ir	0.110831	0.890218	-0.655705
Br	4.328839	-2.981829	0.381643
Br	1.818942	-0.599974	4.739464

Br	-3.162979	-3.830946	-1.775646
Br	-5.342075	0.190351	1.372390
O	-0.663472	2.172741	-2.242537
O	-0.169003	3.945422	-3.521341
N	1.069578	-0.389226	-1.934217
N	-0.950176	2.009646	0.703774
N	1.726906	2.325420	-1.016853
C	0.813256	-0.387694	-3.248051
H	0.132523	0.391826	-3.584737
C	1.344702	-1.336867	-4.095495
H	1.108925	-1.310638	-5.154349
C	2.147197	-2.323617	-3.544674
H	2.558833	-3.112437	-4.169280
C	2.417605	-2.316902	-2.188768
H	3.024204	-3.103540	-1.761510
C	1.886581	-1.320890	-1.369434
C	2.006968	-1.184460	0.087243
C	1.101429	-0.241862	0.659250
C	1.044515	-0.092330	2.045124
H	0.334580	0.599157	2.495760
C	1.901782	-0.811487	2.855034
C	2.847575	-1.674426	2.323262
H	3.542434	-2.201717	2.968877
C	2.894499	-1.847982	0.949730
C	-1.523529	-0.256116	-0.431965
C	-1.713985	-1.485214	-1.060007
H	-0.932912	-1.922409	-1.678538
C	-2.908795	-2.159892	-0.912438
C	-3.948156	-1.632781	-0.163599
H	-4.896131	-2.155083	-0.087369
C	-3.762200	-0.420696	0.478468
C	-2.545341	0.280417	0.400317
C	-2.166679	1.521596	1.080664
C	-2.865058	2.189618	2.087989

H	-3.806631	1.794781	2.440246
C	-2.358840	3.343078	2.652852
H	-2.915804	3.847774	3.438117
C	-1.143073	3.843732	2.214959
H	-0.711874	4.752434	2.622581
C	-0.470874	3.136911	1.242977
H	0.500737	3.461546	0.879460
C	2.915021	2.360421	-0.403288
H	3.084988	1.602325	0.360860
C	3.869892	3.309652	-0.716408
H	4.822880	3.307358	-0.195592
C	3.583892	4.248516	-1.699299
H	4.316810	5.006421	-1.965303
C	2.355196	4.203793	-2.334317
H	2.061077	4.901294	-3.112996
C	1.443809	3.225442	-1.970263
C	0.079536	3.132020	-2.654805

BrIrPic - U-DFT/M05-2X First Triplet State

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Ir	-0.178493	1.063608	0.061121
Br	-4.646378	-2.431811	0.651765
Br	-0.926459	-3.656161	-3.364162
Br	3.204608	-1.978896	3.703653
Br	5.410534	-0.260261	-1.090661
O	0.392504	3.024560	0.793719
O	-0.325194	5.140636	1.001349
N	-1.186391	0.606571	1.778818
N	0.929491	1.407495	-1.634768
N	-1.903845	2.329295	-0.438592
C	-1.092751	1.287010	2.908211
H	-0.437463	2.147194	2.877650
C	-1.765189	0.906635	4.066146

H	-1.650772	1.489872	4.965925
C	-2.548451	-0.258756	4.033439
H	-3.041410	-0.607508	4.929786
C	-2.671476	-0.967748	2.868310
H	-3.237934	-1.882194	2.844613
C	-2.002488	-0.525299	1.688009
C	-2.009834	-1.120748	0.429015
C	-0.959268	-0.632429	-0.525935
C	-0.648838	-1.409596	-1.618932
H	0.159860	-1.122882	-2.276431
C	-1.382530	-2.566099	-1.895565
C	-2.560298	-2.890032	-1.160852
H	-3.207885	-3.677926	-1.516592
C	-2.896157	-2.167578	-0.065698
C	1.518238	0.142081	0.557593
C	1.710696	-0.529107	1.761982
H	0.906180	-0.618089	2.476235
C	2.942760	-1.080029	2.051036
C	4.006800	-0.981450	1.171462
H	4.968876	-1.401113	1.417481
C	3.813357	-0.325847	-0.034416
C	2.575276	0.235262	-0.386014
C	2.201930	0.931963	-1.636150
C	2.977361	1.111584	-2.782204
H	3.975757	0.724702	-2.825083
C	2.464334	1.783340	-3.878090
H	3.078723	1.915208	-4.757723
C	1.170960	2.278251	-3.838646
H	0.732806	2.811121	-4.668548
C	0.437590	2.058860	-2.690247
H	-0.580106	2.404293	-2.593580
C	-3.038860	1.939842	-1.025121
H	-3.090653	0.899389	-1.318351
C	-4.082979	2.820787	-1.249622

H	-4.987759	2.470316	-1.723523
C	-3.937178	4.144748	-0.850983
H	-4.735798	4.855468	-1.013385
C	-2.758117	4.540105	-0.239450
H	-2.576344	5.548389	0.100027
C	-1.757922	3.599601	-0.045279
C	-0.444642	3.986373	0.647263

HIrPic - DFT/M06 Ground state

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Ir	-0.051876	0.072805	-0.188475
H	1.848094	-3.734521	2.527352
H	-1.142842	-1.532249	4.649069
H	-2.832662	-3.772534	-2.359736
H	-5.033740	-0.395724	-0.935688
O	0.269685	1.304886	-1.981727
O	1.503759	2.985506	-2.806597
N	1.333086	-1.335024	-0.750690
N	-1.568595	1.354431	0.380115
N	1.604936	1.402611	0.352054
C	1.892046	-1.372481	-1.967110
H	1.570080	-0.585964	-2.646824
C	2.792546	-2.354969	-2.322577
H	3.222113	-2.358447	-3.319232
C	3.120306	-3.325134	-1.382507
H	3.823150	-4.116673	-1.631186
C	2.541111	-3.283823	-0.129566
H	2.777819	-4.042216	0.611032
C	1.633431	-2.273853	0.183967
C	0.911580	-2.115803	1.437875
C	-0.028527	-1.056446	1.464479
C	-0.764091	-0.880048	2.640269

H	-1.511727	-0.088169	2.694928
C	-0.558603	-1.694062	3.744297
C	0.384614	-2.718620	3.709291
H	0.542067	-3.350604	4.579883
C	1.113869	-2.929878	2.554598
C	-1.646669	-0.965447	-0.840379
C	-2.888069	-0.319771	-0.648739
C	-4.081332	-0.904590	-1.079811
C	-4.064613	-2.139885	-1.696658
H	-4.992157	-2.597014	-2.032844
C	-2.849451	-2.795200	-1.879555
C	-1.662133	-2.219030	-1.456041
H	-0.728719	-2.759490	-1.615058
C	-2.822805	0.963468	0.027785
C	-3.911187	1.775941	0.345873
H	-4.910893	1.463330	0.059691
C	-3.718608	2.964022	1.017938
H	-4.567945	3.596023	1.265470
C	-2.429324	3.342321	1.374993
H	-2.230982	4.268446	1.905079
C	-1.386742	2.509294	1.033330
H	-0.358289	2.754134	1.287729
C	2.264265	1.411488	1.515765
H	1.937156	0.682934	2.256878
C	3.295151	2.298250	1.764701
H	3.806258	2.276156	2.722856
C	3.654391	3.202122	0.773032
H	4.460335	3.912745	0.941065
C	2.972840	3.184008	-0.430953
H	3.198340	3.855928	-1.253902
C	1.949055	2.267613	-0.613443
C	1.177853	2.203954	-1.933817

HIrPic - U-DFT/M05-2X First Triplet State

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Ir	-0.133516	0.025371	-0.190716
H	2.218803	-3.386504	2.655334
H	-0.687653	-1.101303	4.823378
H	-2.630003	-4.021824	-2.207595
H	-5.057586	-0.835233	-0.725218
O	0.040714	1.298864	-1.909922
O	1.165804	2.977894	-2.882096
N	1.339112	-1.233651	-0.795013
N	-1.714506	1.245715	0.406853
N	1.551468	1.454296	0.272372
C	1.848866	-1.305215	-2.037134
H	1.413471	-0.622662	-2.754649
C	2.837682	-2.189593	-2.377392
H	3.213958	-2.212049	-3.388203
C	3.341811	-3.064933	-1.371440
H	4.119202	-3.777232	-1.609854
C	2.833278	-2.998778	-0.105488
H	3.204035	-3.659216	0.665718
C	1.815718	-2.071249	0.215963
C	1.185265	-1.885388	1.472175
C	0.156465	-0.875620	1.533052
C	-0.498987	-0.612292	2.734281
H	-1.274736	0.143093	2.762662
C	-0.178304	-1.309469	3.893538
C	0.811540	-2.305623	3.830466
H	1.060462	-2.860449	4.726569
C	1.474560	-2.601673	2.658698
C	-1.647291	-1.110275	-0.771776
C	-2.923955	-0.558227	-0.537135
C	-4.074868	-1.250569	-0.903328
C	-3.964637	-2.494710	-1.506375

H	-4.857141	-3.033768	-1.792674
C	-2.708857	-3.049292	-1.740493
C	-1.557664	-2.364865	-1.375223
H	-0.585697	-2.803656	-1.552623
C	-2.938364	0.760194	0.106011
C	-4.075513	1.506974	0.404937
H	-5.052985	1.120350	0.162804
C	-3.941489	2.745034	1.005969
H	-4.819315	3.331185	1.240197
C	-2.672617	3.229525	1.300491
H	-2.525502	4.192672	1.764751
C	-1.582983	2.443237	0.979665
H	-0.569894	2.758369	1.182254
C	2.309814	1.453980	1.370588
H	2.030133	0.747879	2.140879
C	3.389525	2.312404	1.506037
H	3.985541	2.283781	2.406271
C	3.684026	3.190348	0.470288
H	4.521623	3.869551	0.550129
C	2.894747	3.178726	-0.669477
H	3.066185	3.825972	-1.516023
C	1.836751	2.286831	-0.732163
C	0.949341	2.208662	-1.971789

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