CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Unveiling Photodeactivation Pathways for a New Iridium(III) Cyclometalated Complex

Daniel Escudero,*[a] Eike Heuser,[b, c] Robert J. Meier,[d] Michael Schäferling,[e] Walter Thiel,[a] and Elisabeth Holder*[b, c]

chem_201301291_sm_miscellaneous_information.pdf

Supporting Information for:

Unveiling photodeactivation pathways for a new iridium(III) cyclometalated complex

Daniel Escudero,*[,a] Eike Heuser,[b,c] Robert J. Meier,[d] Michael Schäferling,[e] Walter Thiel[a] and Elisabeth Holder*[,b,c]

[a]*Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470, Mülheim an der Ruhr, Germany. Fax: +49(0)2083062996; Tel: +49(0)2083062165; E-mail: escudero@kofo.mpg.de*
[b]*Functional Polymers Group and Institute of Polymer Technology, University of Wuppertal, Gaußstr. 20, D-42097 Wuppertal, Germany. Fax: +49-202-439-3880; Tel: +49-202-439-3879; E-mail: holder@uni-wuppertal.de*
[c]*Dutch Polymer Institute (DPI), P.O. Box 513, NL-5600 AX Eindhoven, The Netherlands.*
[d]*Institute of Analytical Chemistry, Chemo- and Biosensors, University of Regensburg, D-93040 Regensburg, Germany.*
[e] *Department of Biotechnology, University of Turku, Tykistökatu 6A, BioCity 6th floor, 20520 Turku, Finland.*

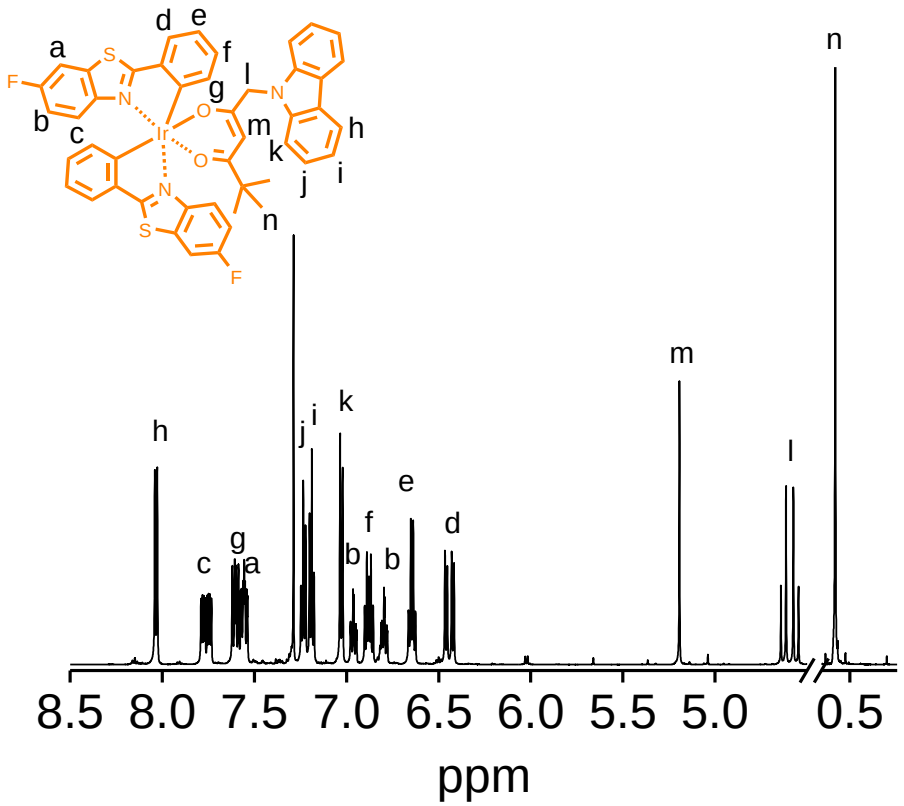

Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of complex **1**. The resonances were assigned with the help of ^{1}H-^{1}H COSY experiments.

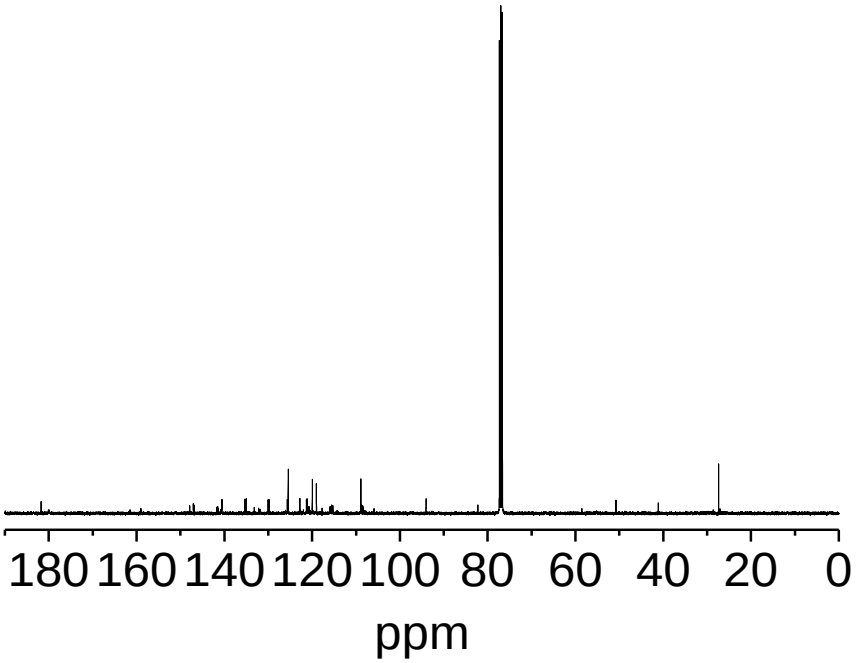

Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) of complex **1**.

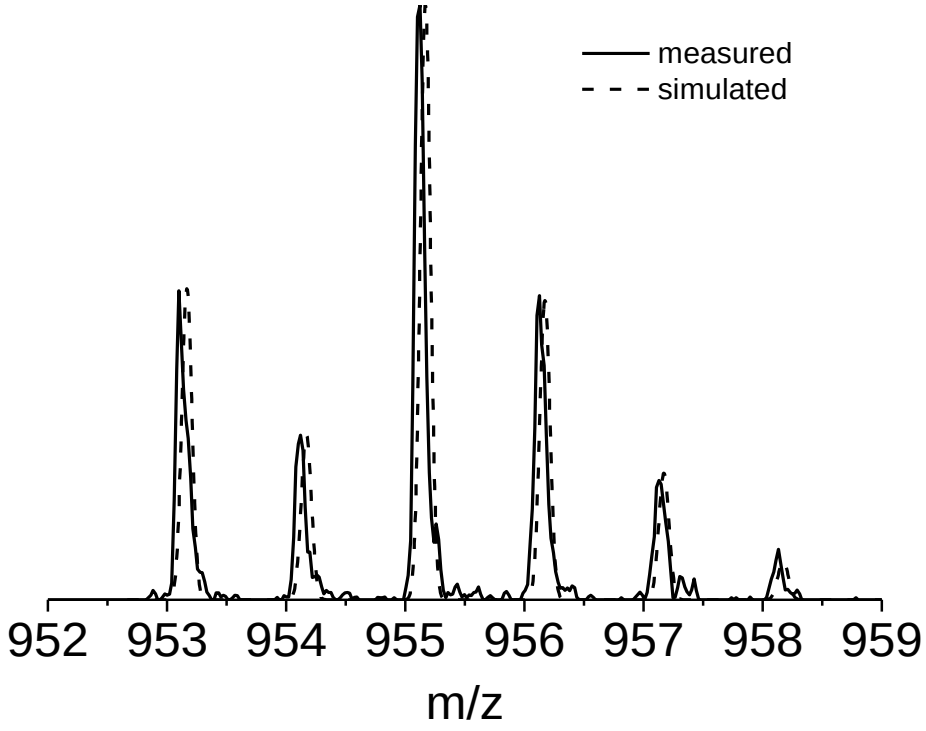

Figure S3. Normalized measured and simulated APLI-MS spectra of complex **1**.

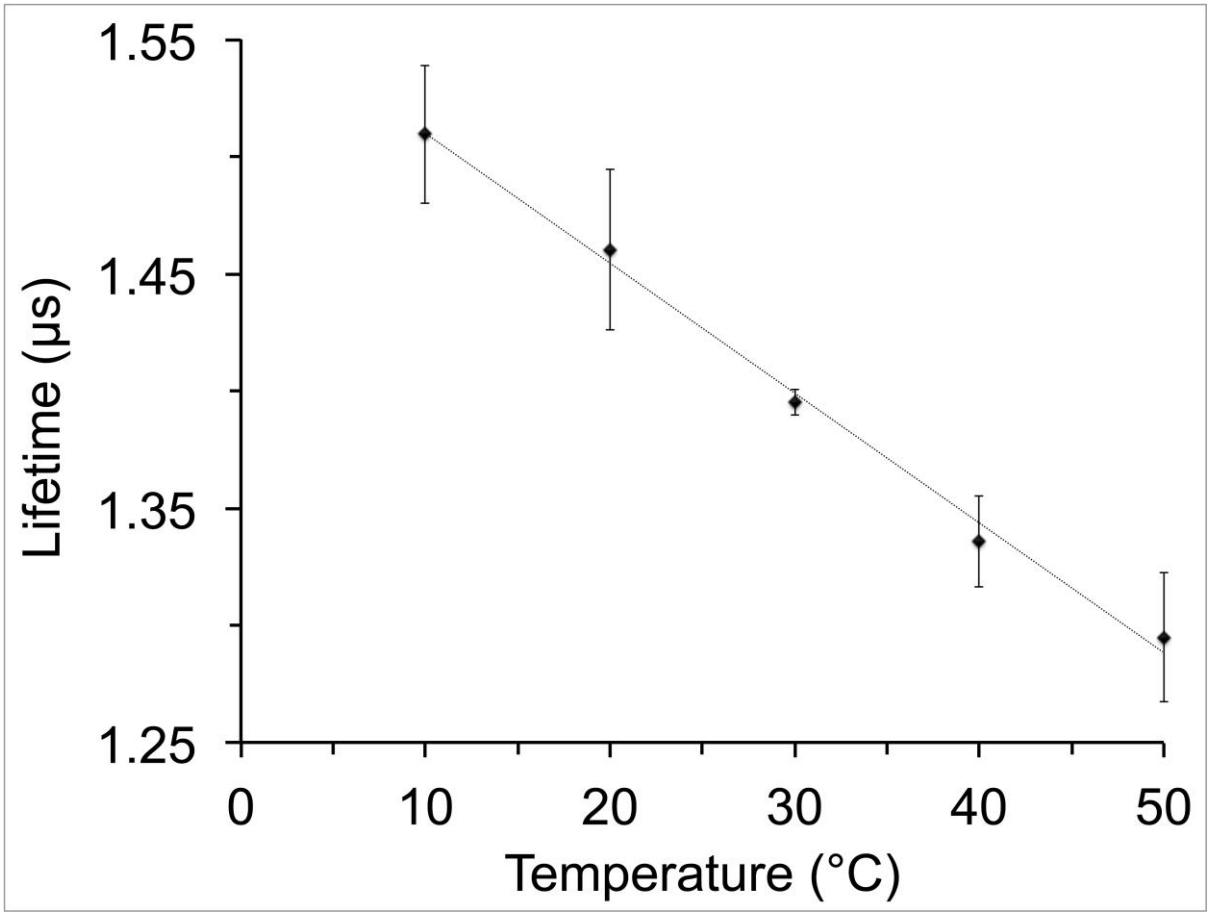

Figure S4. Temperature dependency of the luminescent lifetime of complex **1** at 1000 mbar standard air pressure.

Computational details

All calculations are based on density functional theory (DFT). The geometries of the singlet ground state (S_0), the lowest emitting (T_1) triplet excited state, the lowest ^{3}MC triplet excited states and the transition state (TS) along the $T_1 \rightarrow {}^3$MC transformation were optimized for complex **1**. For these optimizations the hybrid functional B3LYP[1,2] was selected in combination with the 6-31G* basis set for all atoms. Relativistic effects were included for the Ir atom by using the ECP-60-mwb Stuttgart/Dresden pseudopotential.[3] The nature of the stationary points was confirmed by computing the Hessian at the same level of theory. The minimum energy crossing point (MECP) between the S_0 and the ^{3}MC PES was optimized using Harvey´s algorithm,[4] as implemented in the ORCA software;[5] in this case, the B3LYP functional was employed in combination with the def2-svp basis set and the ECP-60-mwb Stuttgart/Dresden pseudopotential for Ir. To get relative energies for S_0, T_1, ^{3}MC, TS and MECP, single-point calculations with the 6-31G* basis set were performed. No spin contamination was observed for the optimized triplet structures. Intrinsic reaction coordinate (IRC) calculations were performed on the S_0 potential energy surface starting at the $S_0/{}^3$MC MECP geometry. The IRC follows the minimum energy reaction pathway in mass-weighted Cartesian coordinates.

The UV-Vis absorption spectrum was obtained by calculating the lowest-lying 130 vertical singlet electronic excitation energies using time-dependent DFT (TD-DFT) at the S_0 optimized geometry. The phosphorescence emission spectra were simulated on the basis of ΔSCF-DFT calculations, which yield the energy difference between the lowest triplet excited state at its optimized geometry (T_1) and the closed-shell ground state at the same geometry in the gas phase. The resulting values are adiabatic in the sense that the lowest triplet state is relaxed to its minimum geometry, but they are computed as vertical transitions to the ground state at the lowest triplet state geometry. This approach is a simple but reliable way to determine emission energies. Both the TD-DFT and ΔSCF-DFT calculations were performed in solution using chloroform as solvent with the polarization continuum model[6,7] and employing the same functional and basis set as in the optimizations. All the calculations apart from the MECP optimization were performed with the Gaussian09 program package.[8]

TDDFT results

Table S1. Main PCM-TDDFT electronic singlet-singlet transition energies (ΔE) with corresponding oscillator strengths (*f*) and assignment for complex **1**.

State	ΔE /nm	*f*	Assignment
S_1	488	0.011	$d_{xy} + \pi_{cycl} \rightarrow \pi^*_{cycl}$ (0.63) MLCT
S_2	477	0.039	$d_{xy} + \pi_{cycl} \rightarrow \pi^*_{cycl}$ (0.63) MLCT
S_3	434	0.055	$d_{yz} \rightarrow \pi^*_{cycl}$ (0.63) MLCT
S_6	399	0.043	$d_{xz} \rightarrow \pi^*_{cycl}$ (0.38) MLCT
S_{15}	337	0.051	$\pi_{anc} \rightarrow \pi^*_{anc}$ (0.52) LC
S_{16}	336	0.100	$\pi_{anc} + \pi_{cycl} \rightarrow \pi^*_{anc}$ (0.53) LLCT
S_{18}	318	0.141	$\pi_{cycl} \rightarrow \pi^*_{cycl}$ (0.67) LC
S_{20}	313	0.243	$\pi_{cycl} \rightarrow \pi^*_{cycl}$ (0.60) LC
S_{34}	283	0.082	$d_{yz} \rightarrow \pi^*_{cycl}$ (0.40) MLCT
S_{37}	278	0.114	$d_{yz} \rightarrow \pi^*_{cycl}$ (0.45) MLCT
S_{39}	274	0.133	$\pi_{anc} \rightarrow \pi^*_{anc}$ (0.55) LC

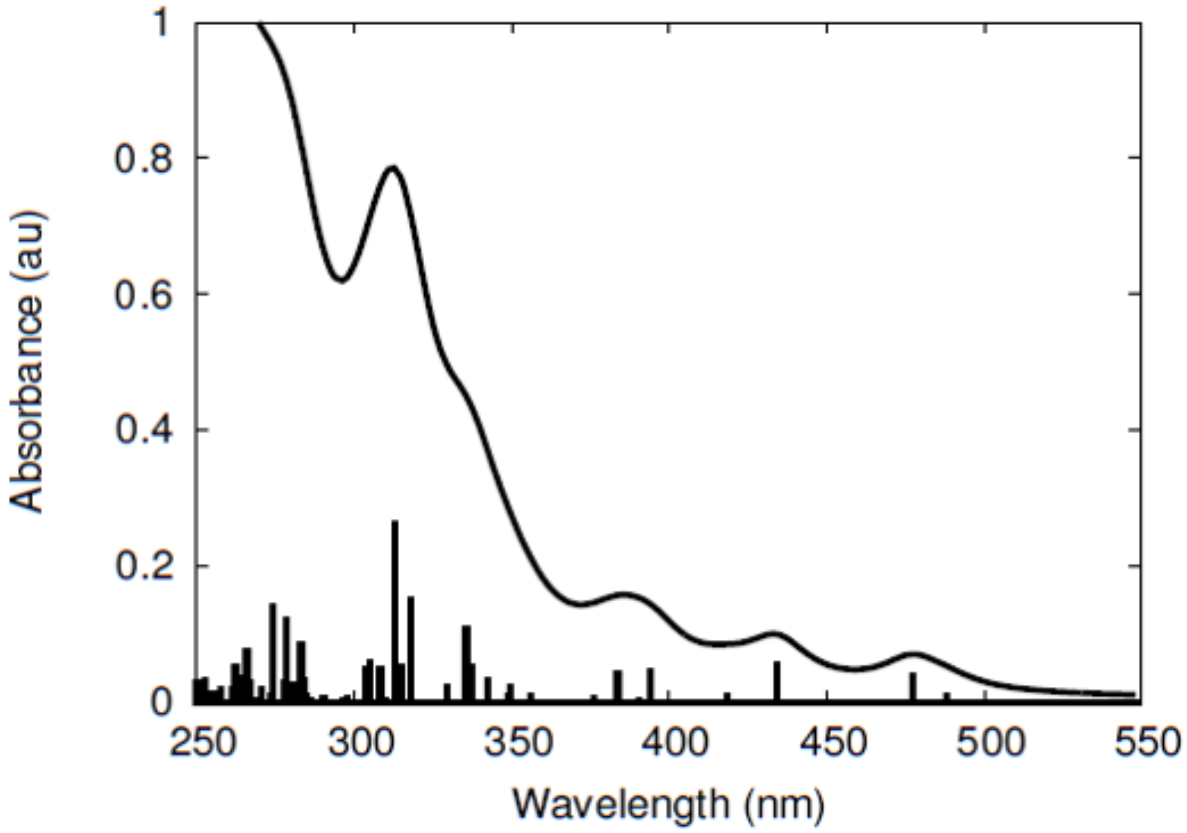

Figure S5. Computed PCM-TDDFT UV-Vis absorption spectrum of complex **1**. The theoretical spectrum is convoluted with a Lorentzian function with a full width at half-maximum (fwhm) of 12 nm; the corresponding transitions are marked with vertical lines.

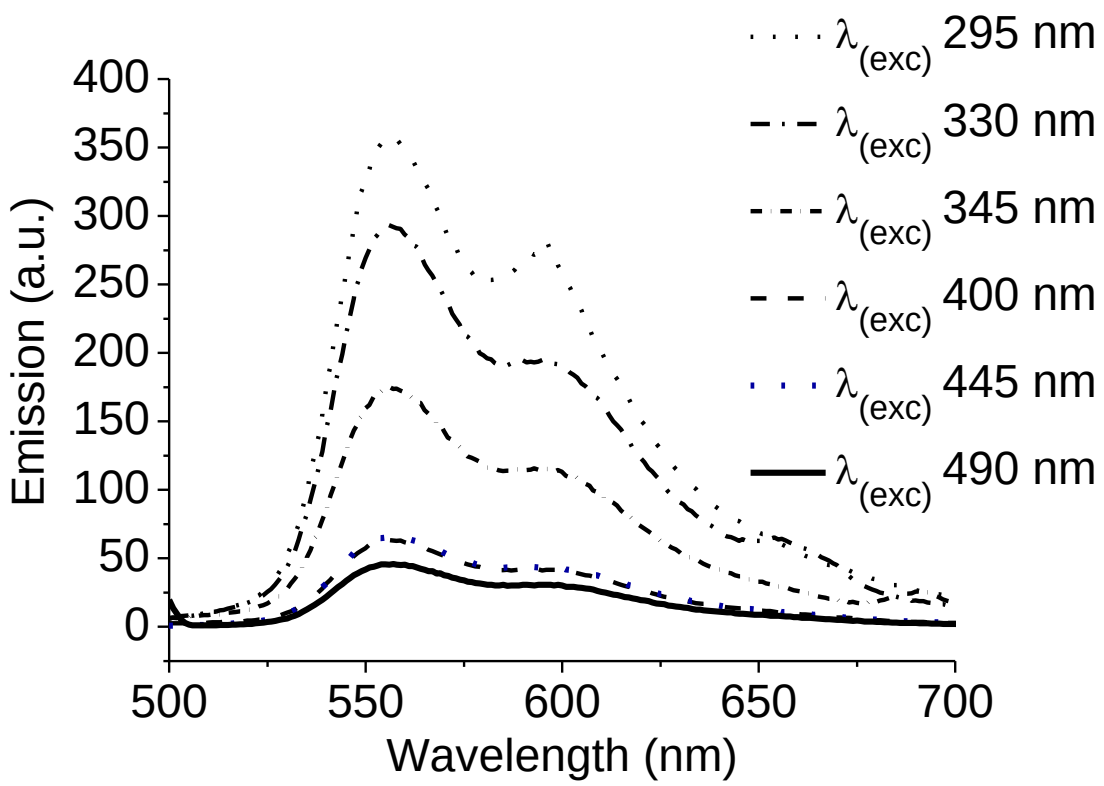

Figure S6. Emission spectra of complex **1** ($CHCl_3$ solution, 10^{-5} M) recorded at different excitation wavelengths.

Cartesian coordinates of the optimized geometries.

S_0

C	-2.433720	-1.422400	-2.587933
C	-2.966977	-1.627560	-3.872072
H	-2.887167	-2.600294	-4.353551
C	-3.602804	-0.578286	-4.521513
H	-4.021108	-0.720846	-5.513569
C	-3.705896	0.665017	-3.880556
H	-4.212272	1.485488	-4.384156
C	-3.170931	0.867834	-2.606808
H	-3.271363	1.845173	-2.143250
C	-4.000572	-1.357264	1.259335
H	-3.722517	-2.322188	0.844685
C	-5.103780	-1.279233	2.111810
H	-5.664512	-2.181973	2.343905
C	-5.502574	-0.057224	2.673093
H	-6.361247	-0.012079	3.336493
C	-4.792893	1.095828	2.366551
H	-5.095719	2.052572	2.787664
C	-3.685625	1.015507	1.504705
Ir	-1.548672	-0.087685	-0.148228
C	-3.246317	-0.217126	0.935276
O	-0.377966	-0.029144	1.717532
C	0.877212	0.134402	1.834443
C	1.802823	0.190135	0.764930
H	2.848694	0.275504	1.025221
C	1.517592	0.166157	-0.600939
O	0.379812	0.125432	-1.181834
C	1.417347	0.275655	3.279402
C	2.670042	0.233639	-1.619050
C	-2.507088	-0.163434	-1.921158
C	2.451337	-0.838783	3.565224
C	2.092708	1.660054	3.428383

C	0.269747	0.167953	4.299017
H	2.005678	-1.833625	3.447524
H	2.811351	-0.752646	4.597538
H	3.319995	-0.781247	2.902576
H	2.939633	1.782311	2.746620
H	2.463612	1.784026	4.453137
H	1.379197	2.468242	3.228787
H	-0.488051	0.939482	4.135719
H	0.669986	0.285463	5.312956
H	-0.234189	-0.801949	4.242004
H	2.547026	-0.608743	-2.307947
H	2.525886	1.137027	-2.223578
C	4.761221	1.351742	-0.750669
C	4.813803	-0.903743	-0.924334
C	4.381692	2.697580	-0.745383
C	6.061406	0.942967	-0.350361
C	4.500860	-2.250015	-1.134813
C	6.094663	-0.501271	-0.461053
C	5.331834	3.637666	-0.348734
H	3.378119	3.006672	-1.022114
C	6.994904	1.908195	0.044550
C	5.495512	-3.193949	-0.884081
H	3.516333	-2.559403	-1.472749
C	7.074230	-1.470559	-0.215454
C	6.626166	3.251313	0.040501
H	5.061254	4.690010	-0.335251
H	7.994765	1.612704	0.351975
C	6.770032	-2.812579	-0.429736
H	5.276215	-4.246891	-1.039173
H	8.059865	-1.178952	0.138240
N	4.019505	0.226929	-1.105361
H	7.342354	4.008856	0.345785
H	7.521950	-3.573674	-0.241702
C	-0.881499	-3.224811	0.126592
C	-1.805819	-2.444153	-1.789415
C	-0.897313	-4.424158	-0.619360
C	-0.419523	-3.232861	1.450326
C	-0.436320	-5.627462	-0.084870
C	0.037339	-4.427173	1.994813
H	-0.436081	-2.315227	2.025018
C	0.028024	-5.593562	1.222663
H	-0.438586	-6.557959	-0.641421
H	0.400690	-4.477096	3.015630
N	-1.382362	-2.130363	-0.572659
S	-1.582763	-4.133182	-2.210620
F	0.479982	-6.737054	1.775436
C	-1.308126	3.114996	-0.216057
C	-2.907594	2.145635	1.064195
C	-1.853165	4.275151	0.376724
C	-0.285805	3.230792	-1.168797
C	-1.378581	5.549652	0.065425
C	0.189035	4.496567	-1.492306
H	0.100486	2.335058	-1.640577
C	-0.354654	5.624924	-0.868562
H	-1.781090	6.452678	0.510480
H	0.972404	4.632871	-2.230341
N	-1.912167	1.937474	0.213396
S	-3.161652	3.835715	1.464363
F	0.128408	6.839584	-1.198298

T_1

C	2.487219	1.392031	-2.558116
C	3.051855	1.576945	-3.829790
H	2.998802	2.545919	-4.321917
C	3.687231	0.511028	-4.456160
H	4.128585	0.640239	-5.439959
C	3.759113	-0.727695	-3.805515
H	4.263520	-1.559510	-4.291455
C	3.195057	-0.911483	-2.540456
H	3.269666	-1.883728	-2.063692
C	3.944560	1.387198	1.316265
H	3.648447	2.347022	0.901787
C	5.045359	1.329916	2.177196
H	5.591229	2.235340	2.426615
C	5.455139	0.088590	2.729429
H	6.311437	0.060875	3.398878

C	4.788809	-1.079050	2.430608
H	5.114242	-2.025694	2.854462
C	3.663941	-1.040640	1.549120
Ir	1.555948	0.089921	-0.117059
C	3.219976	0.240176	0.980372
O	0.370873	0.064247	1.742022
C	-0.884952	-0.098060	1.857788
C	-1.807516	-0.167652	0.786368
H	-2.853637	-0.256783	1.044095
C	-1.517084	-0.160999	-0.577955
O	-0.375345	-0.122973	-1.152588
C	-1.426107	-0.224089	3.303003
C	-2.662771	-0.248162	-1.601291
C	2.537085	0.138423	-1.881370
C	-2.480474	0.875420	3.570821
C	-2.076544	-1.618816	3.468745
C	-0.282164	-0.082058	4.322706
H	-2.053015	1.876623	3.439338
H	-2.839226	0.797838	4.604127
H	-3.347952	0.792580	2.909367
H	-2.917888	-1.765980	2.784924
H	-2.449715	-1.734161	4.493599
H	-1.346953	-2.415901	3.284352
H	0.490103	-0.840886	4.169755
H	-0.682199	-0.193994	5.337319
H	0.202997	0.896869	4.254448
H	-2.550036	0.594134	-2.292146
H	-2.499758	-1.151211	-2.201592
C	-4.733659	-1.398638	-0.730048
C	-4.833759	0.853422	-0.932354
C	-4.324758	-2.735636	-0.706784
C	-6.044429	-1.012998	-0.342314
C	-4.549295	2.203435	-1.158376
C	-6.108309	0.428769	-0.471420
C	-5.256846	-3.690973	-0.303678
H	-3.313468	-3.026743	-0.974988
C	-6.959231	-1.993264	0.059386
C	-5.565864	3.128532	-0.925640
H	-3.569998	2.530241	-1.495251
C	-7.110244	1.379385	-0.244008
C	-6.561350	-3.327949	0.073892
H	-4.963724	-4.736938	-0.275921
H	-7.967013	-1.715853	0.357632
C	-6.834307	2.725023	-0.473711
H	-5.368903	4.183951	-1.093416
H	-8.091382	1.070674	0.107594
N	-4.013993	-0.262030	-1.094064
H	-7.262653	-4.097065	0.384697
H	-7.603937	3.471643	-0.299924
C	0.857911	3.249961	0.077182
C	1.845084	2.432604	-1.789576
C	0.884098	4.430617	-0.698006
C	0.357089	3.284948	1.386559
C	0.396259	5.642152	-0.207568
C	-0.128044	4.486983	1.886393
H	0.368241	2.383235	1.986213
C	-0.107118	5.634483	1.085726
H	0.406105	6.558865	-0.786345
H	-0.521893	4.558640	2.894465
N	1.392577	2.145841	-0.579228
S	1.620511	4.107006	-2.259448
F	-0.586968	6.785161	1.596331
C	1.318174	-3.054417	-0.242098
C	2.911401	-2.131635	1.141859
C	1.855300	-4.240544	0.352775
C	0.328765	-3.177269	-1.248338
C	1.399648	-5.499829	-0.004250
C	-0.124019	-4.439462	-1.608691
H	-0.046657	-2.280567	-1.725634
C	0.404596	-5.571981	-0.982258
H	1.790588	-6.409556	0.438002
H	-0.875252	-4.568954	-2.380773
N	1.863493	-1.901698	0.225190
S	3.112725	-3.851673	1.529119
F	-0.051496	-6.786925	-1.343792

^{3}MC

C	-3.112932	-0.009129	2.520157
C	-3.650198	-0.140474	3.812063
H	-4.364916	0.590601	4.184657
C	-3.272596	-1.206101	4.620773
H	-3.689801	-1.306759	5.618673
C	-2.351607	-2.144464	4.139360
H	-2.053643	-2.980085	4.768374
C	-1.813096	-2.014006	2.858206
H	-1.099391	-2.753068	2.503241
C	-3.904620	-1.852750	-0.886510
H	-4.354342	-0.918762	-0.563129
C	-4.698349	-2.797332	-1.536216
H	-5.750913	-2.591548	-1.714841
C	-4.144461	-4.014636	-1.944072
H	-4.758209	-4.761648	-2.439470
C	-2.797684	-4.269526	-1.704920
H	-2.376401	-5.222703	-2.016292
C	-1.986958	-3.313065	-1.071634
Ir	-1.352214	-0.630098	0.179971
C	-2.529869	-2.060730	-0.646601
O	-0.388254	-0.048006	-1.670754
C	0.747904	0.500160	-1.812816
C	1.508864	1.059977	-0.753462
H	2.452777	1.521276	-1.009187
C	1.082411	1.203435	0.565624
O	0.005705	0.752302	1.094853
C	1.292878	0.600104	-3.255154
C	1.900926	2.044501	1.559364
C	-2.172270	-0.952274	2.008447
C	1.393429	2.090924	-3.658076
C	2.693694	-0.052875	-3.321359
C	0.354289	-0.127230	-4.233669
H	0.410394	2.575587	-3.621194
H	1.769033	2.173499	-4.685040
H	2.070344	2.650925	-3.005339
H	3.425070	0.464523	-2.693240
H	3.062693	-0.024893	-4.353640
H	2.657590	-1.101066	-3.003885
H	0.255240	-1.187085	-3.979762
H	0.756844	-0.052131	-5.250547
H	-0.649540	0.307238	-4.228422
H	1.366084	2.989819	1.712013
H	1.879621	1.528844	2.524157
C	4.371555	1.547506	1.539672
C	3.715071	3.422055	0.456089
C	4.423654	0.366924	2.287761
C	5.545934	2.139983	1.003684
C	2.979195	4.469142	-0.107906
C	5.125630	3.340782	0.310735
C	5.673736	-0.217960	2.492048
H	3.528570	-0.082654	2.707410
C	6.786649	1.529098	1.219804
C	3.679277	5.447856	-0.811996
H	1.898941	4.521336	-0.011265
C	5.802750	4.336743	-0.402995
C	6.844572	0.351771	1.961523
H	5.741048	-1.129477	3.080133
H	7.694184	1.969760	0.815364
C	5.076183	5.386374	-0.959413
H	3.130261	6.272914	-1.257580
H	6.882208	4.290569	-0.521660
N	3.271253	2.333482	1.204572
H	7.802149	-0.129783	2.137249
H	5.591001	6.164503	-1.515568
C	-3.456220	2.293058	-0.256324
C	-3.478197	1.088685	1.639299
C	-4.348261	3.104953	0.484889
C	-3.113544	2.646364	-1.570115
C	-4.903091	4.264213	-0.059305
C	-3.660020	3.798829	-2.121441
H	-2.431374	2.015804	-2.131320
C	-4.537589	4.580709	-1.360955
H	-5.588293	4.904061	0.485400
H	-3.424175	4.109944	-3.133414
N	-2.999257	1.181562	0.425435
S	-4.585846	2.410203	2.078119
F	-5.053563	5.694500	-1.920487
C	1.531898	-3.219468	-0.157955

C	-0.570776	-3.587324	-0.828946
C	1.728726	-4.512300	-0.703157
C	2.620761	-2.525182	0.391596
C	2.982153	-5.127003	-0.695931
C	3.874271	-3.122686	0.399278
H	2.476429	-1.525482	0.785004
C	4.028939	-4.406542	-0.137028
H	3.157626	-6.115752	-1.104844
H	4.738219	-2.608325	0.806071
N	0.234579	-2.749924	-0.239543
S	0.213045	-5.111068	-1.339498
F	5.255373	-4.968429	-0.115553

MECP ($S_0/^3MC$)

C	-3.082706	0.063172	2.446733
C	-3.627722	-0.056209	3.738755
H	-4.324569	0.701395	4.110913
C	-3.294735	-1.136001	4.553872
H	-3.727146	-1.219932	5.553877
C	-2.402550	-2.106460	4.081403
H	-2.132394	-2.955346	4.716613
C	-1.852806	-1.990728	2.802369
H	-1.153313	-2.754631	2.452297
C	-3.861171	-1.828511	-0.981257
H	-4.267066	-0.859983	-0.681459
C	-4.691270	-2.745788	-1.626822
H	-5.734793	-2.491530	-1.832529
C	-4.186311	-3.997697	-1.998610
H	-4.829623	-4.731519	-2.491258
C	-2.854203	-4.312333	-1.729624
H	-2.476206	-5.296650	-2.019831
C	-2.002835	-3.386410	-1.098993
Ir	-1.311363	-0.695220	0.124868
C	-2.500505	-2.101276	-0.706582
O	-0.266579	-0.160108	-1.666257
C	0.859489	0.394201	-1.820452
C	1.596485	0.990374	-0.762667
H	2.550145	1.456102	-1.001946
C	1.121238	1.148765	0.542933
O	0.022150	0.710425	1.014605
C	1.415658	0.455103	-3.261671
C	1.909551	1.970708	1.571274
C	-2.175737	-0.919010	1.945983
C	1.494724	1.932621	-3.711148
C	2.824973	-0.177726	-3.294349
C	0.489725	-0.318479	-4.215415
H	0.501160	2.409119	-3.688481
H	1.869255	1.988463	-4.746823
H	2.169150	2.525965	-3.075278
H	3.545306	0.372592	-2.671129
H	3.208717	-0.176951	-4.327756
H	2.801400	-1.222538	-2.945670
H	0.397580	-1.373745	-3.918959
H	0.894629	-0.278739	-5.239153
H	-0.523587	0.108172	-4.226992
H	1.301509	2.859850	1.808606
H	1.942379	1.381350	2.500848
C	4.405270	1.658087	1.457459
C	3.583636	3.561388	0.553124
C	4.564452	0.420409	2.095727
C	5.522306	2.382594	0.953722
C	2.756612	4.596874	0.097169
C	4.995047	3.604071	0.374272
C	5.860113	-0.085393	2.224061
H	3.709803	-0.135056	2.486462
C	6.812086	1.849433	1.093636
C	3.363372	5.685620	-0.532353
H	1.672261	4.558916	0.220497
C	5.577521	4.708444	-0.265081
C	6.974481	0.617409	1.727518
H	6.010004	-1.046784	2.722687
H	7.679366	2.394165	0.712204
C	4.758542	5.744968	-0.713167
H	2.739525	6.506942	-0.895358
H	6.660043	4.755360	-0.411543
N	3.242599	2.382659	1.211142

H	7.974528	0.192144	1.842699
H	5.200623	6.611438	-1.211720
C	-3.465036	2.468162	-0.251129
C	-3.425345	1.199629	1.590181
C	-4.237155	3.316390	0.586708
C	-3.203372	2.855748	-1.577947
C	-4.745018	4.537057	0.127494
C	-3.703574	4.067187	-2.044247
H	-2.611873	2.200323	-2.220508
C	-4.460400	4.884135	-1.189446
H	-5.337690	5.207503	0.752413
H	-3.521254	4.404007	-3.066450
N	-3.038712	1.305036	0.350577
S	-4.395527	2.580847	2.164325
F	-4.926988	6.048836	-1.663337
C	1.517274	-3.539547	-0.162582
C	-0.601131	-3.746820	-0.837417
C	1.609512	-4.860549	-0.678143
C	2.662216	-2.930045	0.383214
C	2.808399	-5.581663	-0.643954
C	3.859768	-3.635522	0.418326
H	2.599904	-1.907909	0.758664
C	3.912216	-4.944015	-0.088138
H	2.902404	-6.597186	-1.031397
H	4.769069	-3.191023	0.827469
N	0.268614	-2.968223	-0.265330
S	0.056172	-5.340560	-1.311628
F	5.078460	-5.604748	-0.038072

TS ($T_1 \rightarrow {}^3MC$)

C	-2.754704	-0.990445	-2.594033
C	-3.343984	-1.064552	-3.868122
H	-3.605416	-2.030832	-4.293776
C	-3.576378	0.099351	-4.594592
H	-4.030388	0.035281	-5.580003
C	-3.220061	1.351782	-4.068161
H	-3.414750	2.255005	-4.640258
C	-2.625534	1.434489	-2.809388
H	-2.347994	2.406441	-2.411584
C	-4.149613	-0.260408	1.228658
H	-4.096126	-1.285915	0.874493
C	-5.213913	0.125972	2.046196
H	-5.973639	-0.599955	2.324941
C	-5.308297	1.443477	2.510455
H	-6.139387	1.742039	3.143059
C	-4.336294	2.376236	2.155811
H	-4.420719	3.403363	2.504681
C	-3.263033	1.988332	1.341714
Ir	-1.493921	0.240752	-0.243531
C	-3.143867	0.648123	0.856747
O	-0.319015	0.111954	1.583180
C	0.933063	-0.048659	1.754640
C	1.869367	-0.254855	0.719918
H	2.900781	-0.413631	1.001783
C	1.593067	-0.240761	-0.649670
O	0.473081	-0.036406	-1.223209
C	1.433137	-0.006909	3.218261
C	2.730447	-0.460008	-1.662113
C	-2.392552	0.285416	-2.029100
C	2.159971	-1.327976	3.562760
C	2.413715	1.180144	3.373984
C	0.253161	0.184391	4.187461
H	1.493752	-2.190878	3.445319
H	2.494434	-1.303671	4.606802
H	3.038947	-1.495831	2.933720
H	3.290004	1.078361	2.726571
H	2.764234	1.238413	4.411604
H	1.922393	2.129469	3.130507
H	-0.284825	1.115557	3.987481
H	0.627440	0.216796	5.217484
H	-0.469052	-0.634486	4.111692
H	2.422596	-1.274133	-2.326514
H	2.790304	0.434874	-2.293067
C	5.010049	0.191800	-0.795096
C	4.570473	-2.024347	-0.923911

C	4.932990	1.587733	-0.818655
C	6.187018	-0.481854	-0.372348
C	3.971837	-3.273879	-1.110427
C	5.905067	-1.900647	-0.454323
C	6.062205	2.306627	-0.428910
H	4.022256	2.101697	-1.111286
C	7.305694	0.265003	0.014757
C	4.734156	-4.406238	-0.828155
H	2.946007	-3.368420	-1.453636
C	6.647400	-3.054702	-0.177558
C	7.238644	1.655869	-0.018410
H	6.027166	3.392713	-0.437280
H	8.214999	-0.234674	0.338871
C	6.058138	-4.302147	-0.367040
H	4.290823	-5.388969	-0.963813
H	7.670513	-2.977618	0.181444
N	4.043329	-0.751414	-1.136664
H	8.100554	2.245437	0.280786
H	6.624045	-5.204667	-0.154377
C	-1.777355	-3.094480	0.158501
C	-2.514734	-2.119376	-1.741896
C	-2.506994	-4.184463	-0.378116
C	-1.129591	-3.240219	1.394876
C	-2.577727	-5.413267	0.278647
C	-1.201763	-4.457459	2.062515
H	-0.598493	-2.396871	1.818769
C	-1.913606	-5.517863	1.493677
H	-3.129347	-6.259350	-0.115990
H	-0.716343	-4.604839	3.021354
N	-1.771855	-1.961683	-0.641946
S	-3.260500	-3.720704	-1.896073
F	-1.966704	-6.691275	2.158840
C	-0.373070	3.502563	-0.224313
C	-2.212649	2.902947	0.924420
C	-0.580652	4.711461	0.481418
C	0.684593	3.395195	-1.139974
C	0.256421	5.813945	0.301322
C	1.521852	4.487610	-1.327906
H	0.822137	2.466019	-1.682770
C	1.296466	5.666711	-0.606229
H	0.121364	6.751265	0.829198
H	2.348704	4.453799	-2.029310
N	-1.308124	2.520834	0.051960
S	-1.989528	4.555599	1.516647
F	2.126043	6.709657	-0.807416

References

[1] A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648.

[2] C. T. Lee, W. T. Yang, R. G. Parr, *Phys. Rev. B.* **1988**, *37*, 785.

[3] D. Andrae, U. Häusermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta* **1990**, *77***,** 123.

[4] J. Harvey, M. Aschi, H. Schwarz, W. Koch, *Theor. Chim. Acta* **1998**, *99*, 95.

[5] F. Neese. Orca, an ab initio, DFT and semiempirical SCF-MO, package 2.8.0 R2327, University of Bonn: Bonn, Germany, 2011.

[6] M. Cossi, V. Barone, B. Menucci, J. Tomasi, *Chem. Phys. Lett.* **1998**, *286*, 253.

[7] B. Menucci, J. Tomasi, *J. Chem. Phys.* **1997**, *106*, 5151.

[8] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.