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Supporting Information

Spectroscopic Evidence for a New Type of Bonding between a Thioether Radical Cation and a Phenyl Group

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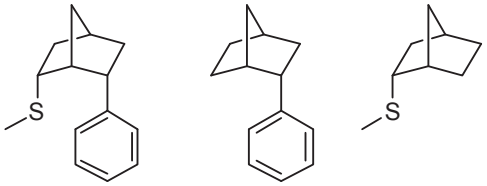
Contents

Citation

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



1 **2** **3**

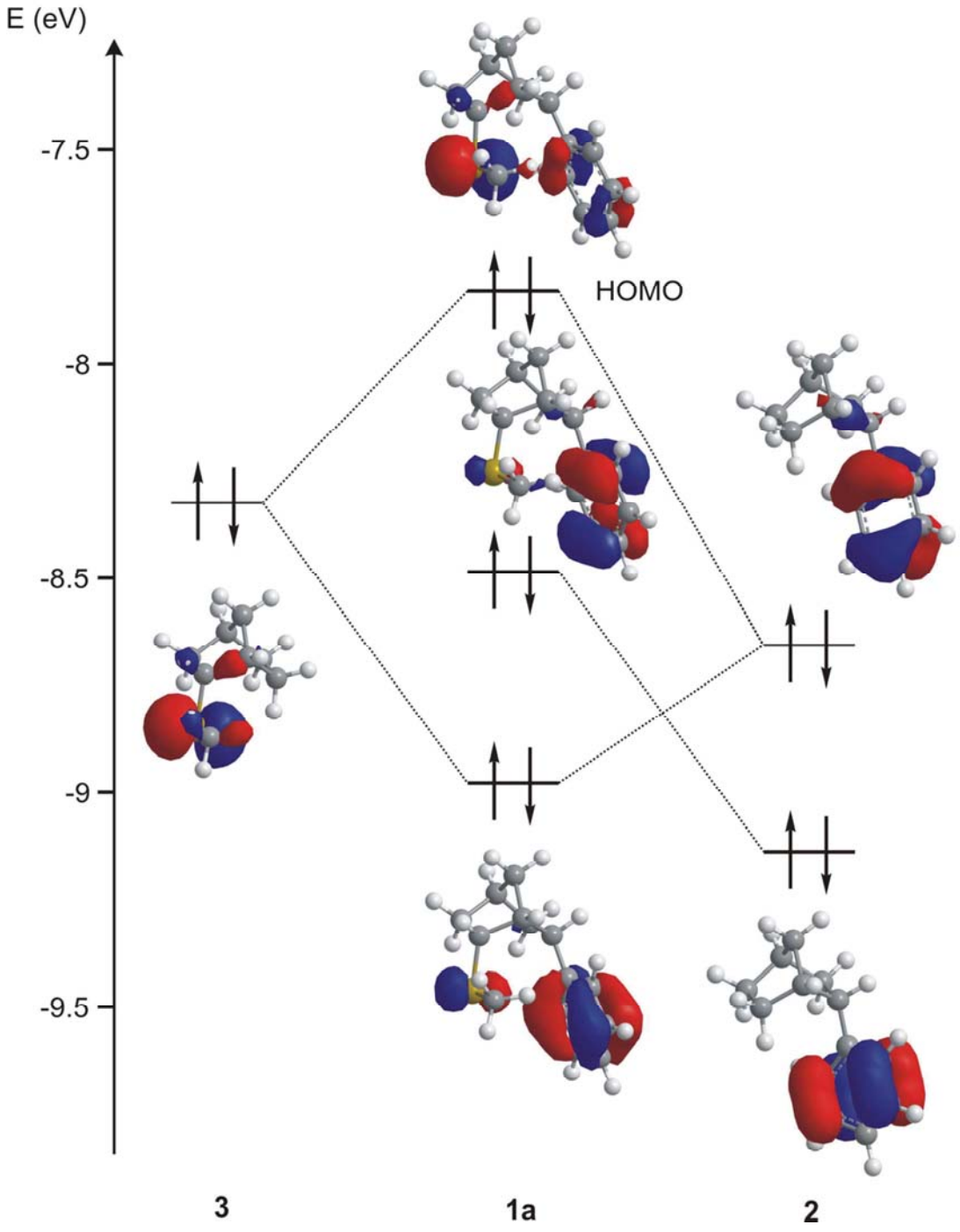


Fig. S1. Orbital interaction diagram of **2** and **3** forming **1a**

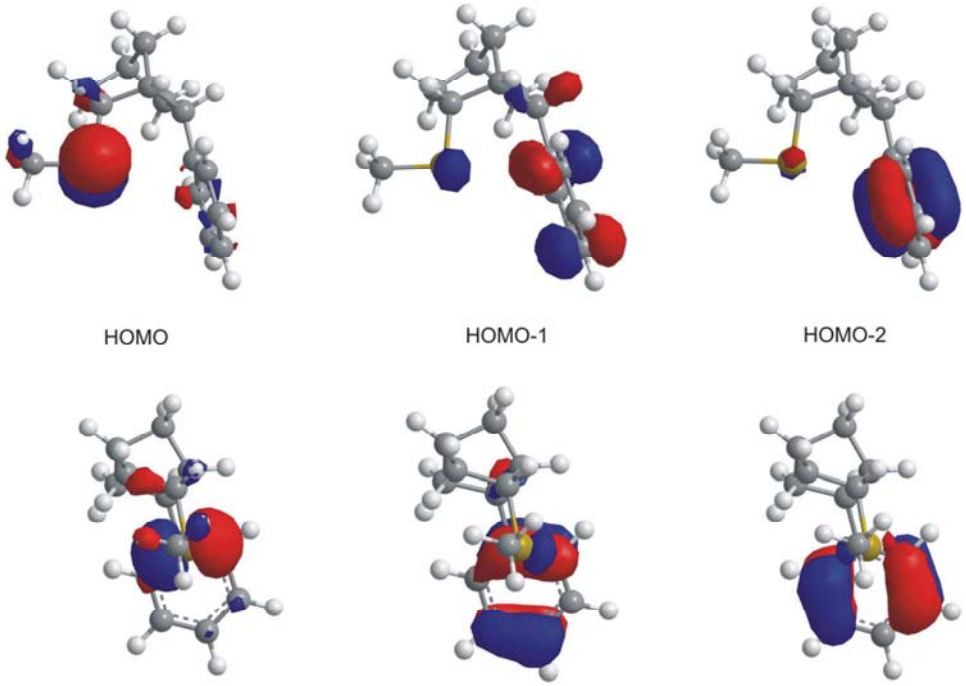


Fig. S2. Molecular orbitals of **1b** that account for the first three observed ionization energies.

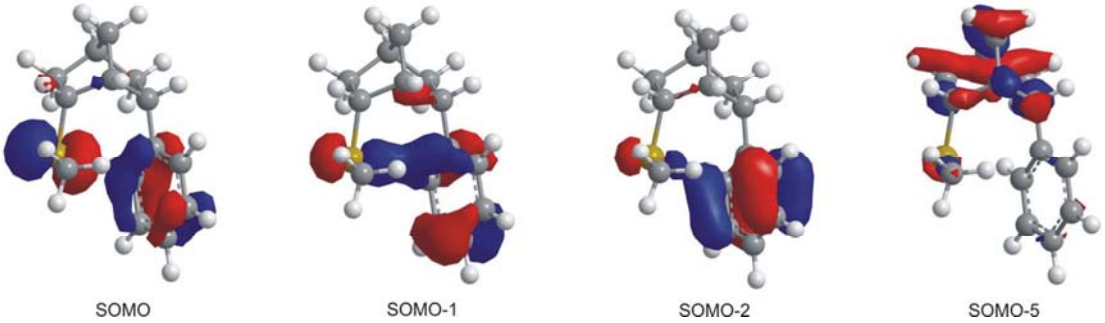


Fig. S3. MOs of **1a**$^{\bullet+}$ that are involved in the main electronic excitations that appear in the EA spectrum in Figure 2**.**

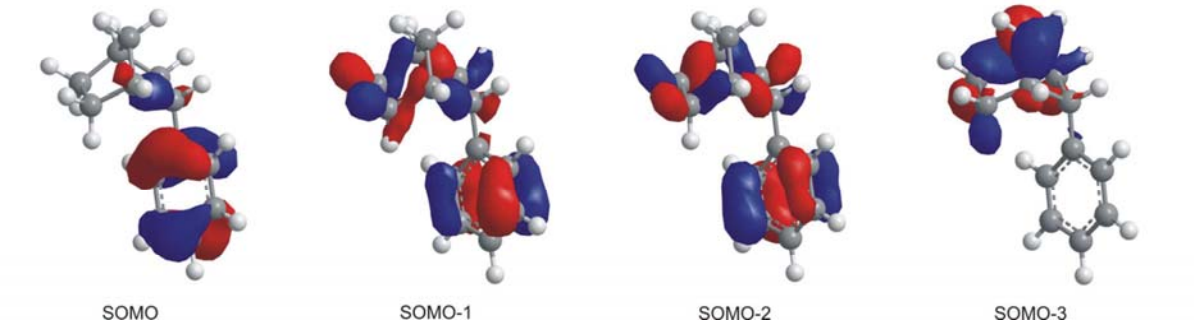


Fig. S4. MOs of **2**$^{\bullet+}$ that are involved in the main electronic excitations that appear in the EA spectrum in Figure S6.

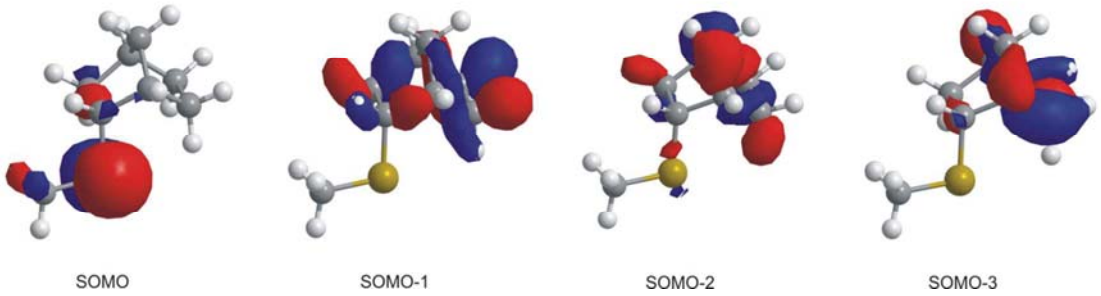


Fig. S5. MOs of $\mathbf{3}^{\bullet+}$ that are involved in the main electronic excitations that appear in the EA spectrum in Figure S6.

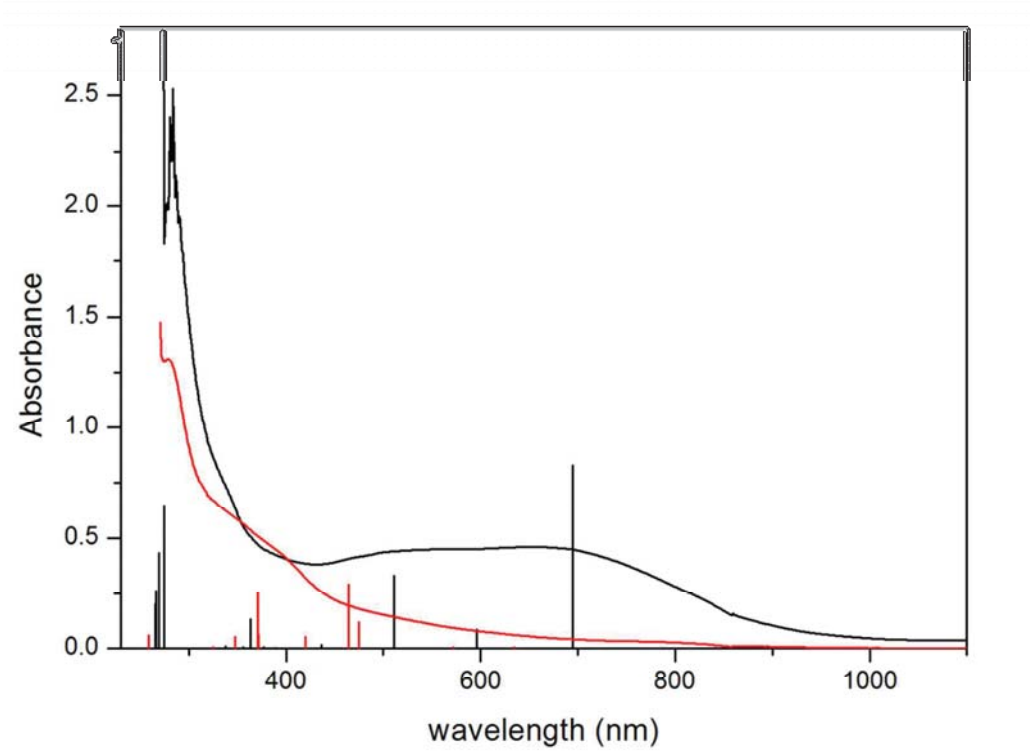


Fig. S6 Difference spectrum obtained on γ-irradiation of 2 (black) and 3 (red) in a Freon mixture at 77K. The bars indicate the main excitation energies and transition moments of $\mathbf{2}^{\bullet+}$ and $\mathbf{3}^{\bullet+}$ calculated by TD-B2PLYP.

Table S1 Energies of the different species calculated with B2PLYP/cc-pVDZ

Species	E(h)	ΔE (kcal/mol)	ZPVE (h)	G (h)	ΔG (kcal/mol)
1a	-941.7823505	0	0.287265	-941.53607	0.04
TS 1a-1b	-941.7796919	1.67	0.286889	-941.53273	1.88
1b	-941.7824469	-0.06	0.287233	-941.536038	0.00
TS 1b-1c	-941.7748374	4.71	0.287122	-941.527688	5.19
1c	-941.7785193	2.40	0.287525	-941.531059	3.33
1a$^{\bullet+}$	-941.519787	0.00	0.287181	-941.27360	0.00
TS **1a$^{\bullet+}$-1b$^{\bullet+}$**	-941.5064255	8.38	0.286755	-941.258773	9.04
1b$^{\bullet+}$	-941.5167601	1.90	0.287198	-941.270239	2.12
TS **1b$^{\bullet+}$-1c$^{\bullet+}$**	-941.5149209	3.05	0.287119	-941.267245	3.95
1c$^{\bullet+}$	-941.5153599	2.78	0.287393	-941.268564	3.29
2	-504.4713103		0.258751	-504.248582	
2$^{\bullet+}$	-504.1695312		0.256748	-503.949788	
3	-710.972344		0.206243	-710.800325	
3$^{\bullet+}$	-710.6785335		0.204888	-710.509142	

Table S2 Comparison of several method modelling the three first electronic transitions of **1a$^{\bullet+}$**. All the TD-DFT calculations were performed on optimized geometry with the corresponding method and basis set.

Method	Difference in energy (cm^{-1})			Sum of absolute differences
	1st	2nd	3rd	
exp_freon	14184	18182	24450	
B3LYP/6-31G*	-3700	-1023	-2455	7177
B3LYP/6-31+G(d,p)	-3821	-1600	-2902	8324
B3LYP/6-311++G(d,p)[a]	-3729	-1628	-2794	8150
M06-2X/6-31G*	996	2016	1112	4124
BH&HLYP/6-31G*	496	-2414	2612	5521
BH&HLYP/6-311G+(d,p)	781	-2801	2077	5659
MPWB1K/6-31+G(d,p)	1050	2210	2340	5601
SAC-CI/6-31G*[b]	987	1120	1668	3775
B2PLYP/cc-pVDZ	-1189	848	339	2376
EOM-CCSD/6-31G*[b]	1813	-239	1940	3992

[a]calculation performed on B3LYP/6-31+G(d,p) optimized geometry
[b]calculation performed on B2PLYP/cc-pVDZ optimized geometry

Table S3 Energies of the orbitals of **1**, **2** and **3** calculated by Koopmans theorem using HF/6-31G* (in eV).

	HOMO	HOMO-1	HOMO-2
1a	8.21	8.77	9.15
1b	8.40	8.61	8.94
exo-SMe-endo-phenyl	8.70	8.84	9.04
endo-SMe-exo-phenyl	8.59	8.95	9.05
2	8.60	8.92	11.38
3	8.87	11.05	11.55

Cartesian coordinates of optimized structures resulting from B2PLYP/cc-pVDZ calculations

1a

H	-3.510906	-1.852591	0.713240
C	-2.674642	-1.239445	0.349774
C	-1.746527	0.960410	-0.080923
C	-0.393032	-1.236150	-0.517123
C	-1.328881	-0.136880	-1.099314
C	-1.281141	-1.868785	0.598203
C	-2.651461	0.187618	0.933097
H	-2.353489	1.697941	-0.632000
H	-0.321559	-1.982026	-1.329151
H	-0.974060	0.275935	-2.054117
H	-0.932571	-1.627050	1.612276
H	-2.243269	0.207469	1.955587
H	-1.300655	-2.965695	0.511650
H	-3.657945	0.631115	0.969622
C	-2.650457	-0.939578	-1.164398
H	-3.511844	-0.339560	-1.497332
H	-2.575099	-1.837809	-1.796228
C	1.049053	-0.869155	-0.206768
C	3.790353	-0.269364	0.198253
C	1.862858	-0.417756	-1.264690
C	1.648708	-1.039205	1.051053
C	3.001766	-0.740512	1.253093
C	3.213298	-0.112274	-1.067922
H	1.431960	-0.313621	-2.264773
H	1.059199	-1.402076	1.893262
H	3.440211	-0.878155	2.244075
H	3.818095	0.238930	-1.907277
H	4.845266	-0.036650	0.357466
S	-0.471118	1.912532	0.820061
C	0.308434	2.813095	-0.555917
H	0.877912	2.133555	-1.206005
H	1.002581	3.537648	-0.107341
H	-0.445915	3.360011	-1.142442

Transition state between **1a** and **1b**

H	3.253776	-2.053116	-0.993462
C	2.449187	-1.467631	-0.526963
C	1.628959	0.753524	0.036807
C	0.271781	-1.413621	0.565471
C	1.298771	-0.348166	1.071843
C	1.076293	-2.167690	-0.545479
C	2.267408	-0.054966	-1.135432
H	2.408614	1.384404	0.491161
H	0.145513	-2.105921	1.415098
H	1.040194	0.056126	2.060764
H	0.610297	-2.114095	-1.538464
H	1.616765	-0.075920	-2.022748
H	1.170217	-3.234734	-0.291424
H	3.223441	0.395189	-1.443525
C	2.609744	-1.163129	0.979361
H	3.506321	-0.569818	1.218706
H	2.604331	-2.069688	1.604715
C	-1.125310	-0.918047	0.232307
C	-3.751419	0.035207	-0.238107
C	-1.995312	-0.619301	1.298259
C	-1.608598	-0.745549	-1.074484
C	-2.906387	-0.272276	-1.308091
C	-3.288702	-0.142941	1.072202
H	-1.646747	-0.761869	2.325219
H	-0.973020	-0.969252	-1.932247
H	-3.255085	-0.143858	-2.335244
H	-3.940147	0.083374	1.919453
H	-4.763124	0.403106	-0.421224
S	0.317242	1.950085	-0.454625
C	0.896743	3.420231	0.457650
H	0.889221	3.246093	1.543683
H	0.190758	4.230893	0.227470
H	1.903861	3.723859	0.134012

1b

H	3.110140	-2.100105	-1.132999
C	2.358013	-1.509464	-0.591472
C	1.704726	0.589221	0.439986
C	0.091997	-1.449159	0.319350
C	1.164005	-0.681629	1.146423
C	0.897647	-1.879041	-0.947955
C	2.513791	0.014210	-0.769997
H	2.393059	1.081696	1.146388
H	-0.107152	-2.365136	0.905227
H	0.867756	-0.494856	2.187262
H	0.579233	-1.341083	-1.852299
H	2.113824	0.362865	-1.733879
H	0.782037	-2.955512	-1.145670
H	3.571734	0.315469	-0.711308
C	2.368959	-1.629856	0.947313
H	3.298904	-1.256720	1.404093
H	2.173392	-2.649245	1.314184
C	-1.266279	-0.795306	0.124929
C	-3.859360	0.319027	-0.123958
C	-1.927248	-0.232402	1.234361
C	-1.944952	-0.808086	-1.104881
C	-3.225544	-0.254564	-1.230352
C	-3.203541	0.323736	1.113340
H	-1.433418	-0.222303	2.208484
H	-1.476457	-1.255287	-1.982381
H	-3.728004	-0.274162	-2.200103
H	-3.687484	0.762438	1.988830
H	-4.856312	0.753670	-0.222097
S	0.450474	1.863889	0.015916
C	1.610720	3.212008	-0.390300
H	2.239428	3.468261	0.476673
H	1.002854	4.086874	-0.660378
H	2.251274	2.948745	-1.245412

Transition state between **1b** and **1c**

H	-3.440213	-1.206399	1.449258
C	-2.590455	-0.939054	0.805612
C	-1.641370	0.727029	-0.689481
C	-0.378314	-1.481134	-0.057597
C	-1.326420	-0.743848	-1.059936
C	-1.256034	-1.580770	1.233671
C	-2.357731	0.588811	0.689332
H	-2.387425	1.068279	-1.423705
H	-0.284034	-2.499997	-0.471067
H	-1.016713	-0.864761	-2.107836
H	-0.826818	-1.061179	2.100747
H	-1.753411	0.954948	1.530962
H	-1.393783	-2.633364	1.524916
H	-3.302275	1.153401	0.693352
C	-2.681186	-1.380164	-0.671030
H	-3.535654	-0.946127	-1.212747
H	-2.698015	-2.474225	-0.793698
C	1.046516	-0.966572	0.068517
C	3.731657	-0.064922	0.157708
C	1.920544	-1.166805	-1.016973
C	1.558066	-0.329905	1.210003
C	2.884385	0.119133	1.254361
C	3.242159	-0.716463	-0.981664
H	1.552474	-1.679873	-1.910088
H	0.923555	-0.169385	2.082514
H	3.255331	0.613995	2.155023
H	3.894466	-0.879802	-1.842547
H	4.765231	0.285604	0.192641
S	-0.235646	1.916271	-0.877856
C	-0.324409	2.953473	0.616858
H	-0.002610	2.409898	1.516994
H	-1.326626	3.379404	0.767505
H	0.382410	3.776389	0.437194

1c

H	-3.296795	-1.794817	1.143460
C	-2.529461	-1.237293	0.588460
C	-1.829239	0.862711	-0.397152
C	-0.322001	-1.299362	-0.455831
C	-1.370562	-0.406178	-1.173319
C	-1.088888	-1.745866	0.834063
C	-2.545805	0.283103	0.861537
H	-2.591844	1.328486	-1.042478
H	-0.236600	-2.192629	-1.102544
H	-1.122076	-0.190074	-2.221416
H	-0.663354	-1.299584	1.746093
H	-2.027753	0.525311	1.799931
H	-1.058407	-2.839048	0.959117
H	-3.569784	0.678953	0.940877
C	-2.630547	-1.279720	-0.951716
H	-3.553170	-0.820807	-1.339361
H	-2.531453	-2.292548	-1.371387
C	1.104165	-0.810332	-0.280403
C	3.820075	-0.044446	-0.027189
C	1.700687	0.060375	-1.210454
C	1.905277	-1.306520	0.765180
C	3.247496	-0.927327	0.894458
C	3.039800	0.444520	-1.082103
H	1.109742	0.461926	-2.033753
H	1.479009	-2.002676	1.490549
H	3.844739	-1.325085	1.718104
H	3.474182	1.133345	-1.810097
H	4.864531	0.258047	0.073166
S	-0.713231	2.306294	-0.162419
C	0.187147	1.998104	1.391365
H	0.795376	1.085674	1.346825
H	-0.490192	1.970831	2.256882
H	0.856697	2.863369	1.503355

1a$^{\bullet+}$

H	3.762780	-1.093650	-1.009437
C	2.836535	-0.748302	-0.534052
C	1.468097	1.115752	0.181322
C	0.659014	-1.308767	0.418670
C	1.406617	-0.121719	1.113894
C	1.637042	-1.697788	-0.738059
C	2.418160	0.670350	-0.976316
H	1.899444	1.958396	0.749306
H	0.655829	-2.117067	1.167527
H	1.036741	0.102703	2.123230
H	1.201619	-1.594892	-1.741915
H	1.928106	0.676158	-1.962576
H	1.940635	-2.748544	-0.631187
H	3.278678	1.351303	-1.036527
C	2.871726	-0.596952	1.000846
H	3.599866	0.147819	1.355246
H	3.044124	-1.542945	1.534138
C	-0.788436	-1.025557	0.106892
C	-3.528462	-0.424421	-0.360227
C	-1.742451	-1.156252	1.135252
C	-1.249918	-0.597888	-1.172894
C	-2.614159	-0.302531	-1.397658
C	-3.086994	-0.860542	0.911124
H	-1.424136	-1.509427	2.119157
H	-0.565794	-0.585962	-2.022347
H	-2.940314	0.000903	-2.393803
H	-3.809600	-0.980657	1.721053
H	-4.585912	-0.212421	-0.526310
S	-0.087111	1.814275	-0.472223
C	-0.979835	2.344960	1.015192
H	-1.372270	1.472308	1.556499
H	-1.803815	2.985301	0.675885
H	-0.293837	2.920224	1.653714

Transition state between **1a**$^{\bullet+}$ and **1b**$^{\bullet+}$

H	3.631839	-0.877264	-1.236341
C	2.722701	-0.680384	-0.653588
C	1.253172	1.009775	0.292461
C	0.714096	-1.499651	0.456844
C	1.403890	-0.275643	1.142521
C	1.661616	-1.793332	-0.752691
C	2.062091	0.672630	-1.018179
H	1.724518	1.848175	0.825868
H	0.768608	-2.334869	1.173338
H	1.115235	-0.127801	2.191456
H	1.160175	-1.791368	-1.729009
H	1.420052	0.593069	-1.908257
H	2.128438	-2.781420	-0.637351
H	2.803212	1.462095	-1.208100
C	2.896618	-0.561400	0.872592
H	3.562605	0.255866	1.187800
H	3.232855	-1.495730	1.344907
C	-0.754488	-1.232431	0.179803
C	-3.454044	-0.387725	-0.206356
C	-1.586655	-0.910418	1.272181
C	-1.312949	-1.155427	-1.103828
C	-2.652566	-0.737776	-1.295543
C	-2.921147	-0.486982	1.083675
H	-1.198264	-0.993691	2.290326
H	-0.724744	-1.416760	-1.983085
H	-3.054865	-0.690888	-2.309530
H	-3.535438	-0.245848	1.953596
H	-4.483939	-0.061696	-0.357398
S	-0.463127	1.589414	-0.024990
C	-0.166243	3.379376	-0.086555
H	0.598099	3.595308	-0.848477
H	0.180948	3.726012	0.898867
H	-1.115869	3.862500	-0.348800

1b$^{\bullet+}$

H	3.575054	-0.735922	-1.437098
C	2.689006	-0.631690	-0.798410
C	1.425299	0.799352	0.692444
C	0.571437	-1.519357	0.020613
C	1.404776	-0.695517	1.070290
C	1.488506	-1.485013	-1.247227
C	2.216127	0.836095	-0.654544
H	1.978162	1.345725	1.477664
H	0.535945	-2.546400	0.416062
H	1.109216	-0.886670	2.110314
H	0.996123	-1.077540	-2.141019
H	1.604129	1.148815	-1.513174
H	1.809442	-2.505231	-1.500555
H	3.060629	1.535432	-0.579957
C	2.847189	-1.075081	0.669997
H	3.611762	-0.514790	1.228447
H	3.044257	-2.151013	0.779817
C	-0.860436	-1.064965	-0.111872
C	-3.566955	-0.211188	-0.254461
C	-1.814263	-1.524495	0.819089
C	-1.303566	-0.152267	-1.118975
C	-2.651531	0.257206	-1.190091
C	-3.141513	-1.105413	0.753146
H	-1.507742	-2.230272	1.594445
H	-0.613328	0.168701	-1.900505
H	-2.969847	0.928015	-1.989954
H	-3.863654	-1.481468	1.480514
H	-4.613595	0.093345	-0.305042
S	-0.230052	1.581727	0.771637
C	-0.000920	3.123585	-0.162391
H	0.809084	3.700041	0.308869
H	-0.945961	3.676523	-0.088036
H	0.242225	2.917557	-1.212620

Transition state between **1b**$^{\bullet+}$ and **1c**$^{\bullet+}$

H	-3.603350	-0.760314	1.431535
C	-2.732314	-0.609239	0.781950
C	-1.525898	0.852148	-0.721646
C	-0.569253	-1.392093	-0.027363
C	-1.450782	-0.655734	-1.085691
C	-1.463532	-1.347903	1.254528
C	-2.368657	0.880452	0.589129
H	-2.052489	1.373319	-1.539702
H	-0.504770	-2.437970	-0.378001
H	-1.163283	-0.842222	-2.128525
H	-0.998690	-0.830706	2.104689
H	-1.832694	1.284096	1.458703
H	-1.700565	-2.367232	1.589819
H	-3.262811	1.501978	0.438149
C	-2.867966	-1.100516	-0.672335
H	-3.663122	-0.595579	-1.240424
H	-3.006791	-2.187914	-0.757070
C	0.863652	-0.913841	0.055124
C	3.635058	-0.325128	0.108718
C	1.664959	-0.971738	-1.129672
C	1.515281	-0.573517	1.269647
C	2.875537	-0.276899	1.292046
C	3.024323	-0.675905	-1.102628
H	1.200110	-1.274401	-2.070969
H	0.957115	-0.568692	2.205751
H	3.359714	-0.026295	2.237584
H	3.612892	-0.731952	-2.019489
H	4.703666	-0.104001	0.138766
S	0.126032	1.648174	-0.772203
C	0.246898	2.690327	0.709892
H	0.251201	2.081022	1.622128
H	-0.592595	3.400344	0.719334
H	1.196118	3.233245	0.612776

1c$^{\bullet+}$

H	-3.580029	-1.003181	1.309225
C	-2.724741	-0.716771	0.684754
C	-1.525237	1.062575	-0.433964
C	-0.635046	-1.330862	-0.409214
C	-1.510378	-0.302557	-1.183488
C	-1.484790	-1.612990	0.876141
C	-2.287198	0.752803	0.889015
H	-2.095651	1.772274	-1.055985
H	-0.626469	-2.242364	-1.035946
H	-1.277170	-0.210504	-2.251928
H	-0.958182	-1.366914	1.808680
H	-1.676327	0.870841	1.794371
H	-1.767224	-2.673575	0.931738
H	-3.149001	1.428587	0.984173
C	-2.934180	-0.788000	-0.840099
H	-3.721494	-0.117707	-1.215100
H	-3.129177	-1.805658	-1.207849
C	0.817952	-0.960436	-0.219892
C	3.587643	-0.348702	-0.002464
C	1.537518	-0.343503	-1.290076
C	1.538301	-1.284627	0.945853
C	2.897724	-0.982858	1.054164
C	2.908094	-0.037731	-1.175611
H	1.036629	-0.171632	-2.244996
H	1.043568	-1.797822	1.770590
H	3.437121	-1.252720	1.964447
H	3.429302	0.424877	-2.015217
H	4.651853	-0.128245	0.095877
S	0.111171	1.897441	-0.385452
C	0.574951	2.121329	1.353660
H	0.674531	1.154136	1.862662
H	-0.176649	2.753447	1.847376
H	1.541954	2.641088	1.332426

2

H	-3.549395	0.492238	1.298735
C	-2.674393	0.269445	0.671846
C	-1.466912	0.605628	-1.413771
C	-0.486004	-0.804837	0.472567
C	-1.363010	-0.813891	-0.819765
C	-1.384903	-0.006238	1.476760
C	-2.366353	1.357043	-0.381585
H	-1.950597	0.563179	-2.402041
H	-0.432851	-1.851393	0.814899
H	-1.041184	-1.576484	-1.543323
H	-0.916945	0.924646	1.828136
H	-1.865367	2.229820	0.066402
H	-0.483887	1.075845	-1.554456
H	-1.595504	-0.616145	2.368659
H	-3.293672	1.720202	-0.851526
C	-2.768251	-0.993580	-0.209727
H	-3.574631	-0.941992	-0.958563
H	-2.875461	-1.923911	0.370266
C	0.944979	-0.343883	0.279913
C	3.638540	0.415857	-0.173895
C	1.343816	1.002403	0.366901
C	1.929657	-1.298569	-0.036883
C	3.259624	-0.928969	-0.262643
C	2.674125	1.378821	0.142520
H	0.613461	1.773750	0.618272
H	1.645224	-2.352602	-0.101381
H	4.002283	-1.693434	-0.501982
H	2.956763	2.431242	0.218923
H	4.676279	0.709662	-0.344449

$2^{\bullet+}$

H	-3.557296	0.461176	1.251228
C	-2.665740	0.253439	0.646245
C	-1.435653	0.604192	-1.425659
C	-0.444827	-0.785240	0.556292
C	-1.324888	-0.812315	-0.846859
C	-1.398806	0.018145	1.490565
C	-2.360181	1.342155	-0.409307
H	-1.919160	0.524259	-2.412311
H	-0.417931	-1.851378	0.829185
H	-0.937829	-1.583832	-1.524192
H	-0.961757	0.955814	1.861936
H	-1.886556	2.228550	0.039701
H	-0.466908	1.094290	-1.592523
H	-1.610233	-0.607901	2.371358
H	-3.285396	1.683842	-0.894451
C	-2.710591	-1.023063	-0.213499
H	-3.494794	-1.003222	-0.987153
H	-2.800188	-1.954268	0.363963
C	0.922937	-0.336102	0.314558
C	3.592480	0.414673	-0.182826
C	1.317246	1.043701	0.378553
C	1.920037	-1.317854	-0.038071
C	3.229020	-0.951576	-0.271605
C	2.626246	1.407934	0.144437
H	0.576800	1.803068	0.628621
H	1.619900	-2.365945	-0.101897
H	3.981611	-1.699857	-0.522413
H	2.930376	2.453697	0.205770
H	4.625685	0.713170	-0.373769

3

H	-2.910650	-1.258630	0.068241
C	-1.992874	-0.654847	0.035838
C	0.382012	-0.492527	0.544089
C	-0.837292	1.354818	-0.701357
C	-0.413216	0.831988	0.686287
C	-1.935666	0.337880	-1.145452
C	-0.697266	-1.496813	0.024356
H	0.732211	-0.799455	1.543176
H	-1.246997	2.372896	-0.614587
H	0.094904	1.578439	1.312795
H	-1.687373	-0.166771	-2.091707
H	-0.464995	-1.873980	-0.984019
H	0.012274	1.390295	-1.397308
H	-2.908388	0.835730	-1.281928
H	-0.769211	-2.367486	0.693148
C	-1.747417	0.282000	1.237191
H	-2.519406	1.059847	1.348419
H	-1.637650	-0.252496	2.194349
S	1.851394	-0.495686	-0.549540
C	2.935206	0.640251	0.376124
H	2.532372	1.663374	0.391803
H	3.905807	0.648564	-0.139197
H	3.083872	0.284147	1.406995

$3^{\bullet+}$

H	-2.400745	-1.636439	-0.938107
C	-1.741952	-0.875710	-0.496680
C	0.435006	-0.390857	0.479405
C	-1.278567	1.442789	0.058122
C	-0.747088	0.415359	1.081989
C	-1.975117	0.554622	-1.022276
C	-0.254112	-1.239872	-0.690043
H	0.902818	-1.057802	1.217745
H	-1.997479	2.107479	0.557042
H	-0.507192	0.827749	2.070483
H	-1.563018	0.699874	-2.031860
H	0.108639	-0.986298	-1.698511
H	-0.495149	2.097411	-0.356022
H	-3.050411	0.773859	-1.076628
H	-0.032461	-2.301301	-0.507552
C	-1.835376	-0.681273	1.026850
H	-2.811725	-0.298551	1.357356
H	-1.589714	-1.581410	1.610446
S	1.748605	0.627834	-0.209466
C	3.222165	-0.384281	0.040984
H	3.398114	-0.479267	1.124316
H	4.062187	0.123301	-0.448766
H	3.048708	-1.378615	-0.398596

Electronic transitions calculated with TD-B2PLYP/cc-pVDZ and the corresponding orbitals involved in the transitions

1a$^{\bullet+}$. Orbital 58 corresponds to the SOMO.

State	wavelength (nm)	Oscillator strength, f
1	769.5	0.009880
2	525.5	0.211608
3	403.4	0.033525
5	385.4	0.017097
7	299.1	0.012287
8	318.0	0.015631
9	313.1	0.002932
10	256.2	0.012385

STATE 1: E= 0.059215 au 1.611 eV 12996.3 cm**-1
56b -> 58b : 0.161074 (c= 0.40134051)
57b -> 58b : 0.809722 (c= 0.89984569)

STATE 2: E= 0.086712 au 2.360 eV 19031.0 cm**-1
54b -> 58b : 0.023432 (c= -0.15307524)
56b -> 58b : 0.758311 (c= 0.87081030)
57b -> 58b : 0.151158 (c= -0.38879055)

STATE 3: E= 0.112958 au 3.074 eV 24791.4 cm**-1
45b -> 58b : 0.016606 (c= 0.12886555)
47b -> 58b : 0.013996 (c= -0.11830388)
50b -> 58b : 0.083517 (c= -0.28899347)
52b -> 58b : 0.147966 (c= -0.38466410)
53b -> 58b : 0.098944 (c= -0.31455302)
54b -> 58b : 0.481728 (c= 0.69406609)
55b -> 58b : 0.054179 (c= 0.23276385)
56b -> 58b : 0.037327 (c= 0.19320155)

STATE 5: E= 0.118234 au 3.217 eV 25949.3 cm**-1
58a -> 59a : 0.030690 (c= 0.17518662)
49b -> 58b : 0.012254 (c= 0.11069836)
51b -> 58b : 0.028532 (c= -0.16891324)
53b -> 58b : 0.017316 (c= -0.13159078)
54b -> 58b : 0.041266 (c= 0.20314044)
55b -> 58b : 0.805945 (c= -0.89774427)
56b -> 60b : 0.010340 (c= -0.10168800)

STATE 7: E= 0.152332 au 4.145 eV 33433.0 cm**-1
57a -> 59a : 0.130838 (c= 0.36171477)
58a -> 59a : 0.054411 (c= 0.23326135)
58a -> 60a : 0.059343 (c= 0.24360390)
45b -> 58b : 0.043909 (c= 0.20954448)
47b -> 58b : 0.137507 (c= -0.37081968)
48b -> 58b : 0.014777 (c= -0.12156149)
51b -> 58b : 0.230652 (c= -0.48026240)
52b -> 58b : 0.051176 (c= -0.22622186)
54b -> 58b : 0.081535 (c= -0.28554287)
55b -> 58b : 0.016713 (c= 0.12928025)
56b -> 59b : 0.010048 (c= 0.10024051)
56b -> 60b : 0.060855 (c= -0.24668772)
57b -> 59b : 0.039656 (c= 0.19913838)

STATE 8: E= 0.143265 au 3.898 eV 31443.0 cm**-1
57a -> 59a : 0.072701 (c= 0.26963055)
58a -> 60a : 0.026785 (c= 0.16366216)
47b -> 58b : 0.017623 (c= -0.13275324)
48b -> 58b : 0.020896 (c= 0.14455314)
49b -> 58b : 0.125108 (c= 0.35370675)
50b -> 58b : 0.114624 (c= 0.33856112)
52b -> 58b : 0.339992 (c= 0.58308876)
53b -> 58b : 0.020695 (c= -0.14385621)
54b -> 58b : 0.123904 (c= 0.35200062)
55b -> 58b : 0.033660 (c= 0.18346621)
56b -> 60b : 0.033493 (c= -0.18300959)
57b -> 59b : 0.015685 (c= 0.12523795)

STATE 9: E= 0.145519 au 3.960 eV 31937.8 cm**-1
47b -> 58b : 0.021689 (c= 0.14727172)
48b -> 58b : 0.125735 (c= -0.35459122)
49b -> 58b : 0.022687 (c= 0.15062153)
50b -> 58b : 0.549944 (c= 0.74158225)
52b -> 58b : 0.172798 (c= -0.41569012)
53b -> 58b : 0.053033 (c= -0.23028921)

STATE 10: E= 0.177849 au 4.840 eV 39033.3 cm**-1
57a -> 59a : 0.184067 (c= 0.42903060)
57a -> 60a : 0.135461 (c= 0.36804962)
58a -> 59a : 0.252388 (c= -0.50238233)
58a -> 60a : 0.012013 (c= -0.10960518)

56b -> 59b : 0.065075 (c= -0.25509806)
56b -> 60b : 0.045639 (c= -0.21363284)
57b -> 60b : 0.223371 (c= -0.47262118)

1b$^{\bullet+}$. Orbital 58 corresponds to the SOMO.

State	wavelength (nm)	Oscillator strength, f
1	768.6	0.018306
2	524.5	0.216024
3	408	0.010829
6	362	0.021727
7	302.1	0.013225
8	310.4	0.011023
9	263.6	0.009188
10	312.9	0.004763

STATE 1: E= 0.059277 au 1.613 eV 13009.9 cm**-1
56b -> 58b : 0.176400 (c= 0.41999947)
57b -> 58b : 0.790130 (c= -0.88889246)

STATE 2: E= 0.086863 au 2.364 eV 19064.2 cm**-1
56b -> 58b : 0.770782 (c= 0.87794168)
57b -> 58b : 0.164530 (c= 0.40562355)

STATE 3: E= 0.111670 au 3.039 eV 24508.7 cm**-1
45b -> 58b : 0.012046 (c= -0.10975243)
46b -> 58b : 0.011759 (c= 0.10843891)
49b -> 58b : 0.013452 (c= 0.11598396)
50b -> 58b : 0.047458 (c= 0.21784941)
52b -> 58b : 0.224452 (c= 0.47376327)
53b -> 58b : 0.176745 (c= 0.42041031)
54b -> 58b : 0.275262 (c= 0.52465455)
55b -> 58b : 0.161704 (c= 0.40212468)
56b -> 58b : 0.012223 (c= -0.11055928)
57b -> 58b : 0.011859 (c= -0.10889732)

STATE 6: E= 0.125882 au 3.425 eV 27628.0 cm**-1
42b -> 58b : 0.010328 (c= 0.10162923)
46b -> 58b : 0.014625 (c= 0.12093570)
50b -> 58b : 0.039528 (c= 0.19881734)
51b -> 58b : 0.021236 (c= -0.14572568)
53b -> 58b : 0.493177 (c= 0.70226581)
54b -> 58b : 0.030776 (c= -0.17543014)
55b -> 58b : 0.333493 (c= -0.57748831)

STATE 7: E= 0.150810 au 4.104 eV 33099.0 cm**-1
57a -> 59a : 0.194071 (c= 0.44053481)
58a -> 59a : 0.011436 (c= -0.10693916)
58a -> 60a : 0.064461 (c= -0.25389253)
46b -> 58b : 0.034569 (c= -0.18592850)

47b -> 58b : 0.082851 (c= -0.28783787)
51b -> 58b : 0.108791 (c= -0.32983524)
52b -> 58b : 0.193455 (c= 0.43983508)
53b -> 58b : 0.018213 (c= -0.13495707)
54b -> 58b : 0.028666 (c= -0.16931050)
55b -> 58b : 0.066418 (c= -0.25771699)
56b -> 59b : 0.051582 (c= -0.22711754)
56b -> 60b : 0.033933 (c= -0.18421011)
57b -> 59b : 0.034403 (c= 0.18547982)
57b -> 60b : 0.015141 (c= -0.12304910)

STATE 8: E= 0.146785 au 3.994 eV 32215.5 cm**-1
57a -> 59a : 0.090779 (c= 0.30129530)
58a -> 60a : 0.017371 (c= -0.13179976)
47b -> 58b : 0.040083 (c= -0.20020823)
48b -> 58b : 0.058827 (c= -0.24254296)
49b -> 58b : 0.099008 (c= -0.31465495)
50b -> 58b : 0.030390 (c= -0.17432631)
51b -> 58b : 0.433976 (c= 0.65876852)
52b -> 58b : 0.019587 (c= -0.13995489)
53b -> 58b : 0.088158 (c= 0.29691469)
56b -> 59b : 0.025713 (c= -0.16035287)
56b -> 60b : 0.018579 (c= -0.13630511)
57b -> 59b : 0.021293 (c= 0.14592071)

STATE 9: E= 0.172877 au 4.704 eV 37942.2 cm**-1
57a -> 59a : 0.088976 (c= 0.29828874)
57a -> 60a : 0.144559 (c= 0.38020947)
58a -> 59a : 0.258510 (c= 0.50843850)
58a -> 60a : 0.036427 (c= 0.19085813)
51b -> 58b : 0.025453 (c= -0.15954074)
52b -> 58b : 0.035011 (c= -0.18711244)
54b -> 58b : 0.019769 (c= 0.14060283)
56b -> 59b : 0.011052 (c= 0.10512865)
56b -> 60b : 0.101406 (c= -0.31844254)
57b -> 59b : 0.052925 (c= 0.23005493)
57b -> 60b : 0.155071 (c= 0.39379094)

STATE 10: E= 0.145608 au 3.962 eV 31957.2 cm**-1
57a -> 59a : 0.014849 (c= -0.12185721)
57a -> 60a : 0.016223 (c= 0.12737095)
58a -> 59a : 0.038804 (c= 0.19698818)
58a -> 60a : 0.012225 (c= 0.11056846)
47b -> 58b : 0.037352 (c= 0.19326619)
48b -> 58b : 0.048029 (c= -0.21915494)
50b -> 58b : 0.064211 (c= 0.25339843)

51b -> 58b : 0.135553 (c= 0.36817463)
52b -> 58b : 0.301293 (c= 0.54890182)
53b -> 58b : 0.023615 (c= -0.15367082)
54b -> 58b : 0.219231 (c= -0.46822079)
56b -> 59b : 0.028349 (c= 0.16837218)
57b -> 60b : 0.023909 (c= 0.15462626)

2$^{\bullet+}$. Orbital 46 corresponds to the SOMO.

State	wavelength (nm)	Oscillator strength, f
1	1099.6	0.000165
2	694.7	0.082900
3	596.3	0.008863
4	511.3	0.033233
5	464.4	0.011335
6	436.5	0.001861
7	376.9	0.000907
8	363.3	0.013213
11	275	0.064839
12	337.7	0.001123
13	265.4	0.020098
14	266.4	0.026245
15	269.7	0.043332

STATE 1: E= 0.041351 au 1.125 eV 9075.5 cm**-1
43b -> 46b : 0.012069 (c= 0.10985688)
44b -> 46b : 0.837749 (c= 0.91528628)
45b -> 46b : 0.119653 (c= -0.34590916)

STATE 2: E= 0.064388 au 1.752 eV 14131.5 cm**-1
41b -> 46b : 0.029317 (c= 0.17122324)
44b -> 46b : 0.111863 (c= 0.33445942)
45b -> 46b : 0.803181 (c= 0.89620354)

STATE 3: E= 0.076833 au 2.091 eV 16863.0 cm**-1
35b -> 46b : 0.020423 (c= -0.14290957)
36b -> 46b : 0.021312 (c= 0.14598717)
38b -> 46b : 0.031500 (c= 0.17748169)
40b -> 46b : 0.026987 (c= 0.16427758)
41b -> 46b : 0.044047 (c= 0.20987471)
42b -> 46b : 0.231940 (c= -0.48160109)
43b -> 46b : 0.576931 (c= 0.75955945)

STATE 4: E= 0.088707 au 2.414 eV 19469.0 cm**-1
45a -> 48a : 0.011495 (c= 0.10721616)
35b -> 46b : 0.013610 (c= 0.11666119)
36b -> 46b : 0.026039 (c= 0.16136702)
37b -> 46b : 0.078442 (c= 0.28007559)
40b -> 46b : 0.080909 (c= 0.28444493)
41b -> 46b : 0.031134 (c= -0.17644861)
42b -> 46b : 0.484452 (c= 0.69602553)
43b -> 46b : 0.215932 (c= 0.46468471)

STATE 5: E= 0.100316 au 2.730 eV 22016.8 cm**-1
45a -> 48a : 0.029209 (c= 0.17090715)
46a -> 47a : 0.010322 (c= -0.10159746)
32b -> 46b : 0.014486 (c= -0.12035910)
33b -> 46b : 0.027516 (c= -0.16587933)
37b -> 46b : 0.175080 (c= -0.41842612)
40b -> 46b : 0.056631 (c= -0.23797341)
41b -> 46b : 0.530252 (c= -0.72818427)
42b -> 46b : 0.018819 (c= -0.13718145)
43b -> 46b : 0.037259 (c= 0.19302618)
45b -> 46b : 0.034616 (c= 0.18605277)

STATE 6: E= 0.103694 au 2.822 eV 22758.2 cm**-1
45a -> 48a : 0.020433 (c= 0.14294271)
32b -> 46b : 0.012460 (c= 0.11162630)
34b -> 46b : 0.045833 (c= -0.21408683)
35b -> 46b : 0.015017 (c= 0.12254322)
36b -> 46b : 0.042444 (c= 0.20601884)
37b -> 46b : 0.075188 (c= 0.27420464)
39b -> 46b : 0.079830 (c= -0.28254268)
40b -> 46b : 0.367369 (c= 0.60610991)
41b -> 46b : 0.066639 (c= -0.25814603)
42b -> 46b : 0.139797 (c= -0.37389450)
43b -> 46b : 0.078713 (c= -0.28055861)

STATE 7: E= 0.122463 au 3.332 eV 26877.5 cm**-1
45a -> 48a : 0.067407 (c= -0.25962810)
32b -> 46b : 0.013087 (c= -0.11439674)
33b -> 46b : 0.052466 (c= 0.22905386)
35b -> 46b : 0.025488 (c= 0.15964877)
36b -> 46b : 0.347169 (c= -0.58921020)
37b -> 46b : 0.147280 (c= 0.38377122)
39b -> 46b : 0.045612 (c= 0.21356971)
41b -> 46b : 0.132513 (c= -0.36402349)
42b -> 46b : 0.037149 (c= -0.19274179)
43b -> 46b : 0.026223 (c= 0.16193608)
44b -> 48b : 0.018339 (c= 0.13542170)

STATE 8: E= 0.126781 au 3.450 eV 27825.1 cm**-1
45a -> 48a : 0.046627 (c= -0.21593219)
32b -> 46b : 0.039368 (c= 0.19841465)
34b -> 46b : 0.069979 (c= 0.26453596)
35b -> 46b : 0.295612 (c= -0.54370255)
36b -> 46b : 0.036271 (c= 0.19044871)
37b -> 46b : 0.044827 (c= 0.21172421)

38b -> 46b : 0.194051 (c= 0.44051175)
39b -> 46b : 0.046850 (c= -0.21644879)
41b -> 46b : 0.128527 (c= -0.35850600)
42b -> 46b : 0.010482 (c= 0.10238285)
44b -> 48b : 0.013655 (c= 0.11685447)

STATE 11: E= 0.164714 au 4.482 eV 36150.6 cm**-1
40a -> 47a : 0.014034 (c= 0.11846545)
41a -> 47a : 0.016242 (c= 0.12744542)
44a -> 47a : 0.088111 (c= 0.29683483)
45a -> 48a : 0.207752 (c= 0.45579819)
46a -> 47a : 0.340281 (c= 0.58333612)
32b -> 46b : 0.015525 (c= -0.12459865)
34b -> 46b : 0.010832 (c= 0.10407514)
35b -> 46b : 0.010371 (c= -0.10184025)
36b -> 46b : 0.047071 (c= -0.21695830)
38b -> 46b : 0.029515 (c= 0.17179995)
44b -> 47b : 0.030194 (c= 0.17376466)
44b -> 48b : 0.064666 (c= -0.25429541)
45b -> 48b : 0.019548 (c= 0.13981311)

STATE 12: E= 0.135740 au 3.694 eV 29791.5 cm**-1
32b -> 46b : 0.082829 (c= -0.28779951)
33b -> 46b : 0.039966 (c= 0.19991424)
34b -> 46b : 0.036336 (c= -0.19061894)
35b -> 46b : 0.103052 (c= 0.32101700)
37b -> 46b : 0.037388 (c= -0.19336075)
38b -> 46b : 0.575354 (c= 0.75852112)
39b -> 46b : 0.031566 (c= 0.17766885)
40b -> 46b : 0.025492 (c= 0.15966237)
43b -> 46b : 0.010375 (c= -0.10185961)

STATE 13: E= 0.182869 au 4.976 eV 40135.1 cm**-1
43a -> 47a : 0.016617 (c= -0.12890761)
44a -> 47a : 0.030330 (c= 0.17415500)
45a -> 47a : 0.693442 (c= 0.83273166)
46a -> 48a : 0.014808 (c= -0.12168764)
32b -> 46b : 0.011962 (c= -0.10937033)
37b -> 46b : 0.010814 (c= 0.10398824)
44b -> 47b : 0.097027 (c= 0.31149138)
44b -> 48b : 0.043485 (c= 0.20853164)
45b -> 48b : 0.012420 (c= -0.11144529)

STATE 14: E= 0.159682 au 4.345 eV 35046.1 cm**-1
45a -> 47a : 0.018275 (c= 0.13518433)
29b -> 46b : 0.020998 (c= 0.14490616)

30b -> 46b : 0.013350 (c= 0.11554307)
32b -> 46b : 0.535954 (c= 0.73208874)
33b -> 46b : 0.108697 (c= 0.32969227)
34b -> 46b : 0.030964 (c= -0.17596658)
36b -> 46b : 0.044959 (c= -0.21203639)
37b -> 46b : 0.107845 (c= -0.32839776)

STATE 15: E= 0.165902 au 4.514 eV 36411.3 cm**-1
44a -> 47a : 0.012842 (c= 0.11332037)
46a -> 47a : 0.029189 (c= 0.17084922)
29b -> 46b : 0.025323 (c= -0.15913118)
31b -> 46b : 0.067412 (c= 0.25963914)
32b -> 46b : 0.042528 (c= -0.20622364)
33b -> 46b : 0.434950 (c= 0.65950736)
34b -> 46b : 0.043834 (c= 0.20936515)
36b -> 46b : 0.105938 (c= 0.32548084)
37b -> 46b : 0.047323 (c= -0.21753945)
38b -> 46b : 0.087348 (c= -0.29554669)
44b -> 48b : 0.017605 (c= 0.13268434)

3$^{\bullet+}$. Orbital 38 corresponds to the SOMO.

State	wavelength (nm)	Oscillator strength, f
1	571.6	0.000862
2	634.3	0.000647
3	475	0.011983
4	464.1	0.029015
5	419.8	0.00531
6	371.3	0.025347
7	347.9	0.005409
8	371.6	0.006363
9	325.4	0.000716
10	258.7	0.005928

STATE 1: E= 0.079711 au 2.169 eV 17494.5 cm**-1
29b -> 38b : 0.133726 (c= 0.36568532)
31b -> 38b : 0.271356 (c= 0.52091832)
32b -> 38b : 0.011055 (c= -0.10514441)
33b -> 38b : 0.049635 (c= -0.22278863)
34b -> 38b : 0.130851 (c= 0.36173307)
36b -> 38b : 0.360331 (c= 0.60027590)

STATE 2: E= 0.071829 au 1.955 eV 15764.6 cm**-1
29b -> 38b : 0.016262 (c= 0.12752134)
30b -> 38b : 0.020831 (c= -0.14432854)
34b -> 38b : 0.012156 (c= -0.11025633)
37b -> 38b : 0.919247 (c= -0.95877371)

STATE 3: E= 0.095926 au 2.610 eV 21053.3 cm**-1
27b -> 38b : 0.025217 (c= -0.15879894)
29b -> 38b : 0.070827 (c= -0.26613255)
30b -> 38b : 0.036942 (c= 0.19220417)
31b -> 38b : 0.092759 (c= -0.30456356)
33b -> 38b : 0.066825 (c= 0.25850503)
34b -> 38b : 0.011361 (c= -0.10658742)
35b -> 38b : 0.341971 (c= 0.58478252)
36b -> 38b : 0.337196 (c= 0.58068607)

STATE 4: E= 0.098182 au 2.672 eV 21548.5 cm**-1
28b -> 38b : 0.013191 (c= -0.11485207)
29b -> 38b : 0.075563 (c= -0.27488687)
31b -> 38b : 0.018257 (c= -0.13511798)
32b -> 38b : 0.042144 (c= 0.20528915)
34b -> 38b : 0.031958 (c= -0.17876801)
35b -> 38b : 0.547398 (c= -0.73986363)

36b -> 38b : 0.245162 (c= 0.49513829)

STATE 5: E= 0.108527 au 2.953 eV 23819.0 cm**-1
23b -> 38b : 0.013492 (c= -0.11615400)
26b -> 38b : 0.015673 (c= -0.12519020)
29b -> 38b : 0.138231 (c= -0.37179453)
30b -> 38b : 0.017592 (c= 0.13263460)
33b -> 38b : 0.170123 (c= 0.41246016)
34b -> 38b : 0.525109 (c= 0.72464415)
35b -> 38b : 0.016382 (c= -0.12799181)
36b -> 38b : 0.023109 (c= -0.15201571)
37b -> 38b : 0.044607 (c= -0.21120333)

STATE 6: E= 0.122712 au 3.339 eV 26932.2 cm**-1
24b -> 38b : 0.012019 (c= 0.10963305)
27b -> 38b : 0.015211 (c= -0.12333489)
29b -> 38b : 0.254266 (c= -0.50424841)
30b -> 38b : 0.025120 (c= -0.15849206)
31b -> 38b : 0.013112 (c= 0.11450846)
32b -> 38b : 0.089811 (c= 0.29968534)
33b -> 38b : 0.496116 (c= -0.70435526)
34b -> 38b : 0.022532 (c= 0.15010800)
35b -> 38b : 0.049566 (c= 0.22263447)

STATE 7: E= 0.130950 au 3.563 eV 28740.2 cm**-1
23b -> 38b : 0.013933 (c= 0.11803936)
26b -> 38b : 0.014264 (c= 0.11943236)
27b -> 38b : 0.025779 (c= 0.16055734)
29b -> 38b : 0.069966 (c= 0.26451043)
30b -> 38b : 0.322229 (c= -0.56765234)
31b -> 38b : 0.249777 (c= -0.49977664)
32b -> 38b : 0.065326 (c= 0.25558913)
34b -> 38b : 0.190969 (c= 0.43699986)
36b -> 38b : 0.014653 (c= 0.12104777)
37b -> 38b : 0.014134 (c= 0.11888441)

STATE 8: E= 0.122601 au 3.336 eV 26907.9 cm**-1
29b -> 38b : 0.023576 (c= -0.15354611)
31b -> 38b : 0.122433 (c= -0.34990407)
32b -> 38b : 0.718710 (c= -0.84776764)
33b -> 38b : 0.093382 (c= -0.30558472)
34b -> 38b : 0.019630 (c= 0.14010544)

STATE 9: E= 0.140023 au 3.810 eV 30731.6 cm**-1
27b -> 38b : 0.010536 (c= 0.10264680)
28b -> 38b : 0.016307 (c= -0.12769767)

29b -> 38b : 0.073748 (c= -0.27156563)
30b -> 38b : 0.502394 (c= -0.70879755)
31b -> 38b : 0.167324 (c= 0.40905292)
32b -> 38b : 0.062736 (c= -0.25047131)
33b -> 38b : 0.093833 (c= 0.30632248)
34b -> 38b : 0.041683 (c= -0.20416378)
35b -> 38b : 0.015928 (c= 0.12620612)

STATE 10: E= 0.176154 au 4.793 eV 38661.4 cm**-1
27b -> 38b : 0.069016 (c= -0.26270975)
28b -> 38b : 0.856286 (c= -0.92535721)
29b -> 38b : 0.049693 (c= 0.22291909)