

## Supporting Information for

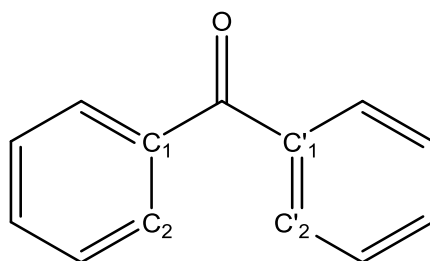
### Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singlet-Triplet Transitions

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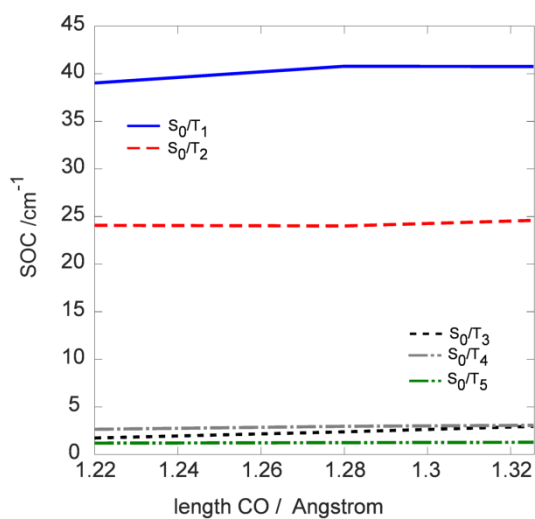
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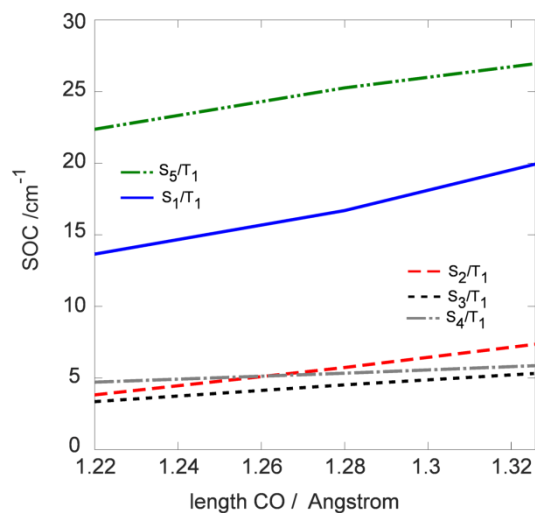
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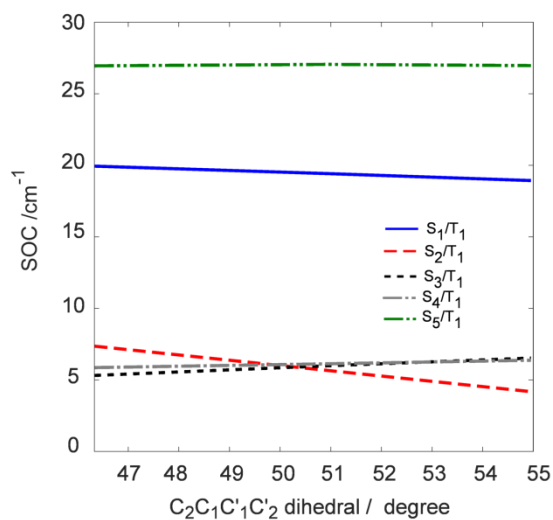
**Figure S1.** Benzophenone structure



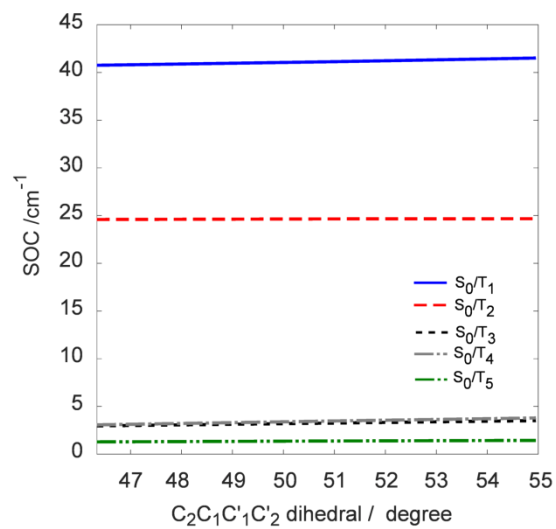
**Figure S2.** S<sub>0</sub>/T<sub>i</sub> spin orbit coupling (cm<sup>-1</sup>) as a function of the stretching of carbonyl bond, computed as a relaxed PES scan of T<sub>1</sub> state.



**Figure S3.**  $S_{\nu}/T_1$  spin orbit coupling ( $\text{cm}^{-1}$ ) as a function of the stretching of carbonyl bond, computed via a relaxed PES scan of  $T_1$  state.



**Figure S4.**  $S_{\nu}/T_1$  spin orbit coupling ( $\text{cm}^{-1}$ ) as a function of the  $C_2C_1C'_1C'_2$  dihedral angle, computed via a relaxed PES scan of  $T_1$  state.



**Figure S5.**  $\text{S}_0/\text{T}_i$  spin orbit coupling ( $\text{cm}^{-1}$ ) with respect the  $\text{C}_2\text{C}_1\text{C}'_1\text{C}'_2$  dihedral angle, computed via a relaxed PES scan of  $\text{T}_1$  state.

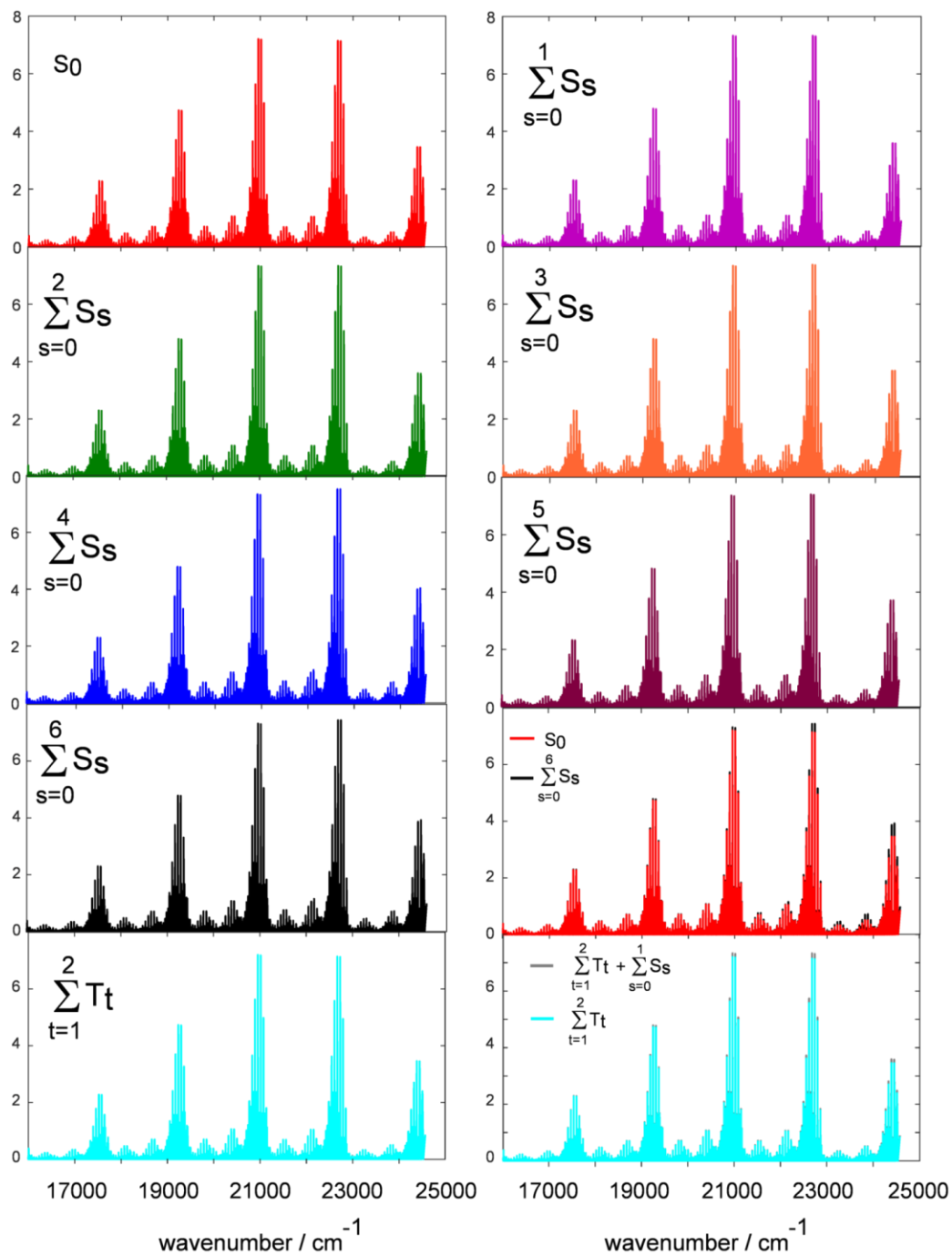
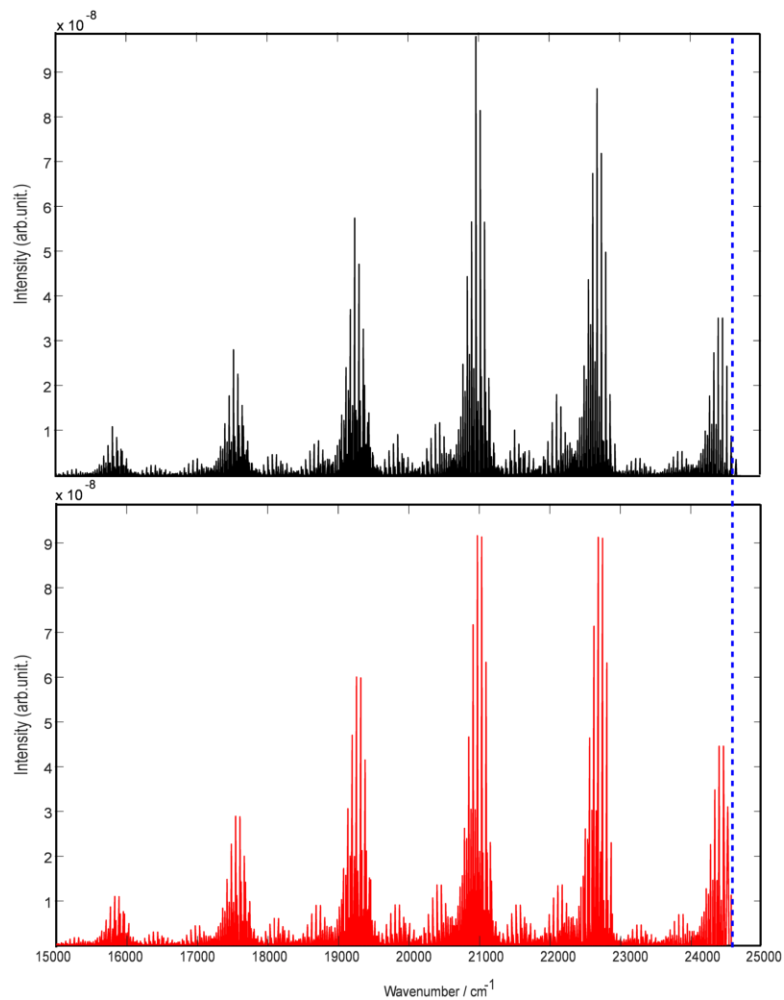


Figure S6. Spectra of  $S_0 \leftarrow T_1$  transition computed with an increasing number of states

## Thermal effects



**Figure S8.** Predicted Spectrum at 77 K (back) and 0 K (red). The 0-0 transition is evidenced by a dashed blue line.

## Optimized geometries (Å)

T1

C	1.296890	0.310535	-0.017767
C	2.432220	1.018851	0.459249
C	3.689769	0.443235	0.419979
C	3.869238	-0.839718	-0.097266
C	2.763437	-1.539922	-0.594901
C	1.503025	-0.975737	-0.576567
H	2.296668	2.004380	0.882559
H	4.539639	0.994021	0.804772
H	4.854521	-1.287228	-0.123254
H	2.897901	-2.528517	-1.017338
H	0.667770	-1.509859	-1.008715
C	-0.000001	0.933207	-0.000007
O	-0.000007	2.256048	-0.000001
C	-1.296887	0.310531	0.017760
C	-1.503018	-0.975745	0.576556
C	-2.763431	-1.539928	0.594898
C	-3.869238	-0.839719	0.097278
C	-3.689772	0.443235	-0.419964
C	-2.432222	1.018849	-0.459248
H	-0.667763	-1.509873	1.008694
H	-2.897891	-2.528526	1.017329
H	-4.854521	-1.287229	0.123273
H	-4.539646	0.994024	-0.804745
H	-2.296675	2.004375	-0.882564

T2

C	-1.30340	0.29760	0.08564
C	-2.29020	0.99403	-0.62096
C	-3.56899	0.47917	-0.73475
C	-3.88802	-0.73389	-0.14509
C	-2.92076	-1.42277	0.57547
C	-1.64410	-0.90899	0.70420
H	-2.03954	1.93427	-1.09355
H	-4.31864	1.02590	-1.29215
H	-4.88707	-1.13922	-0.23830
H	-3.16873	-2.36197	1.05334
H	-0.91364	-1.43165	1.30558
C	0.03459	0.90385	0.21179
O	0.01152	2.14394	0.58957
C	1.30724	0.28296	0.04125
C	1.46593	-1.10630	-0.19733
C	2.71842	-1.64729	-0.35515
C	3.86890	-0.85298	-0.25372
C	3.73154	0.51216	-0.01963
C	2.48511	1.08101	0.12172
H	0.59657	-1.73869	-0.29467
H	2.81543	-2.70519	-0.56430
H	4.84882	-1.29484	-0.37183
H	4.61134	1.14061	0.03631
H	2.38575	2.14792	0.26246

S0

C	0.00000	1.29928	0.34623
C	0.58958	2.41235	0.95587
C	0.57172	3.64925	0.32809

C	-0.05925	3.79672	-0.90563
C	-0.66878	2.70147	-1.50863
C	-0.63124	1.45546	-0.89180
H	1.05456	2.28798	1.92521
H	1.04333	4.50193	0.80107
H	-0.08069	4.76461	-1.39165
H	-1.17432	2.81642	-2.45960
H	-1.11590	0.60975	-1.36169
C	0.00000	0.00000	1.09476
O	0.00000	0.00000	2.31443
C	0.00000	-1.29928	0.34623
C	0.63124	-1.45546	-0.89180
C	0.66878	-2.70147	-1.50863
C	0.05925	-3.79672	-0.90563
C	-0.57172	-3.64925	0.32809
C	-0.58958	-2.41235	0.95587
H	1.11590	-0.60975	-1.36169
H	1.17432	-2.81642	-2.45960
H	0.08069	-4.76461	-1.39165
H	-1.04333	-4.50193	0.80107
H	-1.05456	-2.28798	1.92521

#### S1

C	0.00000	1.29801	0.30467
C	0.43653	2.42639	1.04142
C	0.41922	3.68899	0.47320
C	-0.03093	3.87270	-0.83240
C	-0.48580	2.77136	-1.56171
C	-0.48469	1.50416	-1.00769
H	0.81190	2.29227	2.04692
H	0.76636	4.53733	1.05062
H	-0.03870	4.86060	-1.27491
H	-0.86213	2.90849	-2.56839
H	-0.89416	0.67624	-1.56813
C	0.00000	0.00000	0.93458
O	0.00000	0.00000	2.25131
C	0.00000	-1.29801	0.30467
C	0.48469	-1.50416	-1.00769
C	0.48580	-2.77136	-1.56171
C	0.03093	-3.87270	-0.83240
C	-0.41922	-3.68899	0.47320
C	-0.43653	-2.42639	1.04142
H	0.89416	-0.67624	-1.56813
H	0.86213	-2.90849	-2.56839
H	0.03870	-4.86060	-1.27491
H	-0.76636	-4.53733	1.05062
H	-0.81190	-2.29227	2.04692

#### S2

C	1.31874	0.31513	-0.00628
C	2.50066	1.06713	0.26081
C	3.74862	0.48042	0.22651
C	3.90386	-0.87403	-0.09480
C	2.76282	-1.62187	-0.40147
C	1.50341	-1.05213	-0.35970
H	2.38559	2.11570	0.49817
H	4.62265	1.08189	0.45076
H	4.88538	-1.32896	-0.12044
H	2.86348	-2.66214	-0.69076

H	0.66377	-1.66026	-0.66927
C	0.06331	1.01032	0.03133
O	-0.04566	2.26919	0.09613
C	-1.26127	0.27634	0.00662
C	-1.53961	-0.98822	0.49297
C	-2.86233	-1.55639	0.44662
C	-3.95829	-0.82017	0.00955
C	-3.71548	0.47923	-0.40027
C	-2.39965	1.03683	-0.32320
H	-0.76179	-1.56502	0.97342
H	-2.99027	-2.58329	0.76580
H	-4.94346	-1.25965	-0.04856
H	-4.51362	1.09240	-0.79999
H	-2.23521	2.10028	-0.46025