Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Joint theoretical and experimental study on the phosphorescence of 2,2'-bithiophene

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Table 1.1S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVDZ level of theory.

	x	y	Z
s	-2.291	3.519	0.000
c	-0.230	6.082	0.000
c	2.245	5.314	0.000
c	2.509	2.632	0.000
c	0.234	1.353	0.000
c	-0.234	-1.353	0.000
s	2.291	-3.519	0.000
c	0.230	-6.082	0.000
c	-2.245	-5.314	0.000
c	-2.509	-2.632	0.000
h	-0.983	7.992	0.000
h	3.833	6.622	0.000
h	4.330	1.673	0.000
h	0.983	-7.992	0.000
h	-3.833	-6.622	0.000
h	-4.330	-1.673	0.000

Table 1.2S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVTZ level of theory.

	x	y	Z
s	-2.270	3.504	0.000
c	-0.230	6.049	0.000
c	2.230	5.287	0.000
c	2.494	2.620	0.000
c	0.231	1.348	0.000
c	-0.231	-1.348	0.000
s	2.270	-3.504	0.000
c	0.230	-6.049	0.000
c	-2.230	-5.287	0.000
c	-2.494	-2.620	0.000
h	-0.971	7.944	0.000
h	3.807	6.582	0.000
h	4.300	1.668	0.000
h	0.971	-7.944	0.000
h	-3.807	-6.582	0.000
h	-4.300	-1.668	0.000

Table 1.3S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVQZ level of theory.

	x	y	Z
s	-2.263	3.501	0.000
c	-0.231	6.044	0.000
c	2.231	5.285	0.000
c	2.495	2.619	0.000
c	0.230	1.348	0.000
c	-0.230	-1.348	0.000
s	2.263	-3.501	0.000
c	0.231	-6.044	0.000
c	-2.231	-5.285	0.000
c	-2.495	-2.619	0.000
h	-0.973	7.937	0.000
h	3.806	6.581	0.000
h	4.301	1.668	0.000
h	0.973	-7.937	0.000
h	-3.806	-6.581	0.000
h	-4.301	-1.668	0.000

Table 2.1S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVDZ level of theory.

	x	y	Z
s	-2.282	3.505	0.000
c	-0.244	6.082	0.000
c	2.274	5.322	0.000
c	2.549	2.641	0.000
c	0.239	1.354	0.000
c	-0.239	-1.354	0.000
s	2.282	-3.505	0.000
c	0.244	-6.082	0.000
c	-2.274	-5.322	0.000
c	-2.549	-2.641	0.000
h	-1.017	7.993	0.000
h	3.850	6.655	0.000
h	4.369	1.662	0.000
h	1.017	-7.993	0.000
h	-3.850	-6.655	0.000
h	-4.369	-1.662	0.000

Table 2.2S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVTZ level of theory.

	x	y	Z
s	-2.252	3.474	0.000
c	-0.243	6.029	0.000
c	2.251	5.276	0.000
c	2.525	2.620	0.000
c	0.236	1.344	0.000
c	-0.236	-1.344	0.000
s	2.252	-3.474	0.000
c	0.243	-6.029	0.000
c	-2.251	-5.276	0.000
c	-2.525	-2.620	0.000
h	-1.005	7.919	0.000
h	3.813	6.592	0.000
h	4.325	1.648	0.000
h	1.005	-7.919	0.000
h	-3.813	-6.592	0.000
h	-4.325	-1.648	0.000

Table 2.3S. Ground state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVQZ level of theory.

	x	y	Z
s	-2.241	3.468	0.000
c	-0.244	6.015	0.000
c	2.248	5.268	0.000
c	2.523	2.617	0.000
c	0.235	1.344	0.000
c	-0.235	-1.344	0.000
s	2.241	-3.468	0.000
c	0.244	-6.015	0.000
c	-2.248	-5.268	0.000
c	-2.523	-2.617	0.000
h	-1.005	7.904	0.000
h	3.807	6.584	0.000
h	4.321	1.645	0.000
h	1.005	-7.904	0.000
h	-3.807	-6.584	0.000
h	-4.321	-1.645	0.000

Table 3.1S. Ground state Cartesian atomic coordinates [Å] for the 2T molecule calculated at the CASPT2/aug-cc-pVDZ level of theory.

	x	y	Z
S	-1.212	1.850	0.000
S	1.212	-1.850	0.000
C	-0.134	3.212	0.000
C	0.134	-3.212	0.000
C	-1.193	-2.817	0.000
C	1.193	2.817	0.000
C	-1.340	-1.395	0.000
C	1.340	1.395	0.000
C	-0.123	-0.719	0.000
C	0.123	0.719	0.000
H	-0.543	4.222	0.000
H	0.543	-4.222	0.000
H	-2.026	-3.521	0.000
H	2.026	3.521	0.000
H	-2.303	-0.880	0.000
H	2.303	0.880	0.000

Table 3.2S. Ground state Cartesian atomic coordinates [Å] for the 2T molecule calculated at the CASPT2/aug-cc-pVTZ level of theory.

	x	y	Z
S	1.013	-1.941	0.000
S	-1.013	1.941	0.000
C	-0.174	-3.182	0.000
C	0.174	3.182	0.000
C	-1.445	-2.666	0.000
C	1.445	2.666	0.000
C	-1.455	-1.250	0.000
C	1.455	1.250	0.000
C	-0.190	-0.699	0.000
C	0.190	0.699	0.000
H	0.131	-4.216	0.000
H	-0.131	4.216	0.000
H	-2.334	-3.278	0.000
H	2.334	3.278	0.000
H	-2.354	-0.650	0.000
H	2.354	0.650	0.000

Table 4.1S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVDZ level of theory.

	x	y	Z
s	-2.391	3.498	0.000
c	-0.262	6.041	0.000
c	2.271	5.249	0.000
c	2.577	2.653	0.000
c	0.198	1.276	0.000
c	-0.198	-1.276	0.000
s	2.391	-3.498	0.000
c	0.262	-6.041	0.000
c	-2.271	-5.249	0.000
c	-2.577	-2.653	0.000
h	-0.976	7.966	0.000
h	3.836	6.586	0.000
h	4.393	1.689	0.000
h	0.976	-7.966	0.000
h	-3.836	-6.586	0.000
h	-4.393	-1.689	0.000

Table 4.2S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVTZ level of theory.

	x	y	Z
s	-2.373	3.481	0.000
c	-0.263	6.006	0.000
c	2.256	5.220	0.000
c	2.563	2.640	0.000
c	0.195	1.268	0.000
c	-0.195	-1.268	0.000
s	2.373	-3.481	0.000
c	0.263	-6.006	0.000
c	-2.256	-5.220	0.000
c	-2.563	-2.640	0.000
h	-0.965	7.916	0.000
h	3.809	6.546	0.000
h	4.364	1.684	0.000
h	0.965	-7.916	0.000
h	-3.809	-6.546	0.000
h	-4.364	-1.684	0.000

Table 4.3S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the B3LYP/aug-cc-pVQZ level of theory.

	x	y	Z
s	-2.367	3.478	0.000
c	-0.264	6.000	0.000
c	2.257	5.217	0.000
c	2.564	2.639	0.000
c	0.194	1.269	0.000
c	-0.194	-1.269	0.000
s	2.367	-3.478	0.000
c	0.264	-6.000	0.000
c	-2.257	-5.217	0.000
c	-2.564	-2.639	0.000
h	-0.967	7.908	0.000
h	3.807	6.545	0.000
h	4.364	1.682	0.000
h	0.967	-7.908	0.000
h	-3.807	-6.545	0.000
h	-4.364	-1.682	0.000

Table 5.1S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVDZ level of theory.

	x	y	Z
s	-2.386	3.482	0.000
c	-0.275	6.041	0.000
c	2.296	5.259	0.000
c	2.612	2.654	0.000
c	0.204	1.283	0.000
c	-0.204	-1.283	0.000
s	2.386	-3.482	0.000
c	0.275	-6.041	0.000
c	-2.296	-5.259	0.000
c	-2.612	-2.654	0.000
h	-1.008	7.969	0.000
h	3.850	6.620	0.000
h	4.427	1.667	0.000
h	1.008	-7.969	0.000
h	-3.850	-6.620	0.000
h	-4.427	-1.667	0.000

Table 5.2S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVTZ level of theory.

	x	y	Z
s	-2.360	3.448	0.000
c	-0.276	5.983	0.000
c	2.274	5.210	0.000
c	2.589	2.631	0.000
c	0.201	1.271	0.000
c	-0.201	-1.271	0.000
s	2.360	-3.448	0.000
c	0.276	-5.983	0.000
c	-2.274	-5.210	0.000
c	-2.589	-2.631	0.000
h	-0.996	7.890	0.000
h	3.812	6.555	0.000
h	4.383	1.651	0.000
h	0.996	-7.890	0.000
h	-3.812	-6.555	0.000
h	-4.383	-1.651	0.000

Table 5.3S. The lowest triplet state Cartesian atomic coordinates [a.u.] for the 2T molecule calculated at the CC2/aug-cc-pVQZ level of theory.

	x	y	Z
s	-2.349	3.441	0.000
c	-0.277	5.968	0.000
c	2.271	5.201	0.000
c	2.587	2.626	0.000
c	0.200	1.270	0.000
c	-0.200	-1.270	0.000
s	2.349	-3.441	0.000
c	0.277	-5.968	0.000
c	-2.271	-5.201	0.000
c	-2.587	-2.626	0.000
h	-0.996	7.874	0.000
h	3.806	6.547	0.000
h	4.379	1.648	0.000
h	0.996	-7.874	0.000
h	-3.806	-6.547	0.000
h	-4.379	-1.648	0.000

Table 6.1S. The lowest triplet state Cartesian atomic coordinates [Å] for the 2T molecule calculated at the CASPT2/aug-cc-pVDZ level of theory.

	x	y	Z
S	-1.258	1.840	0.000
S	1.258	-1.840	0.000
C	-0.141	3.191	0.000
C	0.141	-3.191	0.000
C	1.212	2.780	0.000
C	-1.212	-2.780	0.000
C	1.374	1.399	0.000
C	-1.374	-1.399	0.000
C	0.106	0.683	0.000
C	-0.106	-0.683	0.000
H	-0.527	4.210	0.000
H	0.527	-4.210	0.000
H	2.037	3.495	0.000
H	-2.037	-3.495	0.000
H	2.334	0.879	0.000
H	-2.334	-0.879	0.000

Table 6.2S. The lowest triplet state Cartesian atomic coordinates [Å] for the 2T molecule calculated at the CASPT2/aug-cc-pVTZ level of theory.

	x	y	Z
S	-1.187	-1.862	0.000
S	1.187	1.862	0.000
C	0.126	-0.673	0.000
C	-0.126	0.673	0.000
C	1.406	-1.344	0.000
C	-1.406	1.344	0.000
C	1.287	-2.716	0.000
C	-1.287	2.716	0.000
C	-0.042	-3.164	0.000
C	0.042	3.164	0.000
H	2.338	-0.799	0.000
H	-2.338	0.799	0.000
H	2.125	-3.397	0.000
H	-2.125	3.397	0.000
H	-0.390	-4.184	0.000
H	0.390	4.184	0.000

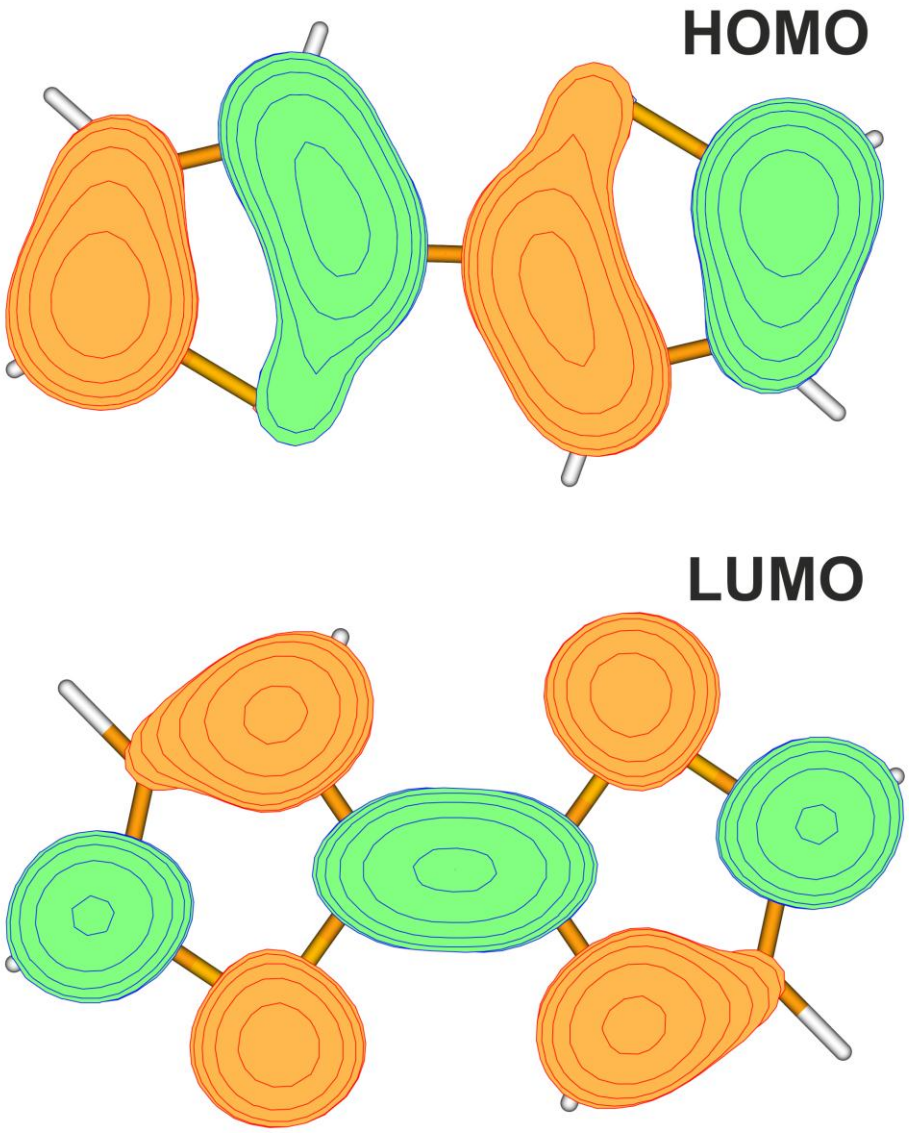

Fig1S. Frontier orbitals of 2T

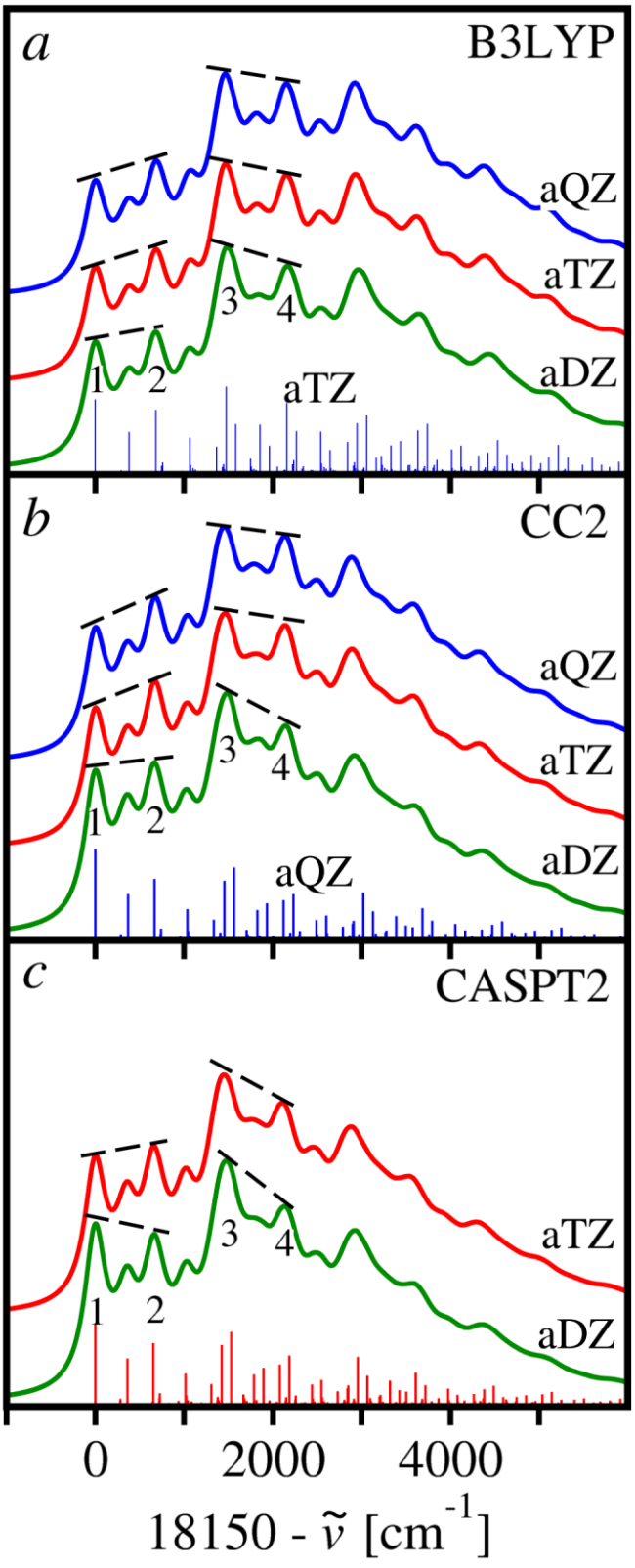

Fig.2S Basis set influence on the theoretical spectra based on the results of the selected quantum chemistry methods.

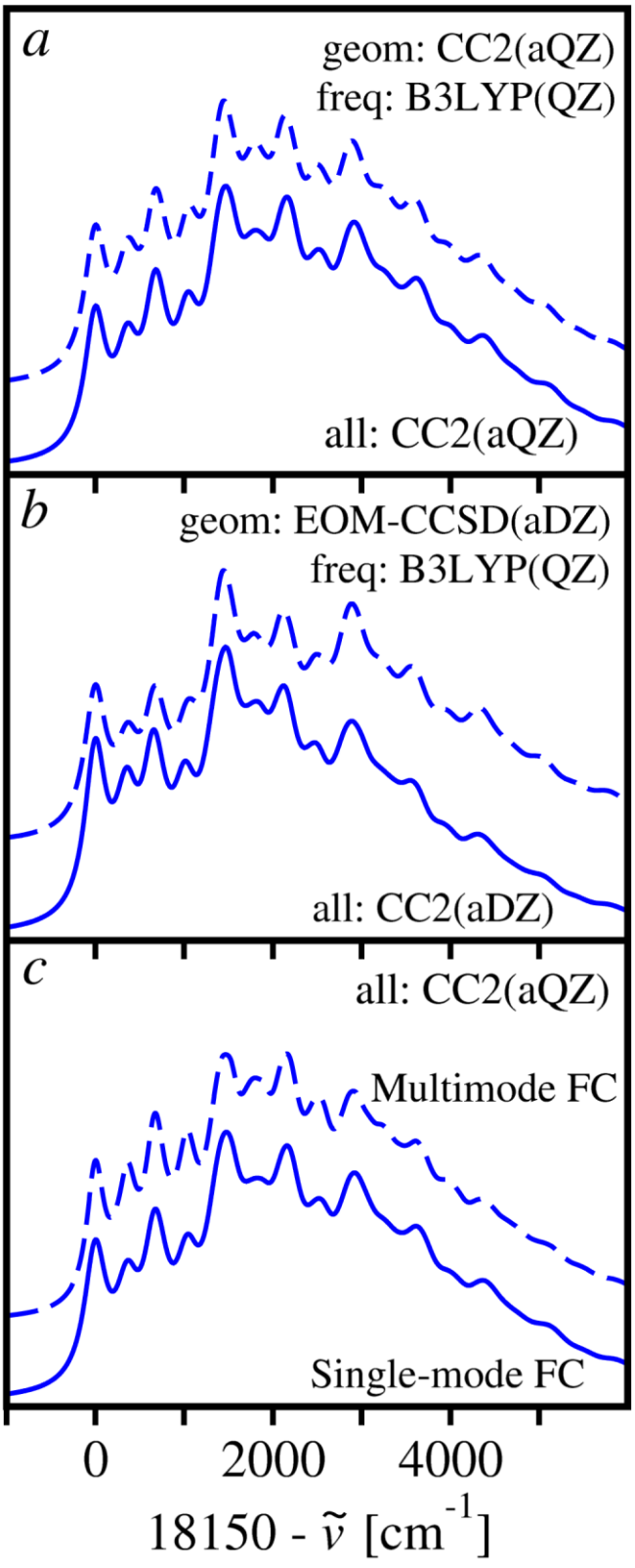

Fig.3S. Effects of various approximations used in the theoretical modeling of the phosphorescence spectrum of 2T.