

Mind the GAP: Quantifying the Breakdown of the Linear Vibronic Coupling Hamiltonian

Supplementary Information

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Contents

S1 TBPe	3
S1-1 Geometry	3
S1-2 Electronic Structure	6
S1-3 LVC parameters	7
S2 TAT-3DBTO2	24
S2-1 Geometry	24
S2-2 Electronic Structure	29
S2-3 LVC parameters	30
S3 Maleimide	46
S3-1 Geometry	46
S3-2 Electronic Structure	46
S3-3 LVC parameters	49
S3-4 Excited-states Dynamics	53
S3-4.1 6-modes Hamiltonian parameters	54
S3-4.2 12-modes Hamiltonian parameters	54

List of Tables

S1 Cartesian coordinates of the GS Minimum of TBPe.	3
S2 Cartesian coordinates of the S1 Minimum of TBPe.	3
S3 Cartesian coordinates of the S1 LVC minimum of TBPe.	4
S4 Cartesian coordinates of the T1 Minimum of TBPe.	5
S5 Cartesian coordinates of the T1 LVC Minimum of TBPe.	5
S6 LVC Analysis for S1 of TBPe.	7
S7 LVC Analysis for T1 of TBPe.	12
S8 LVC Analysis for T2 of TBPe.	17
S9 Cartesian coordinates of the GS Minimum of TAT-3DBTO ₂	24
S10 Cartesian coordinates of the S ₁ C ₃ Minimum of TAT-3DBTO ₂	25
S11 Cartesian coordinates of the S ₁ C ₁ Minimum of TAT-3DBTO ₂	25
S12 Cartesian coordinates of the S ₁ LVC Minimum of TAT-3DBTO ₂	26
S13 Cartesian coordinates of the T ₁ Minimum of TAT-3DBTO ₂	27
S14 Rotation coordinates φ of TAT-3DBTO ₂	28
S15 LVC Analysis for S1 of TAT-3DBTO ₂	30
S16 LVC Analysis for T1 of TAT-3DBTO ₂	37
S17 Cartesian coordinates different minima of Maleimide.	46
S18 Cartesian coordinates different minima of Maleimide.	46

S19	Electronic structure at the ground state optimised geometry. GS stands for the ground state electronic structure: $(\pi_1)^2(\pi_2)^2(n_1)^2(n_2)^2(\pi^*)^0$. Molecular orbitals are shown in figure S5.	46
S20	Electronic structure at the excited states optimised geometries. GS stands for the ground state electronic structure: $(\pi_1)^2(\pi_2)^2(n_1)^2(n_2)^2(\pi^*)^0$. Molecular orbitals are shown in figure S5.	47
S21	LVC Analysis for S1 of Maleimide.	49
S22	LVC Analysis for S2 of Maleimide.	49
S23	LVC Analysis for S3 of Maleimide.	50
S24	LVC Analysis for S4 of Maleimide.	51
S25	Intrastate coupling parameters for the 6-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.	54
S26	Intrastate coupling parameters for the 6-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.	54
S27	Computational details of the 6-modes MCTDH propagations with wavepackets with an initial wavepacket in 1B_2 or 2B_2 . The number of primitive basis and Single Particule Functions are given for each set of combined modes.	54
S28	Intrastate coupling parameters for the 12-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.	55
S29	Intrastate coupling parameters for the 12-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.	55
S30	Computational details of the 12-modes MCTDH propagations with wavepackets with an initial wavepacket in 1B_2 or 2B_2 . The number of primitive basis and Single Particule Functions are given for each set of combined modes.	55

List of Figures

S1	Difference of electronic density associated to the $T_1 \leftarrow \text{GS}$ (left), $S_1 \leftarrow \text{GS}$ (centre) and $T_2 \leftarrow \text{GS}$ (right) for TBPe	6
S2	Definition of the Donor-Acceptor torsion angle φ . \vec{n}_A and \vec{n}_B are the normal vectors to the donor and acceptor units, respectively.	29
S3	Difference of electronic density associated to the $T_1 \leftarrow \text{GS}$ (top) and $S_1 \leftarrow \text{GS}$ (bottom) at the ground state optimised geometry (left) the S_1 minimum (centre) and the T_1 minimum (right). Purple: loss of electronic density. Green: gain.	29
S4	RSMA for all the normal modes of TAT-3DBTO ₂ for S_1 and T_1 as a function of their index. The range of frequencies mentioned in the main text are emphasized in colours.	45
S5	Orbitals involved in the four lowest excited singlet states of Maleimide	47
S6	EOM-CCSD Path between Franck-Condon and the minimum of each of the four lowest excited states.	48
S7	Comparison between the computed adiabatic (full lines) and LVC diabatic (dashed lines) PES along a_1 normal modes.	52
S8	Schematic representation of the coupling selection rules at the C_{2v} ground state minimum of Maleimide . Arrows represent possible vibronic coupling and lowercase irreps correspond to the irreps of the normal modes that enable the coupling.	53
S9	Population kinetics of the lowest excited singlet states of Maleimide using a model Hamiltonian along 12 (full lines) and 6 (dashed lines) normal modes. The initial wavepacket is position at Q_0 in S_4	53

S1 TBPe

S1-1 Geometry

Table S1: Cartesian coordinates of the GS Minimum of TBPe.

At	x	y	z	At	x	y	z	At	x	y	z
C	0.7331	-1.2408	0.0089	H	-0.9613	3.3572	-0.0009	H	5.5821	4.6136	0.0110
C	-0.7358	-1.2416	0.0101	C	3.5973	-3.7721	0.0097	H	5.4668	3.0915	-0.8728
C	-1.4247	0.0012	0.0069	C	-3.5970	-3.7761	0.0187	C	-5.1198	3.6210	-0.0040
C	-0.7372	1.2446	0.0043	C	3.5933	3.7796	0.0058	C	-3.1982	4.5637	-1.2545
C	0.7317	1.2453	0.0057	C	-3.6018	3.7757	-0.0027	C	-3.2006	4.5682	1.2471
C	1.4205	0.0026	0.0079	C	3.1959	-4.5621	-1.2415	H	-5.4701	3.0841	-0.8891
C	2.8371	0.0033	0.0086	C	3.1939	-4.5626	1.2600	H	-5.5917	4.6070	-0.0074
C	3.5375	1.2291	0.0082	C	5.1154	-3.6176	0.0111	H	-5.4723	3.0892	0.8833
C	2.8793	2.4326	0.0066	H	2.1180	-4.7461	1.2962	H	-3.4800	4.0301	2.1562
C	1.4715	2.4085	0.0051	H	3.4717	-4.0232	2.1688	H	-3.7037	5.5392	1.2560
C	3.5387	-1.2217	0.0095	H	3.6970	-5.5336	1.2713	H	-2.1247	4.7515	1.2848
C	2.8817	-2.4260	0.0093	H	2.1200	-4.7448	-1.2798	H	-3.4765	4.0228	-2.1623
C	1.4739	-2.4033	0.0087	H	3.6984	-5.5334	-1.2521	H	-2.1222	4.7466	-1.2912
H	0.9569	-3.3534	0.0084	H	3.4759	-4.0226	-2.1497	H	-3.7008	5.5350	-1.2675
H	4.6214	-1.1774	0.0102	H	5.4677	-3.0835	-0.8749	C	-5.1153	-3.6234	0.0213
H	4.6202	1.1858	0.0093	H	5.5872	-4.6036	0.0118	C	-3.1915	-4.5638	1.2701
H	0.9536	3.3581	0.0032	H	5.4659	-3.0830	0.8975	C	-3.1957	-4.5679	-1.2315
C	-2.8412	0.0003	0.0071	C	5.1115	3.6269	0.0112	H	-3.4694	-4.0233	2.1782
C	-3.5430	1.2253	0.0038	C	3.1860	4.5725	1.2534	H	-2.1154	-4.7459	1.3058
C	-2.8860	2.4296	0.0006	C	3.1938	4.5662	-1.2481	H	-3.6933	-5.5355	1.2834
C	-1.4782	2.4070	0.0011	H	3.4621	4.0354	2.1641	H	-3.4765	-4.0301	-2.1403
C	-1.4753	-2.4049	0.0141	H	2.1099	4.7551	1.2866	H	-3.6975	-5.5396	-1.2402
C	-2.8831	-2.4291	0.0147	H	3.6882	5.5439	1.2637	H	-2.1196	-4.7497	-1.2700
C	-3.5415	-1.2256	0.0109	H	3.4765	4.0249	-2.1544	H	-5.4653	-3.0862	0.9063
H	-0.9572	-3.3544	0.0175	H	3.6952	5.5381	-1.2599	H	-5.5858	-4.6101	0.0260
H	-4.6242	-1.1824	0.0110	H	2.1177	4.7474	-1.2892	H	-5.4694	-3.0929	-0.8660
H	-4.6256	1.1808	0.0038	H	5.4605	3.0946	0.8996				

Table S2: Cartesian coordinates of the S1 Minimum of TBPe.

At	x	y	z	At	x	y	z	At	x	y	z
C	0.7185	-1.2373	0.0051	H	-0.9480	3.3785	-0.0045	H	5.5908	4.5956	0.0161
C	-0.7211	-1.2381	0.0044	C	3.5959	-3.7805	0.0168	H	5.4607	3.0745	-0.8667
C	-1.4114	0.0010	0.0036	C	-3.5955	-3.7846	0.0148	C	-5.1161	3.6088	0.0078
C	-0.7225	1.2408	0.0005	C	3.5914	3.7882	0.0027	C	-3.2147	4.5741	-1.2565
C	0.7171	1.2416	0.0008	C	-3.6000	3.7840	-0.0004	C	-3.2029	4.5848	1.2453
C	1.4074	0.0025	0.0040	C	3.2159	-4.5729	-1.2394	H	-5.4656	3.0676	-0.8750
C	2.8245	0.0033	0.0072	C	3.1937	-4.5790	1.2624	H	-5.6004	4.5887	0.0071
C	3.5193	1.2299	0.0070	C	5.1120	-3.6052	0.0314	H	-5.4564	3.0734	0.8977

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At	x	y	z	At	x	y	z	At	x	y	z
C	2.8568	2.4504	0.0035	H	2.1201	-4.7759	1.2888	H	-3.4690	4.0448	2.1573
C	1.4651	2.4346	-0.0001	H	3.4566	-4.0376	2.1745	H	-3.7203	5.5485	1.2552
C	3.5206	-1.2225	0.0116	H	3.7106	-5.5428	1.2758	H	-2.1295	4.7820	1.2754
C	2.8595	-2.4436	0.0126	H	2.1428	-4.7692	-1.2850	H	-3.4901	4.0265	-2.1612
C	1.4677	-2.4295	0.0087	H	3.7332	-5.5367	-1.2488	H	-2.1414	4.7700	-1.2984
H	0.9439	-3.3750	0.0095	H	3.4946	-4.0267	-2.1439	H	-3.7315	5.5381	-1.2695
H	4.6033	-1.1825	0.0145	H	5.4658	-3.0675	-0.8518	C	-5.1117	-3.6112	0.0401
H	4.6020	1.1912	0.0100	H	5.5963	-4.5851	0.0368	C	-3.1848	-4.5886	1.2541
H	0.9401	3.3795	-0.0033	H	5.4480	-3.0663	0.9209	C	-3.2223	-4.5705	-1.2475
C	-2.8285	0.0002	0.0065	C	5.1078	3.6150	0.0152	H	-3.4423	-4.0518	2.1705
C	-3.5247	1.2260	0.0055	C	3.1901	4.5894	1.2468	H	-2.1110	-4.7853	1.2730
C	-2.8636	2.4472	0.0015	C	3.2084	4.5768	-1.2549	H	-3.7011	-5.5528	1.2661
C	-1.4718	2.4330	-0.0012	H	3.4544	4.0503	2.1599	H	-3.5075	-4.0203	-2.1476
C	-1.4691	-2.4311	0.0069	H	2.1164	4.7855	1.2739	H	-3.7380	-5.5351	-1.2583
C	-2.8608	-2.4469	0.0118	H	3.7063	5.5536	1.2573	H	-2.1492	-4.7646	-1.3007
C	-3.5233	-1.2264	0.0114	H	3.4867	4.0288	-2.1585	H	-5.4421	-3.0746	0.9331
H	-0.9441	-3.3760	0.0048	H	3.7241	5.5414	-1.2675	H	-5.5948	-4.5918	0.0467
H	-4.6060	-1.1877	0.0151	H	2.1350	4.7714	-1.2997	H	-5.4726	-3.0721	-0.8394
H	-4.6073	1.1860	0.0082	H	5.4462	3.0798	0.9060				

Table S3: Cartesian coordinates of the S1 LVC minimum of TBPe.

At	x	y	z	At	x	y	z	At	x	y	z
C	0.7162	-1.2370	0.0097	H	-0.9481	3.3787	0.0013	H	5.5886	4.5961	0.0074
C	-0.7191	-1.2377	0.0097	C	3.5933	-3.7813	0.0133	H	5.4539	3.0759	-0.8766
C	-1.4089	0.0011	0.0079	C	-3.5930	-3.7851	0.0146	C	-5.1138	3.6095	-0.0021
C	-0.7203	1.2406	0.0056	C	3.5888	3.7887	0.0029	C	-3.2046	4.5789	-1.2513
C	0.7149	1.2413	0.0055	C	-3.5974	3.7848	0.0001	C	-3.2084	4.5822	1.2505
C	1.4047	0.0025	0.0075	C	3.2002	-4.5801	-1.2350	H	-5.4571	3.0690	-0.8878
C	2.8234	0.0031	0.0078	C	3.2052	-4.5740	1.2670	H	-5.5983	4.5894	-0.0053
C	3.5179	1.2292	0.0064	C	5.1097	-3.6056	0.0097	H	-5.4604	3.0732	0.8849
C	2.8539	2.4507	0.0046	H	2.1318	-4.7707	1.3056	H	-3.4802	4.0395	2.1593
C	1.4652	2.4345	0.0039	H	3.4778	-4.0279	2.1735	H	-3.7260	5.5460	1.2600
C	3.5190	-1.2222	0.0096	H	3.7226	-5.5378	1.2797	H	-2.1350	4.7791	1.2876
C	2.8563	-2.4443	0.0115	H	2.1269	-4.7777	-1.2682	H	-3.4737	4.0337	-2.1594
C	1.4676	-2.4297	0.0119	H	3.7183	-5.5435	-1.2452	H	-2.1312	4.7759	-1.2857
H	0.9438	-3.3752	0.0134	H	3.4686	-4.0380	-2.1452	H	-3.7222	5.5426	-1.2648
H	4.6015	-1.1829	0.0094	H	5.4525	-3.0686	-0.8783	C	-5.1096	-3.6118	0.0177
H	4.6005	1.1908	0.0070	H	5.5944	-4.5854	0.0103	C	-3.1985	-4.5798	1.2651
H	0.9405	3.3794	0.0024	H	5.4566	-3.0658	0.8944	C	-3.2034	-4.5809	-1.2367
C	-2.8276	0.0004	0.0081	C	5.1054	3.6155	0.0077	H	-3.4681	-4.0360	2.1739
C	-3.5233	1.2257	0.0057	C	3.1935	4.5876	1.2504	H	-2.1248	-4.7752	1.2990
C	-2.8605	2.4477	0.0031	C	3.2001	4.5803	-1.2513	H	-3.7146	-5.5443	1.2778
C	-1.4718	2.4331	0.0033	H	3.4620	4.0468	2.1613	H	-3.4760	-4.0375	-2.1448

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At	x	y	z	At	x	y	z	At	x	y	z
C	-1.4692	-2.4309	0.0115	H	2.1198	4.7836	1.2827	H	-3.7200	-5.5451	-1.2469
C	-2.8579	-2.4471	0.0122	H	3.7099	5.5519	1.2605	H	-2.1299	-4.7766	-1.2741
C	-3.5220	-1.2257	0.0105	H	3.4738	4.0340	-2.1575	H	-5.4532	-3.0724	0.9040
H	-0.9446	-3.3759	0.0128	H	3.7163	5.5447	-1.2643	H	-5.5927	-4.5924	0.0204
H	-4.6046	-1.1874	0.0109	H	2.1265	4.7754	-1.2904	H	-5.4574	-3.0753	-0.8688
H	-4.6059	1.1863	0.0058	H	5.4484	3.0792	0.8962				

Table S4: Cartesian coordinates of the T1 Minimum of TBPe.

At	x	y	z	At	x	y	z	At	x	y	z
C	0.7116	-1.2395	-0.0006	H	-0.9481	3.3843	-0.0009	H	5.6085	4.5746	0.0061
C	-0.7134	-1.2383	-0.0005	C	3.5963	-3.7887	-0.0006	H	5.4633	3.0572	-0.8801
C	-1.4015	0.0011	-0.0005	C	-3.6031	-3.7823	0.0009	C	-5.1118	3.6069	-0.0023
C	-0.7113	1.2393	-0.0006	C	3.6033	3.7820	0.0011	C	-3.2083	4.5866	-1.2508
C	0.7138	1.2382	-0.0003	C	-3.5961	3.7884	-0.0009	C	-3.2104	4.5854	1.2505
C	1.4019	-0.0013	-0.0003	C	3.2104	-4.5855	-1.2520	H	-5.4543	3.0677	-0.8891
C	2.8224	-0.0026	0.0002	C	3.2086	-4.5870	1.2493	H	-5.5997	4.5851	-0.0027
C	3.5199	1.2198	0.0008	C	5.1120	-3.6072	0.0006	H	-5.4561	3.0676	0.8837
C	2.8585	2.4480	0.0008	H	2.1363	-4.7894	1.2838	H	-3.4785	4.0398	2.1587
C	1.4765	2.4367	0.0000	H	3.4753	-4.0424	2.1585	H	-3.7324	5.5465	1.2624
C	3.5177	-1.2262	0.0002	H	3.7307	-5.5481	1.2610	H	-2.1381	4.7877	1.2868
C	2.8542	-2.4533	-0.0004	H	2.1381	-4.7878	-1.2882	H	-3.4749	4.0421	-2.1600
C	1.4722	-2.4395	-0.0008	H	3.7323	-5.5467	-1.2640	H	-2.1360	4.7891	-1.2852
H	0.9483	-3.3845	-0.0014	H	3.4785	-4.0399	-2.1601	H	-3.7303	5.5478	-1.2625
H	4.6000	-1.1853	0.0006	H	5.4561	-3.0675	-0.8852	C	-5.1184	-3.5976	0.0046
H	4.6020	1.1770	0.0013	H	5.5998	-4.5854	0.0006	C	-3.2152	-4.5820	1.2498
H	0.9544	3.3828	-0.0002	H	5.4547	-3.0684	0.8875	C	-3.2207	-4.5792	-1.2515
C	-2.8221	0.0023	-0.0003	C	5.1187	3.5975	0.0052	H	-3.4798	-4.0375	2.1597
C	-3.5175	1.2259	-0.0005	C	3.2152	4.5819	1.2499	H	-2.1432	-4.7864	1.2828
C	-2.8539	2.4531	-0.0008	C	3.2211	4.5788	-1.2514	H	-3.7389	-5.5422	1.2615
C	-1.4720	2.4393	-0.0008	H	3.4796	4.0376	2.1599	H	-3.4891	-4.0327	-2.1590
C	-1.4762	-2.4370	-0.0001	H	2.1432	4.7864	1.2826	H	-3.7444	-5.5394	-1.2631
C	-2.8581	-2.4483	0.0004	H	3.7389	5.5421	1.2615	H	-2.1488	-4.7834	-1.2895
C	-3.5195	-1.2201	0.0002	H	3.4899	4.0321	-2.1587	H	-5.4584	-3.0578	0.8919
H	-0.9539	-3.3830	0.0001	H	3.7448	5.5390	-1.2631	H	-5.6082	-4.5747	0.0055
H	-4.6017	-1.1774	0.0004	H	2.1493	4.7828	-1.2897	H	-5.4628	-3.0574	-0.8809
H	-4.5997	1.1851	-0.0004	H	5.4585	3.0579	0.8927				

Table S5: Cartesian coordinates of the T1 LVC Minimum of TBPe.

At	x	y	z	At	x	y	z	At	x	y	z
C	0.7091	-1.2368	0.0100	H	-0.9544	3.3834	0.0015	H	5.5940	4.5887	0.0082
C	-0.7120	-1.2374	0.0097	C	3.5955	-3.7818	0.0136	H	5.4542	3.0694	-0.8760
C	-1.4017	0.0011	0.0081	C	-3.5951	-3.7856	0.0140	C	-5.1154	3.6040	-0.0023

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At	x	y	z	At	x	y	z	At	x	y	z
C	-0.7133	1.2403	0.0058	C	3.5909	3.7892	0.0029	C	-3.2105	4.5816	-1.2508
C	0.7079	1.2409	0.0055	C	-3.5994	3.7854	0.0002	C	-3.2148	4.5850	1.2504
C	1.3975	0.0025	0.0075	C	3.2044	-4.5844	-1.2326	H	-5.4569	3.0625	-0.8881
C	2.8187	0.0031	0.0076	C	3.2139	-4.5752	1.2687	H	-5.6036	4.5822	-0.0057
C	3.5143	1.2266	0.0061	C	5.1114	-3.5999	0.0070	H	-5.4607	3.0668	0.8847
C	2.8500	2.4528	0.0044	H	2.1415	-4.7770	1.3092	H	-3.4839	4.0412	2.1594
C	1.4696	2.4386	0.0039	H	3.4854	-4.0269	2.1743	H	-3.7368	5.5464	1.2598
C	3.5155	-1.2197	0.0092	H	3.7357	-5.5367	1.2818	H	-2.1423	4.7872	1.2872
C	2.8524	-2.4465	0.0117	H	2.1319	-4.7878	-1.2632	H	-3.4763	4.0353	-2.1593
C	1.4720	-2.4338	0.0127	H	3.7272	-5.5453	-1.2429	H	-2.1379	4.7840	-1.2845
H	0.9501	-3.3799	0.0150	H	3.4679	-4.0422	-2.1443	H	-3.7325	5.5429	-1.2647
H	4.5976	-1.1780	0.0086	H	5.4507	-3.0623	-0.8821	C	-5.1113	-3.6062	0.0175
H	4.5965	1.1859	0.0066	H	5.6000	-4.5778	0.0072	C	-3.2045	-4.5830	1.2637
H	0.9468	3.3842	0.0025	H	5.4585	-3.0585	0.8906	C	-3.2100	-4.5831	-1.2374
C	-2.8230	0.0004	0.0083	C	5.1071	3.6099	0.0082	H	-3.4709	-4.0386	2.1731
C	-3.5198	1.2231	0.0060	C	3.1993	4.5905	1.2499	H	-2.1316	-4.7838	1.2969
C	-2.8567	2.4499	0.0034	C	3.2066	4.5829	-1.2512	H	-3.7250	-5.5452	1.2763
C	-1.4762	2.4373	0.0036	H	3.4647	4.0487	2.1612	H	-3.4798	-4.0382	-2.1456
C	-1.4736	-2.4351	0.0111	H	2.1265	4.7917	1.2815	H	-3.7312	-5.5450	-1.2481
C	-2.8541	-2.4492	0.0119	H	3.7201	5.5525	1.2601	H	-2.1374	-4.7843	-1.2747
C	-3.5185	-1.2231	0.0105	H	3.4774	4.0354	-2.1575	H	-5.4530	-3.0660	0.9040
H	-0.9509	-3.3807	0.0119	H	3.7274	5.5449	-1.2643	H	-5.5982	-4.5850	0.0201
H	-4.6007	-1.1825	0.0110	H	2.1339	4.7834	-1.2900	H	-5.4577	-3.0685	-0.8687
H	-4.6020	1.1814	0.0061	H	5.4480	3.0724	0.8967				

S1-2 Electronic Structure

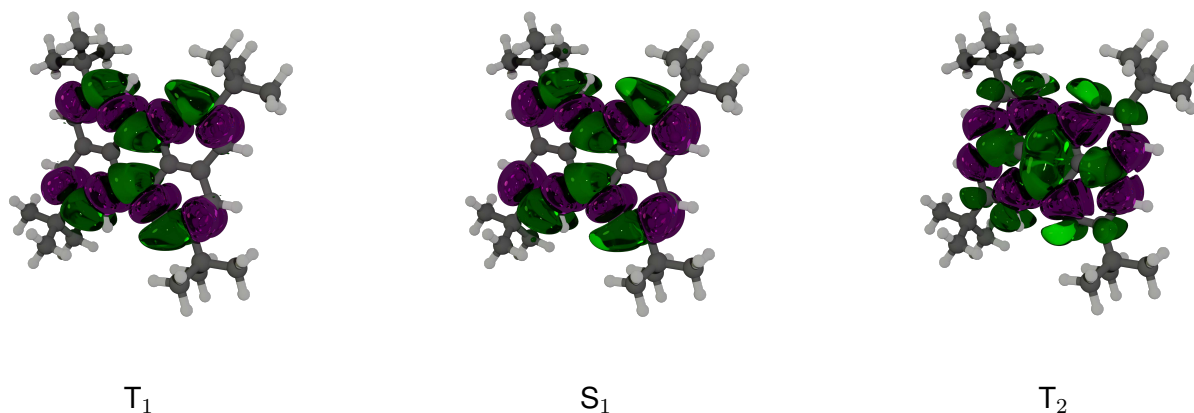


Figure S1: Difference of electronic density associated to the $T_1 \leftarrow GS$ (left), $S_1 \leftarrow GS$ (centre) and $T_2 \leftarrow GS$ (right) for **TBPe**.

S1-3 LVC parameters

Table S6: LVC Analysis for S1 of TBPe.

α	Freq. /cm ⁻¹	κ_α			κ_α^*			ξ
		κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	
1	19.71	0.102	0.000	-0.042	-0.268	-0.001	0.110	0.001
2	25.22	0.103	0.000	-0.033	1.261	-0.009	-0.403	-0.002
3	29.15	-0.108	0.000	0.030	0.540	-0.001	-0.149	-0.002
4	30.92	-0.042	0.000	0.011	-0.422	-0.001	0.110	0.001
5	31.41	-0.040	0.000	0.010	1.404	-0.009	-0.361	0.001
6	48.26	-0.029	0.000	0.005	-0.175	0.000	0.029	0.000
7	72.92	-0.043	0.000	0.005	-2.508	-0.013	0.277	0.000
8	80.77	-0.043	0.000	0.004	-2.378	-0.010	0.237	0.000
9	91.43	1.131	-0.002	-0.100	-3.244	-0.017	0.286	0.009
10	94.40	0.045	0.000	-0.004	4.434	-0.031	-0.379	0.000
11	115.51	-0.001	0.000	0.000	-2.061	-0.005	0.144	0.000
12	122.18	-0.223	0.000	0.015	-2.893	-0.010	0.191	0.000
13	122.91	-0.076	0.000	0.005	-2.919	-0.010	0.192	-0.001
14	153.00	-0.142	0.000	0.007	-0.202	0.000	0.011	0.000
15	166.89	0.272	0.000	-0.013	3.212	-0.009	-0.155	0.001
16	201.34	-0.110	0.000	0.004	8.020	-0.047	-0.321	-0.002
17	223.58	0.011	0.000	0.000	9.687	-0.062	-0.349	0.000
18	228.79	-6.518	-0.028	0.230	-1.275	-0.001	0.045	0.034
19	238.58	-0.020	0.000	0.001	-8.310	-0.043	0.281	0.000
20	238.92	0.178	0.000	-0.006	-2.768	-0.005	0.093	-0.001
21	240.51	0.091	0.000	-0.003	3.582	-0.008	-0.120	-0.001
22	243.91	0.133	0.000	-0.004	-0.450	0.000	0.015	0.000
23	248.58	-0.539	0.000	0.017	9.696	-0.056	-0.315	0.003
24	252.51	-0.442	0.000	0.014	-1.007	-0.001	0.032	0.002
25	253.20	-0.343	0.000	0.011	-17.759	-0.185	0.566	-0.002
26	258.34	11.188	-0.072	-0.349	-7.526	-0.032	0.235	0.052
27	259.22	21.131	-0.255	-0.657	1.222	-0.001	-0.038	-0.094
28	281.31	0.051	0.000	-0.001	-11.276	-0.067	0.323	0.000
29	285.32	0.227	0.000	-0.006	4.852	-0.012	-0.137	-0.001
30	289.15	-0.257	0.000	0.007	-7.270	-0.027	0.203	-0.001
31	290.74	-0.489	0.000	0.014	-6.193	-0.020	0.172	-0.002
32	292.88	-12.108	-0.074	0.333	-11.191	-0.063	0.308	-0.054
33	315.20	-0.076	0.000	0.002	5.508	-0.014	-0.141	0.000
34	322.92	0.090	0.000	-0.002	1.346	-0.001	-0.034	0.000
35	330.98	0.076	0.000	-0.002	1.477	-0.001	-0.036	0.000
36	331.92	-0.192	0.000	0.005	0.236	0.000	-0.006	-0.001
37	336.73	-0.203	0.000	0.005	5.773	-0.015	-0.138	0.001
38	336.98	0.171	0.000	-0.004	3.132	-0.004	-0.075	-0.001
39	337.73	-0.051	0.000	0.001	-2.432	-0.003	0.058	0.000
40	342.64	0.067	0.000	-0.002	-1.002	0.000	0.024	0.001
41	343.67	-0.045	0.000	0.001	4.510	-0.009	-0.106	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
42	349.09	-0.112	0.000	0.003	-2.548	-0.003	0.059	-0.001
43	359.10	-0.355	0.000	0.008	-2.484	-0.003	0.056	-0.001
44	365.63	0.708	0.000	-0.016	4.245	-0.007	-0.094	0.003
45	374.78	-29.524	-0.345	0.635	1.856	-0.001	-0.040	-0.135
46	397.68	0.071	0.000	-0.001	14.672	-0.080	-0.298	0.000
47	398.76	0.015	0.000	0.000	0.569	0.000	-0.012	0.000
48	402.17	0.084	0.000	-0.002	6.468	-0.015	-0.130	0.000
49	411.18	0.088	0.000	-0.002	4.724	-0.008	-0.093	-0.001
50	414.21	0.088	0.000	-0.002	1.631	-0.001	-0.032	0.000
51	427.83	-0.542	0.000	0.010	-2.629	-0.002	0.050	0.002
52	435.71	23.205	-0.183	-0.430	-15.283	-0.079	0.283	-0.104
53	468.07	0.015	0.000	0.000	-2.438	-0.002	0.042	0.000
54	485.28	-0.096	0.000	0.002	-6.270	-0.012	0.104	0.001
55	507.84	10.886	-0.035	-0.173	9.647	-0.027	-0.153	-0.056
56	511.26	-0.671	0.000	0.011	-3.721	-0.004	0.059	0.003
57	521.76	-0.211	0.000	0.003	7.330	-0.015	-0.113	0.001
58	525.67	0.012	0.000	0.000	14.647	-0.060	-0.225	0.000
59	561.37	-0.114	0.000	0.002	-30.260	-0.242	0.435	0.000
60	563.93	-5.758	-0.009	0.082	2.806	-0.002	-0.040	0.033
61	564.55	10.755	-0.030	-0.154	8.748	-0.020	-0.125	-0.059
62	578.88	-0.367	0.000	0.005	-27.124	-0.188	0.378	0.002
63	618.44	-0.018	0.000	0.000	3.168	-0.002	-0.041	-0.001
64	643.48	-0.055	0.000	0.001	-0.241	0.000	0.003	0.000
65	651.09	0.062	0.000	-0.001	7.578	-0.013	-0.094	-0.001
66	660.36	-0.061	0.000	0.001	-9.209	-0.019	0.112	-0.001
67	663.17	-0.035	0.000	0.000	-9.102	-0.019	0.111	0.001
68	679.98	-0.163	0.000	0.002	24.996	-0.136	-0.296	0.001
69	681.57	0.170	0.000	-0.002	3.135	-0.002	-0.037	-0.001
70	691.69	16.873	-0.061	-0.197	-25.020	-0.134	0.292	-0.092
71	692.91	1.118	0.000	-0.013	-1.167	0.000	0.014	-0.006
72	698.96	0.159	0.000	-0.002	-0.204	0.000	0.002	-0.001
73	713.38	-0.119	0.000	0.001	3.090	-0.002	-0.035	0.000
74	821.38	0.081	0.000	-0.001	-7.462	-0.010	0.073	-0.001
75	823.62	0.278	0.000	-0.003	-4.166	-0.003	0.041	-0.002
76	824.47	6.493	-0.008	-0.064	9.726	-0.017	-0.095	0.027
77	826.36	-0.374	0.000	0.004	9.986	-0.018	-0.097	-0.003
78	835.58	-0.070	0.000	0.001	-5.032	-0.004	0.049	0.001
79	846.60	0.084	0.000	-0.001	29.512	-0.152	-0.281	0.000
80	855.57	-0.040	0.000	0.000	15.988	-0.044	-0.151	0.000
81	877.21	-0.071	0.000	0.001	46.915	-0.372	-0.431	0.000
82	879.05	0.006	0.000	0.000	39.765	-0.267	-0.365	0.000
83	898.67	-0.180	0.000	0.002	29.079	-0.139	-0.261	-0.001
84	900.60	0.103	0.000	-0.001	18.890	-0.059	-0.169	0.001
85	902.45	0.082	0.000	-0.001	33.694	-0.186	-0.301	-0.002

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
86	905.76	0.093	0.000	-0.001	17.641	-0.051	-0.157	0.002
87	926.72	-0.033	0.000	0.000	50.742	-0.412	-0.442	0.000
88	928.27	-0.057	0.000	0.000	70.820	-0.801	-0.615	0.000
89	936.91	0.091	0.000	-0.001	-7.464	-0.009	0.064	0.000
90	943.49	-0.030	0.000	0.000	5.090	-0.004	-0.044	0.000
91	943.60	-0.031	0.000	0.000	-5.382	-0.005	0.046	0.000
92	943.77	0.056	0.000	0.000	15.852	-0.039	-0.135	0.000
93	943.96	0.111	0.000	-0.001	-1.387	0.000	0.012	-0.001
94	946.92	-0.452	0.000	0.004	25.147	-0.099	-0.214	0.001
95	947.13	0.032	0.000	0.000	-58.907	-0.543	0.502	0.000
96	947.24	0.075	0.000	-0.001	17.861	-0.050	-0.152	0.000
97	948.23	-0.102	0.000	0.001	14.513	-0.033	-0.123	0.000
98	949.17	0.039	0.000	0.000	-53.752	-0.451	0.457	0.000
99	949.22	-0.006	0.000	0.000	12.153	-0.023	-0.103	0.000
100	949.44	-0.013	0.000	0.000	-12.185	-0.023	0.104	0.000
101	949.50	0.025	0.000	0.000	20.147	-0.063	-0.171	0.000
102	972.23	-18.382	-0.052	0.152	-13.691	-0.029	0.114	0.085
103	995.69	-0.077	0.000	0.001	0.344	0.000	-0.003	0.001
104	1006.22	-0.015	0.000	0.000	0.702	0.000	-0.006	0.000
105	1031.64	-11.740	-0.020	0.092	-37.461	-0.202	0.293	0.037
106	1036.50	-0.021	0.000	0.000	1.754	0.000	-0.014	0.000
107	1037.46	-0.052	0.000	0.000	15.557	-0.035	-0.121	0.000
108	1040.53	0.006	0.000	0.000	11.784	-0.020	-0.091	0.000
109	1041.73	0.028	0.000	0.000	-41.130	-0.241	0.318	0.000
110	1041.84	-0.099	0.000	0.001	-7.756	-0.009	0.060	0.000
111	1042.08	0.070	0.000	-0.001	10.756	-0.016	-0.083	-0.001
112	1042.19	0.031	0.000	0.000	0.948	0.000	-0.007	-0.001
113	1075.14	6.530	-0.006	-0.049	16.555	-0.038	-0.124	-0.006
114	1094.17	-0.156	0.000	0.001	1.218	0.000	-0.009	0.001
115	1139.66	-0.002	0.000	0.000	28.078	-0.103	-0.199	0.000
116	1143.22	0.030	0.000	0.000	0.044	0.000	0.000	0.000
117	1161.39	8.295	-0.009	-0.058	-19.557	-0.049	0.136	-0.066
118	1196.98	-0.004	0.000	0.000	13.260	-0.022	-0.089	0.000
119	1219.19	-0.374	0.000	0.002	9.013	-0.010	-0.060	0.001
120	1239.25	0.032	0.000	0.000	-7.505	-0.007	0.049	0.000
121	1239.30	0.025	0.000	0.000	-1.410	0.000	0.009	0.000
122	1239.53	0.043	0.000	0.000	12.583	-0.019	-0.082	0.000
123	1239.64	0.026	0.000	0.000	1.875	0.000	-0.012	0.000
124	1239.89	0.080	0.000	-0.001	-2.064	-0.001	0.013	-0.001
125	1242.84	0.240	0.000	-0.002	8.853	-0.009	-0.057	0.001
126	1245.47	-0.184	0.000	0.001	-13.866	-0.023	0.090	-0.001
127	1246.17	1.481	0.000	-0.010	-43.374	-0.224	0.281	0.006
128	1246.38	-11.916	-0.017	0.077	-41.501	-0.205	0.269	0.048
129	1249.01	0.731	0.000	-0.005	15.937	-0.030	-0.103	-0.003

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
130	1251.58	0.060	0.000	0.000	-2.521	-0.001	0.016	0.000
131	1286.36	-28.288	-0.092	0.177	-57.047	-0.375	0.358	0.120
132	1290.87	0.386	0.000	-0.002	-75.762	-0.659	0.473	-0.002
133	1301.27	-0.029	0.000	0.000	21.986	-0.055	-0.136	0.000
134	1302.69	0.116	0.000	-0.001	-40.987	-0.191	0.254	0.000
135	1333.48	58.836	-0.385	-0.356	-36.347	-0.147	0.220	-0.256
136	1337.26	0.235	0.000	-0.001	-14.541	-0.023	0.088	-0.002
137	1365.13	0.563	0.000	-0.003	-19.682	-0.042	0.116	-0.003
138	1381.26	2.074	0.000	-0.012	45.835	-0.225	-0.268	-0.009
139	1381.60	0.520	0.000	-0.003	26.966	-0.078	-0.157	-0.002
140	1382.10	25.199	-0.068	-0.147	-9.342	-0.009	0.055	-0.116
141	1382.69	1.192	0.000	-0.007	-16.434	-0.029	0.096	-0.006
142	1382.75	1.409	0.000	-0.008	-0.912	0.000	0.005	-0.007
143	1383.08	0.192	0.000	-0.001	31.604	-0.107	-0.184	0.001
144	1383.10	2.309	-0.001	-0.013	5.422	-0.003	-0.032	-0.010
145	1389.89	0.532	0.000	-0.003	9.558	-0.010	-0.055	-0.002
146	1408.39	-37.162	-0.145	0.213	28.472	-0.085	-0.163	0.199
147	1413.70	-3.308	-0.001	0.019	33.044	-0.114	-0.189	0.014
148	1413.92	-0.970	0.000	0.006	-16.369	-0.028	0.093	0.005
149	1415.75	6.975	-0.005	-0.040	-16.210	-0.028	0.092	-0.031
150	1415.95	40.181	-0.169	-0.229	-11.444	-0.014	0.065	-0.189
151	1420.74	-2.508	-0.001	0.014	-61.984	-0.401	0.352	0.010
152	1426.35	0.146	0.000	-0.001	33.687	-0.118	-0.190	-0.001
153	1428.84	-0.284	0.000	0.002	-7.023	-0.005	0.040	0.001
154	1437.07	129.908	-1.740	-0.729	-6.703	-0.005	0.038	-0.565
155	1461.88	21.123	-0.045	-0.117	10.532	-0.011	-0.058	-0.093
156	1467.06	-1.767	0.000	0.010	-12.780	-0.017	0.070	0.008
157	1470.16	0.094	0.000	-0.001	25.321	-0.065	-0.139	0.000
158	1470.37	0.201	0.000	-0.001	25.685	-0.066	-0.141	-0.001
159	1470.65	-0.070	0.000	0.000	-15.434	-0.024	0.085	0.001
160	1470.75	0.002	0.000	0.000	28.684	-0.083	-0.157	0.000
161	1472.68	-0.204	0.000	0.001	-6.949	-0.005	0.038	0.001
162	1472.76	-0.351	0.000	0.002	0.526	0.000	-0.003	0.001
163	1473.16	0.218	0.000	-0.001	1.494	0.000	-0.008	-0.001
164	1473.32	-0.108	0.000	0.001	-100.721	-1.020	0.551	-0.001
165	1474.38	-0.286	0.000	0.002	24.193	-0.059	-0.132	0.001
166	1476.12	0.056	0.000	0.000	-2.618	-0.001	0.014	0.000
167	1478.91	0.164	0.000	-0.001	30.499	-0.093	-0.166	0.001
168	1480.79	-4.192	-0.002	0.023	0.680	0.000	-0.004	0.022
169	1485.26	-0.158	0.000	0.001	-67.912	-0.460	0.369	0.001
170	1486.03	0.289	0.000	-0.002	-64.085	-0.410	0.348	-0.001
171	1494.75	-0.258	0.000	0.001	35.089	-0.122	-0.189	0.001
172	1494.81	-0.124	0.000	0.001	6.285	-0.004	-0.034	0.001
173	1494.91	0.084	0.000	0.000	21.651	-0.046	-0.117	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
174	1494.95	0.217	0.000	-0.001	31.520	-0.098	-0.170	0.002
175	1496.87	-0.006	0.000	0.000	-40.965	-0.166	0.221	0.000
176	1498.18	0.203	0.000	-0.001	40.580	-0.163	-0.218	-0.001
177	1498.85	9.247	-0.008	-0.050	-0.419	0.000	0.002	-0.045
178	1502.51	0.252	0.000	-0.001	-18.975	-0.036	0.102	-0.001
179	1514.73	2.198	0.000	-0.012	23.851	-0.056	-0.127	-0.011
180	1514.96	11.113	-0.012	-0.059	-26.541	-0.069	0.141	-0.046
181	1515.02	5.579	-0.003	-0.030	25.743	-0.065	-0.137	-0.030
182	1515.43	0.329	0.000	-0.002	57.201	-0.320	-0.304	-0.001
183	1545.91	0.005	0.000	0.000	-60.930	-0.356	0.318	0.000
184	1568.47	1.044	0.000	-0.005	-15.246	-0.022	0.078	-0.004
185	1633.27	133.775	-1.624	-0.661	52.185	-0.247	-0.258	-0.594
186	1641.96	-4.500	-0.002	0.022	-2.119	0.000	0.010	0.020
187	1661.09	-54.069	-0.261	0.263	19.954	-0.036	-0.097	0.255
188	1669.59	0.633	0.000	-0.003	-0.168	0.000	0.001	-0.003
189	1677.42	0.545	0.000	-0.003	7.136	-0.004	-0.034	-0.003
190	1690.87	-1.135	0.000	0.005	2.998	-0.001	-0.014	0.005
191	3039.23	0.042	0.000	0.000	-6.996	-0.002	0.019	0.001
192	3039.29	0.001	0.000	0.000	27.044	-0.036	-0.072	0.000
193	3039.36	-0.032	0.000	0.000	50.952	-0.127	-0.135	-0.001
194	3039.38	-0.128	0.000	0.000	-47.875	-0.112	0.127	-0.002
195	3040.60	-0.001	0.000	0.000	-18.757	-0.017	0.050	0.000
196	3040.64	0.019	0.000	0.000	-11.448	-0.006	0.030	0.000
197	3040.65	-0.008	0.000	0.000	23.527	-0.027	-0.062	0.000
198	3040.72	0.001	0.000	0.000	39.888	-0.078	-0.106	0.001
199	3046.44	-0.050	0.000	0.000	-42.578	-0.088	0.113	-0.001
200	3046.49	-0.110	0.000	0.000	-70.785	-0.244	0.187	0.002
201	3046.57	0.389	0.000	-0.001	-34.418	-0.058	0.091	0.000
202	3046.62	-0.821	0.000	0.002	15.706	-0.012	-0.042	0.006
203	3112.54	0.535	0.000	-0.001	-100.347	-0.479	0.260	0.003
204	3112.61	0.276	0.000	-0.001	57.933	-0.160	-0.150	-0.001
205	3112.66	0.033	0.000	0.000	116.483	-0.646	-0.302	-0.001
206	3112.69	-1.848	0.000	0.005	31.500	-0.047	-0.082	-0.010
207	3115.49	0.010	0.000	0.000	-158.400	-1.194	0.410	0.000
208	3115.51	0.008	0.000	0.000	-51.350	-0.125	0.133	0.000
209	3115.55	-0.014	0.000	0.000	16.746	-0.013	-0.043	0.000
210	3115.59	-0.017	0.000	0.000	57.540	-0.157	-0.149	0.001
211	3120.29	0.025	0.000	0.000	-7.437	-0.003	0.019	-0.001
212	3120.37	0.035	0.000	0.000	10.925	-0.006	-0.028	0.000
213	3120.40	0.002	0.000	0.000	-41.943	-0.084	0.108	-0.002
214	3120.83	-1.628	0.000	0.004	-5.277	-0.001	0.014	-0.007
215	3122.04	-0.018	0.000	0.000	32.735	-0.051	-0.085	0.000
216	3122.05	0.014	0.000	0.000	-7.244	-0.002	0.019	0.000
217	3122.06	-0.025	0.000	0.000	-35.097	-0.058	0.091	0.001

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
218	3122.07	0.006	0.000	0.000	5.818	-0.002	-0.015	0.001
219	3126.02	0.027	0.000	0.000	2.456	0.000	-0.006	0.000
220	3126.06	0.006	0.000	0.000	-28.084	-0.037	0.072	0.000
221	3126.11	0.031	0.000	0.000	-60.455	-0.173	0.156	0.002
222	3126.11	-0.004	0.000	0.000	14.480	-0.010	-0.037	-0.001
223	3127.30	-0.198	0.000	0.001	-66.731	-0.211	0.172	0.001
224	3127.36	-0.069	0.000	0.000	-6.313	-0.002	0.016	0.000
225	3127.53	0.493	0.000	-0.001	31.464	-0.047	-0.081	0.003
226	3127.58	-1.048	0.000	0.003	6.415	-0.002	-0.017	0.006
227	3201.25	-0.060	0.000	0.000	-51.097	-0.121	0.129	0.000
228	3201.59	-0.019	0.000	0.000	-22.012	-0.022	0.055	0.000
229	3206.04	0.403	0.000	-0.001	44.090	-0.090	-0.111	-0.002
230	3206.23	-3.054	0.000	0.008	163.722	-1.239	-0.412	0.011
231	3212.56	0.007	0.000	0.000	28.921	-0.039	-0.073	0.000
232	3212.72	0.085	0.000	0.000	12.553	-0.007	-0.032	0.000
233	3222.07	-4.639	-0.001	0.012	-12.036	-0.007	0.030	0.023
234	3222.15	6.327	-0.002	-0.016	-7.006	-0.002	0.018	-0.029

Table S7: LVC Analysis for T1 of TBPe.

α	Freq. /cm ⁻¹	κ_α			κ_α^*			ξ
		κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	
1	19.71	0.099	0.000	-0.041	0.050	0.000	-0.021	0.000
2	25.22	0.151	0.000	-0.048	1.705	-0.017	-0.545	0.000
3	29.15	-0.164	0.000	0.045	0.136	0.000	-0.038	0.000
4	30.92	-0.049	0.000	0.013	-2.689	-0.035	0.702	0.000
5	31.41	-0.073	0.000	0.019	2.108	-0.021	-0.541	0.000
6	48.26	-0.033	0.000	0.006	-0.031	0.000	0.005	0.000
7	72.92	-0.048	0.000	0.005	-1.439	-0.004	0.159	0.000
8	80.77	-0.032	0.000	0.003	-5.665	-0.059	0.566	0.000
9	91.43	2.677	-0.012	-0.236	-5.364	-0.047	0.473	0.014
10	94.40	0.042	0.000	-0.004	3.510	-0.019	-0.300	0.000
11	115.51	-0.013	0.000	0.001	-3.057	-0.012	0.213	0.000
12	122.18	-0.254	0.000	0.017	-1.242	-0.002	0.082	0.000
13	122.91	-0.079	0.000	0.005	-5.240	-0.033	0.344	0.000
14	153.00	-0.151	0.000	0.008	5.187	-0.026	-0.273	0.001
15	166.89	0.323	0.000	-0.016	2.434	-0.005	-0.118	0.001
16	201.34	-0.141	0.000	0.006	11.005	-0.089	-0.441	0.000
17	223.58	-0.002	0.000	0.000	4.963	-0.016	-0.179	0.000
18	228.79	-8.422	-0.046	0.297	0.859	0.000	-0.030	0.034
19	238.58	-0.030	0.000	0.001	-15.624	-0.152	0.528	0.000
20	238.92	0.251	0.000	-0.008	-4.352	-0.012	0.147	-0.001
21	240.51	0.118	0.000	-0.004	-1.453	-0.001	0.049	0.000
22	243.91	0.146	0.000	-0.005	10.591	-0.068	-0.350	-0.001

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
23	248.58	-0.645	0.000	0.021	13.932	-0.116	-0.452	0.002
24	252.51	-0.540	0.000	0.017	2.184	-0.003	-0.070	0.002
25	253.20	-0.401	0.000	0.013	-19.755	-0.228	0.629	-0.001
26	258.34	13.198	-0.100	-0.412	-16.653	-0.159	0.520	0.044
27	259.22	24.955	-0.356	-0.776	-1.062	-0.001	0.033	-0.080
28	281.31	0.055	0.000	-0.002	-18.906	-0.188	0.542	0.000
29	285.32	0.268	0.000	-0.008	6.004	-0.019	-0.170	-0.001
30	289.15	-0.292	0.000	0.008	3.040	-0.005	-0.085	-0.001
31	290.74	-0.545	0.000	0.015	-2.701	-0.004	0.075	-0.002
32	292.88	-13.656	-0.094	0.376	-5.224	-0.014	0.144	-0.042
33	315.20	-0.093	0.000	0.002	6.525	-0.020	-0.167	0.000
34	322.92	0.092	0.000	-0.002	5.574	-0.014	-0.139	0.000
35	330.98	0.085	0.000	-0.002	0.488	0.000	-0.012	0.000
36	331.92	-0.203	0.000	0.005	-0.958	0.000	0.023	-0.001
37	336.73	-0.224	0.000	0.005	9.225	-0.037	-0.221	0.001
38	336.98	0.171	0.000	-0.004	-0.748	0.000	0.018	-0.001
39	337.73	-0.054	0.000	0.001	-1.506	-0.001	0.036	0.000
40	342.64	0.060	0.000	-0.001	-0.713	0.000	0.017	0.000
41	343.67	-0.065	0.000	0.002	0.914	0.000	-0.021	0.000
42	349.09	-0.114	0.000	0.003	-3.580	-0.005	0.083	0.000
43	359.10	-0.405	0.000	0.009	-10.289	-0.044	0.231	-0.001
44	365.63	0.807	0.000	-0.018	12.391	-0.062	-0.273	0.002
45	374.78	-33.798	-0.452	0.727	-0.092	0.000	0.002	-0.110
46	397.68	0.085	0.000	-0.002	4.341	-0.007	-0.088	0.000
47	398.76	0.012	0.000	0.000	-5.922	-0.013	0.120	0.000
48	402.17	0.099	0.000	-0.002	11.561	-0.049	-0.232	0.000
49	411.18	0.093	0.000	-0.002	29.964	-0.324	-0.588	-0.001
50	414.21	0.111	0.000	-0.002	-5.167	-0.010	0.101	0.000
51	427.83	-0.667	0.000	0.013	-6.982	-0.017	0.132	0.002
52	435.71	29.252	-0.291	-0.542	4.166	-0.006	-0.077	-0.090
53	468.07	-0.024	0.000	0.000	-3.503	-0.004	0.060	0.000
54	485.28	-0.150	0.000	0.002	-4.263	-0.006	0.071	0.001
55	507.84	12.529	-0.046	-0.199	4.263	-0.005	-0.068	-0.050
56	511.26	-0.743	0.000	0.012	-9.771	-0.028	0.154	0.003
57	521.76	-0.178	0.000	0.003	14.741	-0.062	-0.228	0.001
58	525.67	0.013	0.000	0.000	-19.137	-0.103	0.294	0.000
59	561.37	-0.062	0.000	0.001	-8.648	-0.020	0.124	0.000
60	563.93	-1.823	-0.001	0.026	4.037	-0.004	-0.058	0.009
61	564.55	3.191	-0.003	-0.046	22.241	-0.130	-0.318	-0.015
62	578.88	-0.169	0.000	0.002	2.620	-0.002	-0.037	0.001
63	618.44	-0.029	0.000	0.000	6.750	-0.011	-0.088	0.000
64	643.48	-0.025	0.000	0.000	-2.959	-0.002	0.037	0.000
65	651.09	0.068	0.000	-0.001	-15.595	-0.055	0.193	0.000
66	660.36	-0.054	0.000	0.001	-8.888	-0.018	0.109	0.000

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
67	663.17	-0.010	0.000	0.000	8.937	-0.018	-0.109	0.000
68	679.98	-0.191	0.000	0.002	-17.268	-0.065	0.205	0.001
69	681.57	0.156	0.000	-0.002	8.356	-0.015	-0.099	-0.001
70	691.69	15.670	-0.053	-0.183	-11.979	-0.031	0.140	-0.066
71	692.91	1.038	0.000	-0.012	4.994	-0.005	-0.058	-0.004
72	698.96	0.166	0.000	-0.002	-3.871	-0.003	0.045	-0.001
73	713.38	-0.127	0.000	0.001	-34.415	-0.246	0.389	0.000
74	821.38	0.086	0.000	-0.001	-6.065	-0.007	0.060	0.000
75	823.62	0.279	0.000	-0.003	3.250	-0.002	-0.032	-0.001
76	824.47	6.434	-0.007	-0.063	6.725	-0.008	-0.066	0.019
77	826.36	-0.354	0.000	0.003	16.246	-0.047	-0.159	-0.001
78	835.58	-0.071	0.000	0.001	-9.337	-0.015	0.090	0.000
79	846.60	0.077	0.000	-0.001	-3.482	-0.002	0.033	0.000
80	855.57	-0.046	0.000	0.000	-38.350	-0.255	0.362	0.000
81	877.21	-0.079	0.000	0.001	-9.735	-0.016	0.090	0.000
82	879.05	-0.002	0.000	0.000	11.216	-0.021	-0.103	0.000
83	898.67	-0.123	0.000	0.001	70.551	-0.821	-0.633	0.000
84	900.60	0.138	0.000	-0.001	-12.973	-0.028	0.116	0.000
85	902.45	0.097	0.000	-0.001	35.222	-0.204	-0.315	0.000
86	905.76	0.144	0.000	-0.001	50.052	-0.410	-0.446	0.000
87	926.72	-0.039	0.000	0.000	64.128	-0.658	-0.558	0.000
88	928.27	-0.061	0.000	0.001	55.898	-0.499	-0.486	0.000
89	936.91	0.091	0.000	-0.001	-1.039	0.000	0.009	0.000
90	943.49	-0.064	0.000	0.001	32.169	-0.163	-0.275	0.000
91	943.60	-0.027	0.000	0.000	-7.164	-0.008	0.061	0.000
92	943.77	0.051	0.000	0.000	22.538	-0.080	-0.193	0.000
93	943.96	0.134	0.000	-0.001	-26.509	-0.110	0.227	0.000
94	946.92	-0.181	0.000	0.002	59.185	-0.548	-0.504	-0.003
95	947.13	-0.011	0.000	0.000	-71.525	-0.800	0.609	0.000
96	947.24	0.068	0.000	-0.001	26.765	-0.112	-0.228	0.000
97	948.23	-0.106	0.000	0.001	17.236	-0.046	-0.147	0.000
98	949.17	0.034	0.000	0.000	-28.124	-0.123	0.239	0.000
99	949.22	-0.005	0.000	0.000	41.142	-0.264	-0.350	0.000
100	949.44	-0.005	0.000	0.000	-9.493	-0.014	0.081	0.000
101	949.50	0.041	0.000	0.000	34.725	-0.188	-0.295	0.000
102	972.23	-20.971	-0.067	0.174	-22.507	-0.077	0.187	0.067
103	995.69	-0.064	0.000	0.001	-3.824	-0.002	0.031	0.001
104	1006.22	-0.059	0.000	0.000	3.359	-0.002	-0.027	0.001
105	1031.64	-21.275	-0.065	0.166	-38.586	-0.214	0.302	0.058
106	1036.50	-0.055	0.000	0.000	-9.712	-0.013	0.076	0.000
107	1037.46	-0.129	0.000	0.001	33.158	-0.157	-0.258	0.000
108	1040.53	0.015	0.000	0.000	7.667	-0.008	-0.059	0.000
109	1041.73	0.033	0.000	0.000	-22.261	-0.070	0.172	0.000
110	1041.84	-0.131	0.000	0.001	9.335	-0.012	-0.072	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
111	1042.08	0.100	0.000	-0.001	23.132	-0.076	-0.179	0.000
112	1042.19	0.027	0.000	0.000	7.927	-0.009	-0.061	0.000
113	1075.14	15.745	-0.034	-0.118	9.288	-0.012	-0.070	-0.030
114	1094.17	-0.175	0.000	0.001	23.633	-0.076	-0.174	0.001
115	1139.66	0.072	0.000	-0.001	20.446	-0.054	-0.145	0.000
116	1143.22	0.062	0.000	0.000	4.336	-0.002	-0.031	0.000
117	1161.39	-2.929	-0.001	0.020	2.192	-0.001	-0.015	-0.014
118	1196.98	0.047	0.000	0.000	26.360	-0.086	-0.178	0.000
119	1219.19	-0.423	0.000	0.003	-8.026	-0.008	0.053	0.001
120	1239.25	0.023	0.000	0.000	-11.379	-0.015	0.074	0.000
121	1239.30	0.034	0.000	0.000	-17.513	-0.037	0.114	0.000
122	1239.53	0.057	0.000	0.000	20.735	-0.051	-0.135	0.000
123	1239.64	0.026	0.000	0.000	-9.097	-0.010	0.059	0.000
124	1239.89	0.123	0.000	-0.001	17.406	-0.036	-0.113	0.000
125	1242.84	0.334	0.000	-0.002	12.038	-0.017	-0.078	0.001
126	1245.47	-0.267	0.000	0.002	-12.563	-0.019	0.081	-0.001
127	1246.17	2.289	-0.001	-0.015	-7.075	-0.006	0.046	0.007
128	1246.38	-18.354	-0.040	0.119	-79.618	-0.754	0.515	0.062
129	1249.01	1.044	0.000	-0.007	6.808	-0.005	-0.044	-0.003
130	1251.58	0.045	0.000	0.000	5.720	-0.004	-0.037	0.000
131	1286.36	-42.625	-0.209	0.267	-51.728	-0.308	0.324	0.137
132	1290.87	0.536	0.000	-0.003	-56.751	-0.370	0.355	-0.002
133	1301.27	0.028	0.000	0.000	4.349	-0.002	-0.027	0.000
134	1302.69	0.133	0.000	-0.001	-106.410	-1.288	0.659	-0.001
135	1333.48	85.840	-0.819	-0.519	-42.608	-0.202	0.258	-0.279
136	1337.26	0.373	0.000	-0.002	-29.190	-0.094	0.176	-0.002
137	1365.13	0.760	0.000	-0.004	-22.710	-0.056	0.134	-0.003
138	1381.26	2.729	-0.001	-0.016	25.513	-0.070	-0.149	-0.009
139	1381.60	0.685	0.000	-0.004	38.494	-0.159	-0.225	-0.002
140	1382.10	32.828	-0.116	-0.192	-20.309	-0.044	0.119	-0.109
141	1382.69	1.590	0.000	-0.009	-19.147	-0.039	0.112	-0.006
142	1382.75	1.838	0.000	-0.011	2.682	-0.001	-0.016	-0.007
143	1383.08	0.231	0.000	-0.001	41.391	-0.184	-0.241	0.000
144	1383.10	3.046	-0.001	-0.018	-3.768	-0.002	0.022	-0.010
145	1389.89	0.706	0.000	-0.004	2.738	-0.001	-0.016	-0.002
146	1408.39	-39.643	-0.165	0.227	50.989	-0.274	-0.292	0.158
147	1413.70	-4.266	-0.002	0.024	34.917	-0.128	-0.199	0.014
148	1413.92	-1.178	0.000	0.007	-19.884	-0.041	0.113	0.004
149	1415.75	8.455	-0.007	-0.048	14.475	-0.022	-0.082	-0.028
150	1415.95	48.879	-0.250	-0.278	-24.972	-0.065	0.142	-0.171
151	1420.74	-3.569	-0.001	0.020	-40.475	-0.171	0.230	0.012
152	1426.35	0.246	0.000	-0.001	47.387	-0.233	-0.268	-0.001
153	1428.84	-0.307	0.000	0.002	-1.905	0.000	0.011	0.000
154	1437.07	172.460	-3.067	-0.968	-5.853	-0.004	0.033	-0.579

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
155	1461.88	32.229	-0.105	-0.178	16.777	-0.029	-0.093	-0.101
156	1467.06	-2.575	-0.001	0.014	-24.456	-0.060	0.134	0.009
157	1470.16	0.098	0.000	-0.001	8.209	-0.007	-0.045	0.000
158	1470.37	0.235	0.000	-0.001	23.341	-0.055	-0.128	-0.001
159	1470.65	-0.092	0.000	0.001	-20.841	-0.044	0.114	0.000
160	1470.75	0.030	0.000	0.000	24.699	-0.061	-0.135	0.000
161	1472.68	-0.280	0.000	0.002	30.504	-0.094	-0.167	0.001
162	1472.76	-0.474	0.000	0.003	46.283	-0.216	-0.253	0.002
163	1473.16	0.284	0.000	-0.002	25.088	-0.063	-0.137	-0.001
164	1473.32	-0.147	0.000	0.001	-81.327	-0.665	0.445	0.001
165	1474.38	-0.382	0.000	0.002	-31.616	-0.100	0.173	0.001
166	1476.12	0.091	0.000	0.000	9.513	-0.009	-0.052	0.000
167	1478.91	0.177	0.000	-0.001	74.536	-0.557	-0.406	0.001
168	1480.79	-6.751	-0.005	0.037	58.325	-0.340	-0.318	0.023
169	1485.26	-0.213	0.000	0.001	-62.320	-0.388	0.338	0.001
170	1486.03	0.383	0.000	-0.002	-129.533	-1.673	0.703	-0.001
171	1494.75	-0.359	0.000	0.002	-44.785	-0.199	0.242	0.001
172	1494.81	-0.136	0.000	0.001	-13.030	-0.017	0.070	0.001
173	1494.91	0.112	0.000	-0.001	-8.274	-0.007	0.045	0.000
174	1494.95	0.252	0.000	-0.001	9.893	-0.010	-0.053	0.001
175	1496.87	0.005	0.000	0.000	-35.730	-0.126	0.193	0.000
176	1498.18	0.241	0.000	-0.001	54.959	-0.299	-0.296	-0.001
177	1498.85	11.095	-0.012	-0.060	19.474	-0.037	-0.105	-0.038
178	1502.51	0.314	0.000	-0.002	-11.051	-0.012	0.059	-0.001
179	1514.73	3.158	-0.001	-0.017	21.787	-0.046	-0.116	-0.011
180	1514.96	15.947	-0.025	-0.085	-15.466	-0.023	0.082	-0.049
181	1515.02	8.016	-0.006	-0.043	21.461	-0.045	-0.114	-0.032
182	1515.43	0.462	0.000	-0.002	55.242	-0.298	-0.294	-0.001
183	1545.91	-0.025	0.000	0.000	-19.736	-0.037	0.103	0.000
184	1568.47	1.365	0.000	-0.007	-18.988	-0.034	0.098	-0.004
185	1633.27	181.472	-2.988	-0.896	104.612	-0.993	-0.517	-0.603
186	1641.96	-6.127	-0.003	0.030	9.573	-0.008	-0.047	0.021
187	1661.09	-76.682	-0.525	0.372	28.190	-0.071	-0.137	0.257
188	1669.59	0.896	0.000	-0.004	15.116	-0.020	-0.073	-0.003
189	1677.42	0.797	0.000	-0.004	8.581	-0.007	-0.041	-0.003
190	1690.87	-1.586	0.000	0.008	-4.728	-0.002	0.023	0.006
191	3039.23	-0.044	0.000	0.000	-68.534	-0.229	0.182	0.001
192	3039.29	0.005	0.000	0.000	6.753	-0.002	-0.018	0.000
193	3039.36	0.018	0.000	0.000	25.061	-0.031	-0.067	-0.001
194	3039.38	0.142	0.000	0.000	-75.551	-0.278	0.200	-0.002
195	3040.60	-0.009	0.000	0.000	-42.109	-0.086	0.112	0.000
196	3040.64	0.015	0.000	0.000	-18.776	-0.017	0.050	0.000
197	3040.65	-0.008	0.000	0.000	46.253	-0.104	-0.123	0.000
198	3040.72	0.004	0.000	0.000	35.049	-0.060	-0.093	0.000

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
199	3046.44	-0.027	0.000	0.000	8.628	-0.004	-0.023	0.000
200	3046.49	-0.053	0.000	0.000	-80.254	-0.313	0.212	0.001
201	3046.57	0.188	0.000	0.000	-134.900	-0.885	0.357	0.004
202	3046.62	-0.398	0.000	0.001	182.764	-1.625	-0.484	0.009
203	3112.54	0.513	0.000	-0.001	-44.395	-0.094	0.115	0.002
204	3112.61	0.263	0.000	-0.001	152.149	-1.102	-0.394	-0.001
205	3112.66	0.031	0.000	0.000	172.075	-1.410	-0.446	-0.001
206	3112.69	-1.757	0.000	0.005	-16.753	-0.013	0.043	-0.008
207	3115.49	0.009	0.000	0.000	-128.763	-0.789	0.333	0.000
208	3115.51	0.010	0.000	0.000	-38.412	-0.070	0.099	0.000
209	3115.55	-0.014	0.000	0.000	48.636	-0.113	-0.126	0.000
210	3115.59	-0.014	0.000	0.000	46.130	-0.101	-0.119	0.000
211	3120.29	0.018	0.000	0.000	-68.323	-0.222	0.177	0.000
212	3120.37	0.031	0.000	0.000	11.274	-0.006	-0.029	0.000
213	3120.40	0.002	0.000	0.000	-14.417	-0.010	0.037	0.000
214	3120.83	-1.420	0.000	0.004	-61.419	-0.179	0.159	0.000
215	3122.04	-0.015	0.000	0.000	-154.998	-1.140	0.400	0.000
216	3122.05	0.014	0.000	0.000	-12.578	-0.008	0.032	0.000
217	3122.06	-0.021	0.000	0.000	-65.793	-0.205	0.170	0.000
218	3122.07	0.005	0.000	0.000	17.095	-0.014	-0.044	0.000
219	3126.02	0.027	0.000	0.000	-52.097	-0.129	0.134	0.000
220	3126.06	0.008	0.000	0.000	-80.763	-0.309	0.208	0.000
221	3126.11	0.035	0.000	0.000	-89.627	-0.381	0.231	0.000
222	3126.11	-0.006	0.000	0.000	19.080	-0.017	-0.049	0.000
223	3127.30	-0.210	0.000	0.001	-56.975	-0.154	0.147	0.001
224	3127.36	-0.073	0.000	0.000	31.519	-0.047	-0.081	0.000
225	3127.53	0.521	0.000	-0.001	40.542	-0.078	-0.105	0.003
226	3127.58	-1.106	0.000	0.003	7.675	-0.003	-0.020	0.007
227	3201.25	-0.102	0.000	0.000	-16.560	-0.013	0.042	0.000
228	3201.59	-0.037	0.000	0.000	-6.733	-0.002	0.017	0.000
229	3206.04	0.697	0.000	-0.002	5.231	-0.001	-0.013	-0.003
230	3206.23	-5.382	-0.001	0.014	112.017	-0.580	-0.282	0.017
231	3212.56	0.009	0.000	0.000	11.000	-0.006	-0.028	0.000
232	3212.72	0.126	0.000	0.000	46.501	-0.100	-0.117	0.000
233	3222.07	-7.598	-0.003	0.019	-25.169	-0.029	0.063	0.026
234	3222.15	10.263	-0.005	-0.026	74.969	-0.259	-0.188	-0.032

Table S8: LVC Analysis for T2 of TBPe.

α	Freq. /cm ⁻¹	κ_α			κ_α^*			ξ
		κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	
1	19.71	0.176	0.000	-0.072	-0.042	0.000	0.017	0.001
2	25.22	0.055	0.000	-0.018	1.591	-0.015	-0.509	0.000
3	29.15	-0.001	0.000	0.000	0.775	-0.003	-0.215	0.000

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
4	30.92	-0.033	0.000	0.009	-1.321	-0.008	0.345	0.000
5	31.41	0.052	0.000	-0.013	-0.665	-0.002	0.171	0.000
6	48.26	0.032	0.000	-0.005	-0.352	0.000	0.059	0.000
7	72.92	-0.001	0.000	0.000	-3.823	-0.030	0.423	0.000
8	80.77	-0.052	0.000	0.005	0.543	-0.001	-0.054	0.000
9	91.43	1.641	-0.004	-0.145	-3.093	-0.016	0.273	0.011
10	94.40	0.058	0.000	-0.005	0.844	-0.001	-0.072	0.000
11	115.51	-0.030	0.000	0.002	-6.759	-0.059	0.472	0.000
12	122.18	-0.152	0.000	0.010	-1.295	-0.002	0.086	0.000
13	122.91	-0.073	0.000	0.005	2.479	-0.007	-0.163	0.000
14	153.00	-0.094	0.000	0.005	8.673	-0.073	-0.457	-0.001
15	166.89	0.090	0.000	-0.004	2.647	-0.006	-0.128	0.001
16	201.34	-0.045	0.000	0.002	0.419	0.000	-0.017	0.000
17	223.58	-0.029	0.000	0.001	10.057	-0.067	-0.363	0.000
18	228.79	-10.659	-0.074	0.376	-0.428	0.000	0.015	0.054
19	238.58	0.007	0.000	0.000	-4.051	-0.010	0.137	0.000
20	238.92	0.142	0.000	-0.005	-2.327	-0.003	0.079	0.000
21	240.51	-0.103	0.000	0.003	0.369	0.000	-0.012	0.001
22	243.91	0.083	0.000	-0.003	7.549	-0.035	-0.250	0.000
23	248.58	-0.224	0.000	0.007	7.494	-0.033	-0.243	0.001
24	252.51	-0.168	0.000	0.005	1.691	-0.002	-0.054	0.000
25	253.20	-0.066	0.000	0.002	-0.016	0.000	0.001	0.000
26	258.34	4.169	-0.010	-0.130	-21.805	-0.273	0.681	0.019
27	259.22	8.008	-0.037	-0.249	2.060	-0.002	-0.064	-0.035
28	281.31	0.036	0.000	-0.001	-7.642	-0.031	0.219	0.000
29	285.32	0.035	0.000	-0.001	-0.462	0.000	0.013	0.001
30	289.15	-0.167	0.000	0.005	-6.511	-0.022	0.182	0.000
31	290.74	-0.318	0.000	0.009	-0.283	0.000	0.008	-0.001
32	292.88	-7.159	-0.026	0.197	-1.977	-0.002	0.054	-0.023
33	315.20	-0.107	0.000	0.003	6.819	-0.022	-0.174	0.000
34	322.92	0.084	0.000	-0.002	1.676	-0.001	-0.042	0.000
35	330.98	0.088	0.000	-0.002	0.765	0.000	-0.019	0.000
36	331.92	-0.184	0.000	0.004	0.576	0.000	-0.014	-0.001
37	336.73	-0.148	0.000	0.004	-7.156	-0.023	0.171	0.001
38	336.98	0.115	0.000	-0.003	0.963	0.000	-0.023	0.000
39	337.73	-0.050	0.000	0.001	-1.329	-0.001	0.032	0.000
40	342.64	0.088	0.000	-0.002	2.537	-0.003	-0.060	0.000
41	343.67	-0.040	0.000	0.001	3.888	-0.007	-0.091	0.000
42	349.09	-0.079	0.000	0.002	-3.046	-0.004	0.070	0.000
43	359.10	-0.249	0.000	0.006	-1.555	-0.001	0.035	-0.001
44	365.63	0.422	0.000	-0.009	1.722	-0.001	-0.038	0.001
45	374.78	-18.556	-0.136	0.399	3.446	-0.005	-0.074	-0.080
46	397.68	0.028	0.000	-0.001	-8.682	-0.028	0.176	0.000
47	398.76	-0.008	0.000	0.000	-4.353	-0.007	0.088	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
48	402.17	0.096	0.000	-0.002	3.847	-0.005	-0.077	0.000
49	411.18	0.075	0.000	-0.001	13.344	-0.064	-0.262	-0.001
50	414.21	0.063	0.000	-0.001	-4.529	-0.007	0.088	0.000
51	427.83	-0.541	0.000	0.010	-4.348	-0.007	0.082	0.002
52	435.71	22.707	-0.175	-0.420	-23.029	-0.180	0.426	-0.093
53	468.07	0.023	0.000	0.000	-14.696	-0.068	0.253	0.000
54	485.28	-0.081	0.000	0.001	-17.210	-0.090	0.286	0.001
55	507.84	14.942	-0.065	-0.237	1.799	-0.001	-0.029	-0.077
56	511.26	-0.876	0.000	0.014	15.423	-0.069	-0.243	0.005
57	521.76	-0.181	0.000	0.003	26.006	-0.192	-0.402	0.001
58	525.67	-0.010	0.000	0.000	-6.905	-0.013	0.106	0.000
59	561.37	-0.104	0.000	0.001	24.592	-0.160	-0.353	0.000
60	563.93	-3.977	-0.004	0.057	-0.875	0.000	0.013	0.012
61	564.55	7.324	-0.014	-0.105	21.761	-0.124	-0.311	-0.022
62	578.88	-0.237	0.000	0.003	15.332	-0.060	-0.214	0.001
63	618.44	-0.052	0.000	0.001	-17.833	-0.076	0.233	0.000
64	643.48	-0.019	0.000	0.000	-11.130	-0.029	0.140	0.000
65	651.09	0.073	0.000	-0.001	-1.679	-0.001	0.021	0.000
66	660.36	-0.042	0.000	0.001	10.152	-0.023	-0.124	0.000
67	663.17	-0.056	0.000	0.001	18.783	-0.079	-0.228	0.000
68	679.98	-0.081	0.000	0.001	-17.120	-0.064	0.203	0.001
69	681.57	0.101	0.000	-0.001	9.940	-0.021	-0.118	-0.001
70	691.69	8.859	-0.017	-0.103	9.667	-0.020	-0.113	-0.073
71	692.91	0.596	0.000	-0.007	10.957	-0.026	-0.128	-0.005
72	698.96	0.098	0.000	-0.001	-4.490	-0.004	0.052	-0.001
73	713.38	-0.102	0.000	0.001	-7.517	-0.012	0.085	0.001
74	821.38	-0.067	0.000	0.001	0.655	0.000	-0.006	0.000
75	823.62	-0.195	0.000	0.002	-2.902	-0.002	0.028	0.000
76	824.47	-4.669	-0.004	0.046	5.296	-0.005	-0.052	-0.012
77	826.36	0.218	0.000	-0.002	-10.012	-0.018	0.098	0.000
78	835.58	-0.141	0.000	0.001	-10.357	-0.019	0.100	0.000
79	846.60	0.081	0.000	-0.001	-7.178	-0.009	0.068	0.000
80	855.57	0.014	0.000	0.000	-1.285	0.000	0.012	0.000
81	877.21	-0.081	0.000	0.001	-50.789	-0.436	0.467	0.000
82	879.05	-0.012	0.000	0.000	-43.774	-0.323	0.402	0.000
83	898.67	-0.184	0.000	0.002	30.581	-0.154	-0.274	0.000
84	900.60	0.078	0.000	-0.001	-3.157	-0.002	0.028	0.001
85	902.45	0.047	0.000	0.000	33.974	-0.190	-0.304	0.000
86	905.76	-0.019	0.000	0.000	-4.352	-0.003	0.039	0.000
87	926.72	0.048	0.000	0.000	46.234	-0.342	-0.402	0.000
88	928.27	-0.141	0.000	0.001	39.741	-0.252	-0.345	0.000
89	936.91	0.084	0.000	-0.001	-2.944	-0.001	0.025	0.000
90	943.49	0.070	0.000	-0.001	-2.483	-0.001	0.021	-0.001
91	943.60	0.029	0.000	0.000	14.744	-0.034	-0.126	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
92	943.77	0.044	0.000	0.000	40.989	-0.264	-0.350	0.000
93	943.96	0.066	0.000	-0.001	13.339	-0.028	-0.114	0.000
94	946.92	-0.910	0.000	0.008	32.439	-0.165	-0.276	0.005
95	947.13	0.055	0.000	0.000	-86.467	-1.170	0.736	-0.001
96	947.24	0.107	0.000	-0.001	10.296	-0.017	-0.088	0.000
97	948.23	-0.090	0.000	0.001	-15.051	-0.035	0.128	0.000
98	949.17	0.039	0.000	0.000	-37.621	-0.221	0.320	0.000
99	949.22	0.018	0.000	0.000	16.132	-0.041	-0.137	0.000
100	949.44	-0.021	0.000	0.000	9.584	-0.014	-0.081	0.000
101	949.50	0.024	0.000	0.000	29.359	-0.135	-0.249	0.000
102	972.23	-6.251	-0.006	0.052	-4.396	-0.003	0.036	0.020
103	995.69	-0.111	0.000	0.001	-1.026	0.000	0.008	0.000
104	1006.22	-0.160	0.000	0.001	7.602	-0.009	-0.061	0.000
105	1031.64	-10.172	-0.015	0.080	-13.305	-0.025	0.104	0.039
106	1036.50	-0.052	0.000	0.000	-8.961	-0.011	0.070	0.000
107	1037.46	-0.042	0.000	0.000	17.302	-0.043	-0.135	0.000
108	1040.53	-0.055	0.000	0.000	22.932	-0.075	-0.178	0.000
109	1041.73	-0.010	0.000	0.000	-26.336	-0.099	0.204	0.000
110	1041.84	-0.057	0.000	0.000	10.588	-0.016	-0.082	0.000
111	1042.08	0.063	0.000	0.000	12.360	-0.022	-0.096	0.000
112	1042.19	0.110	0.000	-0.001	14.400	-0.029	-0.111	0.000
113	1075.14	33.756	-0.157	-0.253	-1.403	0.000	0.011	-0.106
114	1094.17	-0.242	0.000	0.002	1.391	0.000	-0.010	0.001
115	1139.66	-0.110	0.000	0.001	15.473	-0.031	-0.110	0.000
116	1143.22	-0.186	0.000	0.001	-9.287	-0.011	0.066	-0.001
117	1161.39	39.126	-0.195	-0.272	1.289	0.000	-0.009	-0.128
118	1196.98	-0.373	0.000	0.003	3.464	-0.001	-0.023	0.001
119	1219.19	-0.605	0.000	0.004	-4.317	-0.002	0.029	0.003
120	1239.25	0.071	0.000	0.000	1.416	0.000	-0.009	0.000
121	1239.30	-0.058	0.000	0.000	-31.298	-0.117	0.204	0.000
122	1239.53	-0.059	0.000	0.000	23.618	-0.067	-0.154	0.000
123	1239.64	0.008	0.000	0.000	-2.413	-0.001	0.016	0.000
124	1239.89	0.053	0.000	0.000	32.818	-0.129	-0.213	0.000
125	1242.84	-0.186	0.000	0.001	13.492	-0.022	-0.088	0.000
126	1245.47	-0.049	0.000	0.000	12.177	-0.018	-0.079	-0.001
127	1246.17	-1.965	0.000	0.013	-22.306	-0.059	0.144	-0.004
128	1246.38	16.219	-0.031	-0.105	-16.009	-0.030	0.104	-0.037
129	1249.01	-0.753	0.000	0.005	1.010	0.000	-0.007	0.001
130	1251.58	0.114	0.000	-0.001	16.190	-0.031	-0.104	0.000
131	1286.36	-16.751	-0.032	0.105	-51.937	-0.311	0.326	0.078
132	1290.87	0.351	0.000	-0.002	-47.696	-0.261	0.298	-0.001
133	1301.27	-0.092	0.000	0.001	45.628	-0.237	-0.283	0.000
134	1302.69	0.289	0.000	-0.002	-0.108	0.000	0.001	0.000
135	1333.48	70.975	-0.560	-0.429	-54.819	-0.334	0.332	-0.323

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
136	1337.26	0.519	0.000	-0.003	-12.604	-0.018	0.076	-0.003
137	1365.13	0.451	0.000	-0.003	-7.455	-0.006	0.044	-0.002
138	1381.26	3.118	-0.001	-0.018	-16.792	-0.030	0.098	-0.012
139	1381.60	0.672	0.000	-0.004	15.711	-0.026	-0.092	-0.002
140	1382.10	36.562	-0.143	-0.213	5.002	-0.003	-0.029	-0.142
141	1382.69	1.419	0.000	-0.008	-9.329	-0.009	0.054	-0.007
142	1382.75	2.138	0.000	-0.012	-10.460	-0.012	0.061	-0.009
143	1383.08	0.508	0.000	-0.003	31.765	-0.108	-0.185	-0.001
144	1383.10	3.420	-0.001	-0.020	11.960	-0.015	-0.070	-0.013
145	1389.89	0.139	0.000	-0.001	-18.012	-0.035	0.105	0.000
146	1408.39	-86.327	-0.784	0.494	34.700	-0.127	-0.199	0.324
147	1413.70	-1.351	0.000	0.008	35.439	-0.132	-0.202	0.003
148	1413.92	-1.107	0.000	0.006	-30.139	-0.095	0.172	0.004
149	1415.75	8.139	-0.007	-0.046	-29.517	-0.091	0.168	-0.027
150	1415.95	45.494	-0.217	-0.259	14.182	-0.021	-0.081	-0.161
151	1420.74	1.592	0.000	-0.009	-18.041	-0.034	0.102	-0.008
152	1426.35	0.144	0.000	-0.001	14.796	-0.023	-0.084	-0.001
153	1428.84	0.204	0.000	-0.001	-15.563	-0.025	0.088	-0.001
154	1437.07	14.669	-0.022	-0.082	-16.270	-0.027	0.091	0.020
155	1461.88	47.250	-0.226	-0.261	11.274	-0.013	-0.062	-0.146
156	1467.06	-3.024	-0.001	0.017	11.707	-0.014	-0.064	0.010
157	1470.16	-0.582	0.000	0.003	10.372	-0.011	-0.057	0.002
158	1470.37	-0.333	0.000	0.002	-3.118	-0.001	0.017	0.001
159	1470.65	0.000	0.000	0.000	-8.839	-0.008	0.048	0.000
160	1470.75	0.072	0.000	0.000	12.482	-0.016	-0.068	0.000
161	1472.68	-0.105	0.000	0.001	19.871	-0.040	-0.109	0.000
162	1472.76	-0.299	0.000	0.002	0.380	0.000	-0.002	0.001
163	1473.16	0.218	0.000	-0.001	20.691	-0.043	-0.113	-0.001
164	1473.32	-0.081	0.000	0.000	-65.225	-0.428	0.357	0.000
165	1474.38	0.035	0.000	0.000	3.808	-0.001	-0.021	0.000
166	1476.12	0.035	0.000	0.000	34.115	-0.117	-0.186	0.000
167	1478.91	-0.451	0.000	0.002	66.654	-0.445	-0.364	-0.001
168	1480.79	-21.789	-0.048	0.119	30.335	-0.092	-0.165	0.070
169	1485.26	-0.452	0.000	0.002	-59.133	-0.349	0.321	0.002
170	1486.03	-0.049	0.000	0.000	-26.372	-0.069	0.143	0.000
171	1494.75	-0.014	0.000	0.000	32.245	-0.103	-0.174	0.000
172	1494.81	-0.049	0.000	0.000	6.242	-0.004	-0.034	0.000
173	1494.91	0.085	0.000	0.000	15.779	-0.025	-0.085	0.000
174	1494.95	0.139	0.000	-0.001	45.738	-0.207	-0.247	0.000
175	1496.87	0.183	0.000	-0.001	-12.493	-0.015	0.067	-0.001
176	1498.18	0.454	0.000	-0.002	44.424	-0.195	-0.239	-0.002
177	1498.85	18.569	-0.034	-0.100	-19.813	-0.039	0.107	-0.087
178	1502.51	0.109	0.000	-0.001	-15.279	-0.023	0.082	0.000
179	1514.73	3.585	-0.001	-0.019	-8.320	-0.007	0.044	-0.015

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
180	1514.96	17.679	-0.031	-0.094	-10.808	-0.011	0.058	-0.063
181	1515.02	8.944	-0.008	-0.048	32.439	-0.103	-0.173	-0.041
182	1515.43	0.512	0.000	-0.003	34.813	-0.119	-0.185	-0.001
183	1545.91	-0.142	0.000	0.001	-30.335	-0.088	0.158	0.000
184	1568.47	0.713	0.000	-0.004	-14.856	-0.021	0.076	-0.004
185	1633.27	90.455	-0.742	-0.447	47.889	-0.208	-0.236	-0.567
186	1641.96	-3.377	-0.001	0.017	-2.931	-0.001	0.014	0.021
187	1661.09	-123.710	-1.365	0.601	2.271	0.000	-0.011	0.555
188	1669.59	1.580	0.000	-0.008	-21.093	-0.039	0.102	-0.007
189	1677.42	1.878	0.000	-0.009	-8.006	-0.006	0.038	-0.008
190	1690.87	-1.532	0.000	0.007	-9.202	-0.007	0.044	0.008
191	3039.23	0.002	0.000	0.000	-50.706	-0.125	0.135	0.000
192	3039.29	0.004	0.000	0.000	5.828	-0.002	-0.015	0.000
193	3039.36	-0.008	0.000	0.000	-4.226	-0.001	0.011	0.000
194	3039.38	-0.007	0.000	0.000	-46.501	-0.105	0.123	0.000
195	3040.60	-0.006	0.000	0.000	-19.204	-0.018	0.051	0.000
196	3040.64	0.018	0.000	0.000	3.181	0.000	-0.008	0.000
197	3040.65	-0.008	0.000	0.000	-46.529	-0.106	0.123	0.000
198	3040.72	0.002	0.000	0.000	24.806	-0.030	-0.066	0.000
199	3046.44	-0.045	0.000	0.000	96.760	-0.455	-0.256	0.000
200	3046.49	-0.089	0.000	0.000	-95.174	-0.441	0.252	0.000
201	3046.57	0.314	0.000	-0.001	-134.236	-0.877	0.355	0.000
202	3046.62	-0.664	0.000	0.002	100.384	-0.490	-0.266	0.000
203	3112.54	0.061	0.000	0.000	-137.050	-0.894	0.355	0.001
204	3112.61	0.031	0.000	0.000	149.306	-1.061	-0.387	0.000
205	3112.66	0.006	0.000	0.000	45.765	-0.100	-0.119	0.000
206	3112.69	-0.189	0.000	0.000	7.898	-0.003	-0.020	-0.001
207	3115.49	-0.001	0.000	0.000	-50.967	-0.124	0.132	0.000
208	3115.51	0.018	0.000	0.000	-13.979	-0.009	0.036	0.000
209	3115.55	-0.012	0.000	0.000	48.581	-0.112	-0.126	0.000
210	3115.59	-0.004	0.000	0.000	54.051	-0.139	-0.140	0.000
211	3120.29	-0.008	0.000	0.000	8.857	-0.004	-0.023	0.000
212	3120.37	0.000	0.000	0.000	12.493	-0.007	-0.032	0.000
213	3120.40	-0.001	0.000	0.000	3.068	0.000	-0.008	0.000
214	3120.83	0.386	0.000	-0.001	-44.789	-0.095	0.116	0.001
215	3122.04	-0.008	0.000	0.000	-64.646	-0.198	0.167	0.000
216	3122.05	0.011	0.000	0.000	-35.590	-0.060	0.092	0.000
217	3122.06	0.005	0.000	0.000	-41.172	-0.080	0.106	0.000
218	3122.07	0.030	0.000	0.000	12.157	-0.007	-0.031	0.000
219	3126.02	0.018	0.000	0.000	-47.182	-0.106	0.122	0.000
220	3126.06	-0.007	0.000	0.000	-51.453	-0.126	0.133	0.000
221	3126.11	0.002	0.000	0.000	-60.407	-0.173	0.156	0.000
222	3126.11	-0.011	0.000	0.000	-6.108	-0.002	0.016	0.000
223	3127.30	0.159	0.000	0.000	5.690	-0.002	-0.015	0.000

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
224	3127.36	0.067	0.000	0.000	16.833	-0.013	-0.043	0.000
225	3127.53	-0.382	0.000	0.001	32.246	-0.049	-0.083	-0.001
226	3127.58	0.860	0.000	-0.002	-29.304	-0.041	0.076	-0.002
227	3201.25	-0.073	0.000	0.000	40.821	-0.077	-0.103	0.000
228	3201.59	-0.011	0.000	0.000	27.985	-0.036	-0.070	0.000
229	3206.04	0.111	0.000	0.000	30.676	-0.043	-0.077	-0.002
230	3206.23	-0.983	0.000	0.002	74.128	-0.254	-0.186	0.014
231	3212.56	-0.082	0.000	0.000	2.661	0.000	-0.007	0.000
232	3212.72	0.202	0.000	-0.001	69.444	-0.222	-0.174	0.000
233	3222.07	-10.135	-0.005	0.025	-1.371	0.000	0.003	0.038
234	3222.15	13.684	-0.009	-0.034	66.155	-0.201	-0.166	-0.048

S2 TAT-3DBTO2

S2-1 Geometry

Table S9: Cartesian coordinates of the GS Minimum of TAT-3DBTO₂.

At	x	y	z	At	x	y	z	At	x	y	z
C	1.3951	-0.0057	1.6208	C	-3.1715	3.8658	1.8773	O	-7.5445	3.6524	0.2362
C	0.7104	-1.2426	1.6630	C	-4.4109	4.3027	1.4133	O	-6.4651	5.5698	-1.0049
C	0.7209	1.2366	1.6630	C	-4.8744	3.7934	0.2122	H	5.1312	-1.8044	1.5906
C	-0.6926	1.2111	1.6208	C	-4.1440	2.8767	-0.5487	H	0.7919	-4.2104	2.1426
C	-0.7025	-1.2054	1.6208	C	-2.8992	2.4606	-0.0911	H	5.0697	-4.2660	1.8776
C	-1.4314	0.0061	1.6630	C	-1.7621	-4.6795	1.8773	H	2.9045	-5.4396	2.1902
N	2.7664	-0.2518	1.6105	C	-1.5208	-5.9713	1.4133	H	3.2503	2.7910	2.1426
C	2.9732	-1.6303	1.7017	C	-0.8480	-6.1180	0.2122	H	3.2586	5.2351	2.1902
C	1.7228	-2.2817	1.7801	C	-0.4192	-5.0272	-0.5487	H	1.1596	6.5235	1.8776
C	1.1146	2.6329	1.7801	C	-0.6813	-3.7411	-0.0911	H	-1.0030	5.3459	1.5906
N	-1.1651	2.5216	1.6105	S	6.8347	3.4874	-0.5647	H	-4.0422	1.4194	2.1426
C	-0.0747	3.3901	1.7017	C	5.7152	3.7269	-1.9376	H	-4.1282	-3.5416	1.5906
C	-2.8375	-0.3511	1.7801	C	4.5590	2.9569	-1.7854	H	-6.2293	-2.2575	1.8776
N	-1.6012	-2.2699	1.6105	S	-6.4376	4.1753	-0.5647	H	-6.1630	0.2044	2.1902
C	-2.8985	-1.7597	1.7017	C	-6.0852	3.0861	-1.9376	H	5.0375	0.3108	2.8352
C	4.1832	-2.3226	1.7049	C	-4.8403	2.4697	-1.7854	H	6.8397	1.8295	1.9893
C	1.7177	-3.6687	1.9918	S	-0.3972	-7.6628	-0.5647	H	2.6634	1.1161	-0.6507
C	4.1403	-3.7010	1.8649	C	0.3700	-6.8130	-1.9376	H	-2.7879	4.2072	2.8352
C	2.9189	-4.3638	2.0314	C	0.2813	-5.4267	-1.7854	H	-5.0042	5.0086	1.9893
C	2.3183	3.3219	1.9918	C	5.9242	4.5604	-3.0230	H	-2.2982	1.7485	-0.6507
C	2.3197	4.7098	2.0314	C	4.9271	4.6215	-3.9971	H	-2.2495	-4.5180	2.8352
C	1.1350	5.4361	1.8649	C	3.7631	3.8632	-3.8642	H	-1.8355	-6.8381	1.9893
C	-0.0802	4.7840	1.7049	C	3.5703	3.0297	-2.7633	H	-0.3652	-2.8646	-0.6507
C	-4.0360	0.3468	1.9918	C	-6.9115	2.8503	-3.0230	H	6.8356	5.1468	-3.1103
C	-4.1030	-2.4614	1.7049	C	-6.4659	1.9563	-3.9971	H	5.0585	5.2657	-4.8631
C	-5.2753	-1.7351	1.8649	C	-5.2272	1.3273	-3.8642	H	2.9928	3.9243	-4.6296
C	-5.2386	-0.3460	2.0314	C	-4.4089	1.5771	-2.7633	H	2.6554	2.4487	-2.6713
C	-1.3416	-3.5732	1.1297	C	0.9873	-7.4107	-3.0230	H	-7.8750	3.3464	-3.1103
C	3.7653	0.6248	1.1297	C	1.5387	-6.5777	-3.9971	H	-7.0895	1.7480	-4.8631
C	-2.4237	2.9485	1.1297	C	1.4641	-5.1906	-3.8642	H	-4.8950	0.6296	-4.6296
C	4.9336	0.8137	1.8773	C	0.8386	-4.6068	-2.7633	H	-3.4484	1.0753	-2.6713
C	5.9317	1.6686	1.4133	O	0.6091	-8.3599	0.2362	H	1.0395	-8.4932	-3.1103
C	5.7224	2.3246	0.2122	O	-1.5911	-8.3838	-1.0049	H	2.0310	-7.0137	-4.8631
C	4.5633	2.1505	-0.5487	O	6.9353	4.7075	0.2362	H	1.9022	-4.5540	-4.6296
C	3.5805	1.2805	-0.0911	O	8.0561	2.8140	-1.0049	H	0.7930	-3.5240	-2.6713

Table S10: Cartesian coordinates of the S_1 C_3 Minimum of TAT-3DBTO₂.

At	x	y	z	At	x	y	z	At	x	y	z
C	1.4036	0.0022	1.5017	C	-3.2155	3.6926	2.0122	O	-7.6182	3.1149	0.6455
C	0.7084	-1.2556	1.5475	C	-4.5201	4.0635	1.6856	O	-6.9889	5.3799	-0.2633
C	0.7332	1.2412	1.5475	C	-5.0259	3.6900	0.4532	H	5.1195	-1.7502	1.3415
C	-0.7037	1.2145	1.5017	C	-4.2657	2.9872	-0.5082	H	0.8266	-4.2383	1.9582
C	-0.6999	-1.2167	1.5017	C	-2.9642	2.6180	-0.1750	H	5.0935	-4.2336	1.5612
C	-1.4415	0.0143	1.5475	C	-1.5902	-4.6310	2.0122	H	2.9472	-5.4402	1.8852
N	2.7537	-0.2522	1.4338	C	-1.2591	-5.9463	1.6856	H	3.2572	2.8350	1.9582
C	2.9672	-1.6237	1.5045	C	-0.6827	-6.1976	0.4532	H	3.2378	5.2724	1.8852
C	1.7215	-2.2870	1.6167	C	-0.4542	-5.1878	-0.5082	H	1.1197	6.5279	1.5612
C	1.1199	2.6344	1.6167	C	-0.7851	-3.8761	-0.1750	H	-1.0440	5.3087	1.3415
N	-1.1585	2.5109	1.4338	S	6.7685	3.8167	-0.1211	H	-4.0837	1.4033	1.9582
C	-0.0774	3.3816	1.5045	C	5.9375	3.8750	-1.6970	H	-4.0755	-3.5585	1.3415
C	-2.8414	-0.3473	1.6167	C	4.8651	2.9691	-1.7422	H	-6.2132	-2.2943	1.5612
N	-1.5952	-2.2587	1.4338	S	-6.6896	3.9534	-0.1211	H	-6.1849	0.1678	1.8852
C	-2.8898	-1.7578	1.5045	C	-6.3246	3.2046	-1.6970	H	4.7998	0.4484	2.9818
C	4.1865	-2.2929	1.4634	C	-5.0039	2.7288	-1.7422	H	6.5653	2.1367	2.3930
C	1.7379	-3.6809	1.7914	S	-0.0789	-7.7701	-0.1211	H	2.9509	0.9996	-0.8668
C	4.1599	-3.6770	1.5898	C	0.3871	-7.0795	-1.6970	H	-2.7883	3.9326	2.9818
C	2.9491	-4.3589	1.7699	C	0.1388	-5.6978	-1.7422	H	-5.1331	4.6174	2.3930
C	2.3189	3.3455	1.7914	C	6.2651	4.7036	-2.7573	H	-2.3411	2.0558	-0.8668
C	2.3004	4.7335	1.7699	C	5.4902	4.6257	-3.9138	H	-2.0116	-4.3810	2.9818
C	1.1044	5.4411	1.5898	C	4.4159	3.7318	-3.9818	H	-1.4322	-6.7541	2.3930
C	-0.1075	4.7721	1.4634	C	4.0979	2.9051	-2.9092	H	-0.6098	-3.0554	-0.8668
C	-4.0567	0.3354	1.7914	C	-7.2060	3.0739	-2.7573	H	7.1045	5.3914	-2.6866
C	-4.0790	-2.4791	1.4634	C	-6.7511	2.4418	-3.9138	H	5.7230	5.2609	-4.7649
C	-5.2643	-1.7641	1.5898	C	-5.4397	1.9584	-3.9818	H	3.8194	3.6801	-4.8901
C	-5.2495	-0.3746	1.7699	C	-4.5648	2.0963	-2.9092	H	3.2610	2.2137	-2.9832
C	-1.3170	-3.6091	1.0830	C	0.9409	-7.7775	-2.7573	H	-8.2213	3.4570	-2.6866
C	3.7841	0.6640	1.0830	C	1.2609	-7.0675	-3.9138	H	-7.4176	2.3258	-4.7649
C	-2.4671	2.9451	1.0830	C	1.0239	-5.6901	-3.9818	H	-5.0967	1.4676	-4.8901
C	4.8056	0.9384	2.0122	C	0.4670	-5.0014	-2.9092	H	-3.5476	1.7173	-2.9832
C	5.7792	1.8828	1.6856	O	1.1115	-8.1550	0.6455	H	1.1168	-8.8483	-2.6866
C	5.7086	2.5076	0.4532	O	-1.1647	-8.7425	-0.2633	H	1.6946	-7.5867	-4.7649
C	4.7199	2.2006	-0.5082	O	6.5067	5.0401	0.6455	H	1.2774	-5.1477	-4.8901
C	3.7493	1.2581	-0.1750	O	8.1536	3.3626	-0.2633	H	0.2866	-3.9310	-2.9832

Table S11: Cartesian coordinates of the S_1 C_1 Minimum of TAT-3DBTO₂.

At	x	y	z	At	x	y	z	At	x	y	z
C	1.4283	-0.0225	1.4505	C	-3.1792	3.7922	1.9425	O	-7.6247	3.3816	0.6253
C	0.7318	-1.2592	1.5442	C	-4.4635	4.1984	1.5824	O	-6.7908	5.4471	-0.5713
C	0.7529	1.2378	1.4963	C	-4.9909	3.7136	0.3978	H	5.1239	-1.7427	1.1809
C	-0.6954	1.2055	1.5397	C	-4.2826	2.8653	-0.4574	H	0.8718	-4.2519	2.0114

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At	x	y	z	At	x	y	z	At	x	y	z
C	-0.6745	-1.2153	1.5662	C	-2.9970	2.4734	-0.0991	H	5.1284	-4.2315	1.4737
C	-1.4136	0.0196	1.6543	C	-1.6928	-4.6420	1.9563	H	3.0046	-5.4312	1.9091
N	2.7671	-0.2826	1.3190	C	-1.4751	-5.9567	1.5467	H	3.2904	2.8013	1.6937
C	2.9764	-1.6407	1.3987	C	-0.8870	-6.1649	0.3110	H	3.3068	5.2284	1.4841
C	1.7390	-2.3047	1.5758	C	-0.5160	-5.1196	-0.5387	H	1.1683	6.4927	1.2737
C	1.1313	2.6161	1.5146	C	-0.7536	-3.8102	-0.1341	H	-1.0147	5.3095	1.2801
N	-1.1653	2.5066	1.4959	S	6.4866	4.1137	0.1140	H	-4.0165	1.4137	2.2342
C	-0.0735	3.3733	1.4634	C	5.9639	3.9769	-1.5738	H	-4.0908	-3.5334	1.5621
C	-2.8188	-0.3426	1.7978	C	5.0299	2.9226	-1.7447	H	-6.1945	-2.2659	1.9336
N	-1.5741	-2.2497	1.5338	S	-6.6347	4.0349	-0.2309	H	-6.1333	0.1879	2.2956
C	-2.8781	-1.7443	1.6777	C	-6.3265	3.0547	-1.6933	H	4.6547	0.5485	3.0462
C	4.2071	-2.3028	1.3380	C	-5.0451	2.4968	-1.6665	H	6.2841	2.4082	2.5912
C	1.7701	-3.6893	1.7903	S	-0.4875	-7.7532	-0.4102	H	3.1792	0.8347	-1.0114
C	4.1946	-3.6757	1.5077	C	0.1839	-6.9808	-1.8749	H	-2.7356	4.1168	2.8804
C	2.9891	-4.3555	1.7483	C	0.1019	-5.5877	-1.7951	H	-5.0399	4.8615	2.2227
C	2.3554	3.3239	1.5705	C	6.3495	4.8138	-2.6110	H	-2.4082	1.8122	-0.7297
C	2.3542	4.7036	1.4826	C	5.7958	4.6143	-3.8718	H	-2.1215	-4.4279	2.9320
C	1.1488	5.4088	1.3611	C	4.8605	3.5815	-4.0661	H	-1.7462	-6.7926	2.1869
C	-0.0852	4.7535	1.3628	C	4.4789	2.7459	-3.0298	H	-0.4840	-2.9645	-0.7613
C	-4.0103	0.3458	2.0552	C	-7.2136	2.8461	-2.7353	H	7.0751	5.6052	-2.4343
C	-4.0702	-2.4561	1.6998	C	-6.7926	2.0427	-3.7956	H	6.0861	5.2512	-4.7035
C	-5.2444	-1.7376	1.9085	C	-5.5173	1.4759	-3.7899	H	4.4328	3.4306	-5.0559
C	-5.2110	-0.3555	2.1053	C	-4.6377	1.6969	-2.7309	H	3.7647	1.9444	-3.2115
C	-1.3277	-3.5845	1.1182	C	0.7315	-7.6389	-2.9627	H	-8.2031	3.2965	-2.7264
C	3.8180	0.6451	1.0236	C	1.2171	-6.8613	-4.0146	H	-7.4629	1.8603	-4.6320
C	-2.4652	2.9239	1.1107	C	1.1484	-5.4687	-3.9547	H	-5.2029	0.8537	-4.6245
C	4.7158	1.0216	2.0717	C	0.5934	-4.8235	-2.8504	H	-3.6458	1.2507	-2.7437
C	5.6160	2.0516	1.8092	O	0.5694	-8.4021	0.3639	H	0.7816	-8.7245	-2.9933
C	5.6351	2.6451	0.5576	O	-1.7113	-8.4881	-0.7237	H	1.6544	-7.3451	-4.8845
C	4.8053	2.1863	-0.5363	O	5.8544	5.2896	0.7548	H	1.5360	-4.8762	-4.7801
C	3.8825	1.1752	-0.2527	O	7.9468	4.0110	0.2653	H	0.5531	-3.7371	-2.8172

Table S12: Cartesian coordinates of the S_1 LVC Minimum of TAT-3DBTO₂.

At	x	y	z	At	x	y	z	At	x	y	z
C	1.3906	-0.0421	1.5478	C	-3.2197	3.7173	2.0349	O	-7.5815	3.3553	0.3936
C	0.6866	-1.2940	1.5888	C	-4.4963	4.1318	1.6467	O	-6.7366	5.6490	-0.4564
C	0.7312	1.2013	1.6113	C	-4.9344	3.7854	0.3666	H	5.0992	-1.8305	1.4270
C	-0.7054	1.1893	1.5540	C	-4.1337	3.0550	-0.5737	H	0.7755	-4.2635	2.0657
C	-0.7210	-1.2424	1.5243	C	-2.8671	2.6392	-0.1733	H	5.0484	-4.3068	1.7006
C	-1.4544	-0.0052	1.5694	C	-1.6963	-4.6811	1.9345	H	2.8914	-5.4842	2.0443
N	2.7427	-0.3028	1.4832	C	-1.3894	-5.9975	1.5721	H	3.2702	2.7389	2.1017
C	2.9472	-1.6767	1.5769	C	-0.7495	-6.2162	0.3610	H	3.2722	5.1823	2.1716
C	1.6921	-2.3282	1.6862	C	-0.4161	-5.1634	-0.5310	H	1.1735	6.4759	1.8985

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At	x	y	z	At	x	y	z	At	x	y	z
C	1.1311	2.5832	1.7444	C	-0.7286	-3.8541	-0.1660	H	-1.0024	5.2936	1.5909
N	-1.1465	2.4941	1.5311	S	6.7395	3.6313	-0.4746	H	-4.0888	1.4040	1.9563
C	-0.0577	3.3504	1.6591	C	5.7070	3.7616	-1.9330	H	-4.1219	-3.5571	1.3190
C	-2.8561	-0.3571	1.6268	C	4.5887	2.9122	-1.8524	H	-6.2514	-2.2769	1.5309
N	-1.6263	-2.2782	1.4405	S	-6.5389	4.1624	-0.3136	H	-6.2034	0.1812	1.8713
C	-2.9185	-1.7690	1.5089	C	-6.0877	3.3968	-1.9134	H	4.9574	0.3439	2.8314
C	4.1590	-2.3597	1.5551	C	-4.7865	2.8516	-1.8876	H	6.7124	1.9695	2.0700
C	1.6946	-3.7181	1.8934	S	-0.2109	-7.8004	-0.2709	H	2.7203	1.0015	-0.7960
C	4.1195	-3.7412	1.7103	C	0.4200	-7.0357	-1.7684	H	-2.8409	3.9400	3.0372
C	2.9010	-4.4067	1.8985	C	0.2422	-5.6351	-1.7531	H	-5.1373	4.7042	2.3368
C	2.3373	3.2703	1.9627	C	5.9404	4.5842	-3.0236	H	-2.2129	2.0641	-0.8501
C	2.3323	4.6580	2.0165	C	5.0179	4.5555	-4.0780	H	-2.1680	-4.4591	2.8902
C	1.1459	5.3891	1.8662	C	3.8952	3.7159	-4.0191	H	-1.6344	-6.8329	2.2338
C	-0.0720	4.7410	1.6916	C	3.6738	2.8954	-2.9168	H	-0.4848	-3.0065	-0.8127
C	-4.0692	0.3347	1.7915	C	-6.8869	3.3224	-3.0563	H	6.8191	5.2295	-3.0538
C	-4.1153	-2.4784	1.4509	C	-6.3622	2.6800	-4.2233	H	5.1732	5.1879	-4.9491
C	-5.2970	-1.7548	1.5712	C	-5.0657	2.1308	-4.2220	H	3.1830	3.7026	-4.8490
C	-5.2695	-0.3661	1.7582	C	-4.2764	2.2092	-3.0640	H	2.7946	2.2478	-2.8897
C	-1.3429	-3.6219	1.0662	C	1.0213	-7.7002	-2.8277	H	-7.8914	3.7563	-3.0424
C	3.7489	0.6020	1.0526	C	1.4626	-6.9323	-3.9185	H	-6.9630	2.6092	-5.1390
C	-2.4325	2.9513	1.1289	C	1.2967	-5.5341	-3.9241	H	-4.6674	1.6333	-5.1409
C	4.8742	0.8412	1.8685	C	0.6911	-4.8802	-2.8527	H	-3.2692	1.7765	-3.0825
C	5.8430	1.7545	1.4479	O	0.8890	-8.3307	0.5620	H	1.1423	-8.7880	-2.8066
C	5.6659	2.3943	0.2322	O	-1.3592	-8.6835	-0.5733	H	1.9374	-7.4231	-4.7668
C	4.5566	2.1398	-0.6082	O	6.6839	4.8703	0.3215	H	1.6456	-4.9466	-4.7813
C	3.5960	1.2265	-0.1854	O	8.0592	3.0641	-0.8100	H	0.5698	-3.7907	-2.8759

Table S13: Cartesian coordinates of the T₁ Minimum of TAT-3DBTO₂.

At	x	y	z	At	x	y	z	At	x	y	z
C	1.4151	-0.0298	1.6193	C	-3.1117	3.9068	1.8267	O	-7.4962	3.7067	0.2102
C	0.6944	-1.2895	1.6697	C	-4.3509	4.3475	1.3668	O	-6.4108	5.6144	-1.0400
C	0.7406	1.2303	1.6608	C	-4.8258	3.8312	0.1732	H	5.1158	-1.8919	1.6330
C	-0.6605	1.2256	1.5638	C	-4.1060	2.9038	-0.5871	H	0.7418	-4.2322	2.1942
C	-0.6829	-1.2485	1.5599	C	-2.8621	2.4822	-0.1346	H	5.0236	-4.3471	1.9740
C	-1.4317	0.0098	1.6172	C	-1.8763	-4.6962	1.7753	H	2.8459	-5.4929	2.2844
N	2.7733	-0.2994	1.5915	C	-1.6431	-5.9873	1.3085	H	3.2752	2.7138	2.2367
C	2.9641	-1.6885	1.7319	C	-0.9015	-6.1422	0.1489	H	3.3212	5.1621	2.3207
C	1.7067	-2.3275	1.8179	C	-0.3912	-5.0533	-0.5653	H	1.2596	6.4930	1.9539
C	1.1445	2.6061	1.8126	C	-0.6396	-3.7667	-0.1050	H	-0.9168	5.3676	1.5747
N	-1.1220	2.5372	1.5580	S	6.7496	3.4883	-0.6533	H	-3.9459	1.4849	2.2428
C	-0.0332	3.3900	1.7024	C	5.5705	3.7640	-1.9681	H	-4.1814	-3.4790	1.6274
C	-2.7901	-0.3209	1.8106	C	4.4236	2.9840	-1.7914	H	-6.2437	-2.1279	1.9636
N	-1.6133	-2.2894	1.5579	S	-6.3897	4.2208	-0.5972	H	-6.1041	0.3246	2.3106

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At	x	y	z	At	x	y	z	At	x	y	z
C	-2.8993	-1.7481	1.7197	C	-6.0509	3.1250	-1.9683	H	5.1305	0.1919	2.7140
C	4.1600	-2.3920	1.7574	C	-4.8113	2.4972	-1.8183	H	6.8817	1.7352	1.8328
C	1.6785	-3.7067	2.0490	S	-0.4476	-7.6878	-0.6185	H	2.5747	1.1270	-0.6197
C	4.0993	-3.7748	1.9449	C	0.4283	-6.8442	-1.9285	H	-2.7207	4.2513	2.7804
C	2.8758	-4.4198	2.1116	C	0.3726	-5.4576	-1.7621	H	-4.9361	5.0620	1.9404
C	2.3591	3.2696	2.0724	C	5.7306	4.6312	-3.0357	H	-2.2672	1.7648	-0.6936
C	2.3801	4.6522	2.1282	C	4.6950	4.7160	-3.9664	H	-2.4132	-4.5376	2.7065
C	1.2106	5.4069	1.9291	C	3.5405	3.9469	-3.8094	H	-2.0175	-6.8508	1.8530
C	-0.0109	4.7853	1.7177	C	3.3960	3.0807	-2.7271	H	-0.2602	-2.8946	-0.6310
C	-3.9815	0.4162	2.0711	C	-6.8834	2.8911	-3.0494	H	6.6355	5.2244	-3.1422
C	-4.1119	-2.4026	1.7508	C	-6.4504	1.9874	-4.0201	H	4.7883	5.3863	-4.8175
C	-5.2770	-1.6312	1.9415	C	-5.2176	1.3463	-3.8886	H	2.7401	4.0256	-4.5418
C	-5.1973	-0.2462	2.1238	C	-4.3927	1.5945	-2.7926	H	2.4882	2.4918	-2.6160
C	-1.3771	-3.5895	1.0726	C	1.0921	-7.4479	-2.9827	H	-7.8425	3.3958	-3.1359
C	3.7647	0.5599	1.0832	C	1.7276	-6.6213	-3.9097	H	-7.0796	1.7807	-4.8825
C	-2.3766	2.9782	1.0796	C	1.6876	-5.2340	-3.7619	H	-4.8955	0.6409	-4.6513
C	4.9773	0.7200	1.7767	C	1.0143	-4.6442	-2.6929	H	-3.4368	1.0837	-2.7012
C	5.9472	1.5937	1.2952	O	0.4878	-8.4256	0.2313	H	1.1156	-8.5304	-3.0817
C	5.6817	2.2968	0.1302	O	-1.6298	-8.3715	-1.1429	H	2.2582	-7.0618	-4.7504
C	4.4828	2.1440	-0.5807	O	6.8816	4.6861	0.1779	H	2.1908	-4.6021	-4.4902
C	3.5199	1.2686	-0.1022	O	7.9583	2.8442	-1.1694	H	0.9962	-3.5616	-2.5895

	φ_1	φ_2	φ_3
GS ^{SYM}	57.29	57.29	57.29
S ₁ ^{SYM}	67.27	67.27	67.27
S ₁ ^{MIN}	77.47	61.04	59.84
S ₁ ^{LVC}	66.59	62.88	60.98
T ₁ ^{MIN}	52.51	54.47	50.88

Table S14: Rotation coordinates φ of TAT-3DBTO₂.

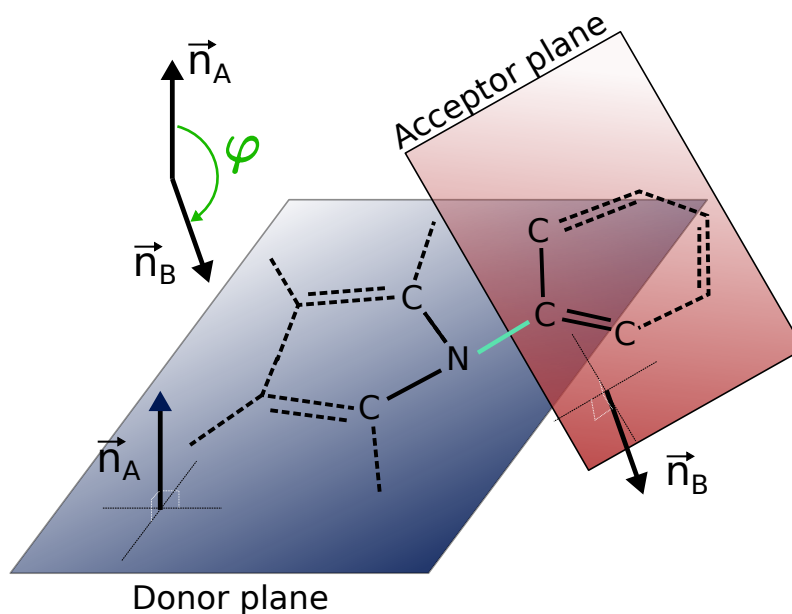


Figure S2: Definition of the Donor-Acceptor torsion angle φ . \vec{n}_A and \vec{n}_B are the normal vectors to the donor and acceptor units, respectively.

S2-2 Electronic Structure

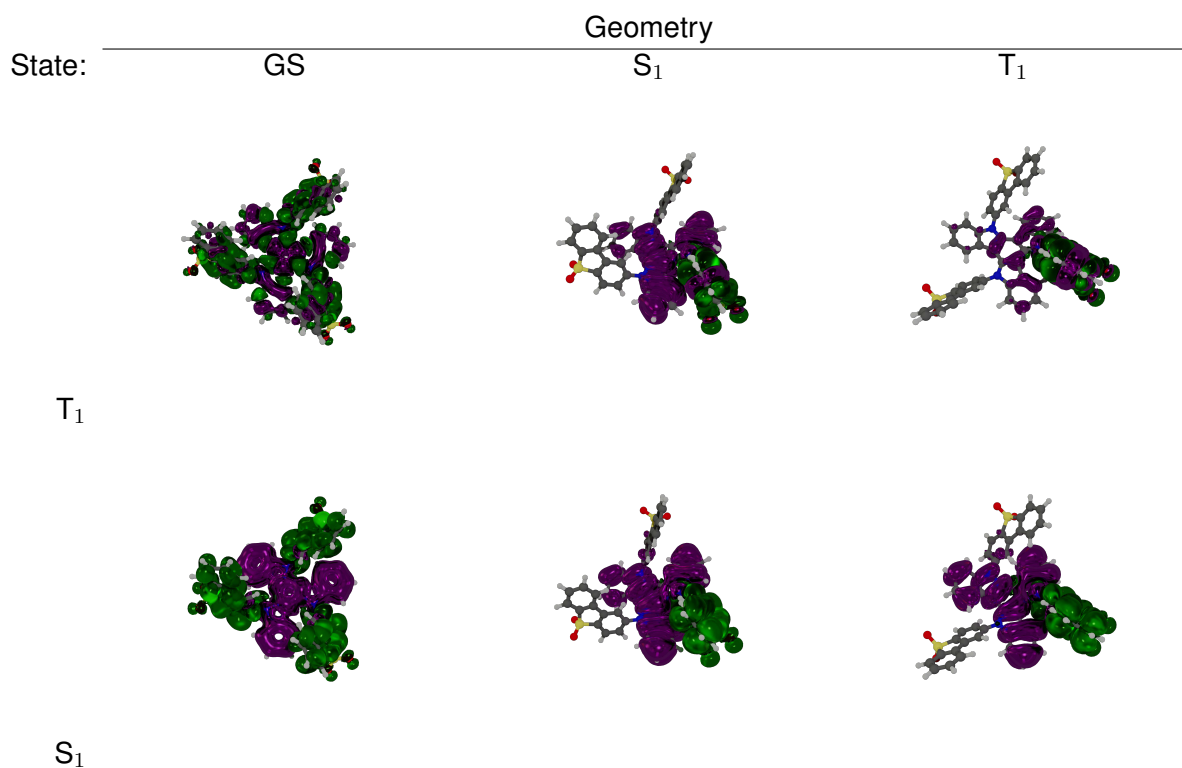


Figure S3: Difference of electronic density associated to the $T_1 \leftarrow GS$ (top) and $S_1 \leftarrow GS$ (bottom) at the ground state optimised geometry (left) the S_1 minimum (centre) and the T_1 minimum (right). Purple: loss of electronic density. Green: gain.

S2-3 LVC parameters

Table S15: LVC Analysis for S1 of TAT-3DBTO₂.

α	Freq. /cm ⁻¹	κ_{α}			κ_{α}^*			ξ
		κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	
1	7.27	2.244	-0.103	-2.489	-1.930	-0.076	2.140	0.004
2	8.11	0.904	-0.015	-0.900	-0.021	-0.000	0.021	0.001
3	13.90	6.964	-0.517	-4.040	10.845	-1.254	-6.291	-0.003
4	16.87	-2.219	-0.043	1.061	-6.322	-0.351	3.022	0.003
5	20.01	-0.904	-0.006	0.364	-9.645	-0.689	3.888	0.007
6	21.72	-0.536	-0.002	0.199	-11.714	-0.936	4.350	0.009
7	26.17	2.755	-0.043	-0.849	6.008	-0.204	-1.851	-0.003
8	27.20	5.955	-0.193	-1.766	13.579	-1.005	-4.027	-0.006
9	27.28	-5.387	-0.158	1.593	-1.880	-0.019	0.556	-0.003
10	52.89	1.683	-0.008	-0.257	7.781	-0.170	-1.187	-0.005
11	53.53	1.155	-0.004	-0.174	6.529	-0.118	-0.984	-0.005
12	54.84	1.215	-0.004	-0.179	-3.222	-0.028	0.474	0.004
13	81.36	-0.807	-0.001	0.080	0.000	-0.000	-0.000	-0.001
14	82.52	0.377	-0.000	-0.037	-2.820	-0.014	0.276	0.003
15	83.34	-0.054	-0.000	0.005	3.926	-0.027	-0.380	-0.003
16	92.20	-0.164	-0.000	0.014	7.464	-0.090	-0.653	-0.006
17	92.59	-0.193	-0.000	0.017	3.230	-0.017	-0.281	-0.003
18	98.64	-6.598	-0.065	0.540	-7.699	-0.089	0.630	0.001
19	106.64	-6.629	-0.061	0.501	-4.360	-0.026	0.330	-0.002
20	113.36	1.293	-0.002	-0.092	-9.483	-0.118	0.675	0.009
21	114.43	-0.996	-0.001	0.070	-7.869	-0.080	0.555	0.006
22	122.31	0.897	-0.001	-0.059	-4.205	-0.021	0.277	0.004
23	123.08	0.848	-0.001	-0.056	14.951	-0.269	-0.980	-0.012
24	124.37	10.782	-0.139	-0.699	26.701	-0.850	-1.732	-0.013
25	135.02	6.728	-0.050	-0.402	-8.045	-0.071	0.481	0.012
26	144.39	0.151	-0.000	-0.008	-10.176	-0.106	0.568	0.009
27	144.89	-0.052	-0.000	0.003	-10.467	-0.112	0.583	0.009
28	158.02	-0.343	-0.000	0.018	10.037	-0.094	-0.512	-0.009
29	159.46	0.369	-0.000	-0.019	8.140	-0.062	-0.412	-0.007
30	161.93	-2.310	-0.005	0.115	1.965	-0.004	-0.098	-0.004
31	173.08	0.975	-0.001	-0.045	-7.487	-0.048	0.349	0.007
32	173.40	0.272	-0.000	-0.013	-4.143	-0.015	0.193	0.004
33	174.49	9.308	-0.074	-0.430	4.381	-0.016	-0.203	0.004
34	190.80	-0.189	-0.000	0.008	12.709	-0.125	-0.537	-0.011
35	191.18	0.058	-0.000	-0.002	10.231	-0.081	-0.432	-0.009
36	236.90	-0.551	-0.000	0.019	-7.480	-0.035	0.255	0.006
37	237.25	-0.697	-0.000	0.024	48.286	-1.456	-1.642	-0.041
38	238.02	-2.128	-0.003	0.072	-25.688	-0.411	0.870	0.020
39	239.23	4.018	-0.010	-0.135	-47.632	-1.405	1.606	0.044
40	246.13	-0.242	-0.000	0.008	69.319	-2.893	-2.272	-0.059
41	246.29	0.745	-0.000	-0.024	-6.211	-0.023	0.203	0.006

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
42	257.54	6.887	-0.027	-0.216	-26.333	-0.399	0.825	0.028
43	282.13	-0.121	-0.000	0.003	-3.123	-0.005	0.089	0.003
44	282.85	0.343	-0.000	-0.010	-18.872	-0.187	0.538	0.016
45	296.86	7.952	-0.032	-0.216	15.663	-0.122	-0.426	-0.007
46	302.95	-6.493	-0.021	0.173	-55.137	-1.487	1.468	0.041
47	314.98	-0.127	-0.000	0.003	-1.342	-0.001	0.034	0.001
48	315.29	0.485	-0.000	-0.012	19.535	-0.179	-0.500	-0.016
49	316.37	-0.769	-0.000	0.020	-16.041	-0.121	0.409	0.013
50	330.08	0.418	-0.000	-0.010	-44.607	-0.893	1.090	0.038
51	330.19	-0.022	-0.000	0.001	-73.111	-2.399	1.786	0.062
52	355.94	-3.160	-0.004	0.072	92.085	-3.531	-2.087	-0.080
53	376.88	-0.387	-0.000	0.008	25.402	-0.254	-0.544	-0.022
54	377.11	-0.174	-0.000	0.004	50.190	-0.990	-1.073	-0.042
55	387.54	-6.282	-0.015	0.131	-36.499	-0.509	0.760	0.025
56	388.06	-0.068	-0.000	0.001	67.727	-1.752	-1.408	-0.057
57	388.36	-0.589	-0.000	0.012	10.332	-0.041	-0.215	-0.009
58	399.76	-3.207	-0.004	0.065	-3.299	-0.004	0.067	0.000
59	400.25	8.754	-0.028	-0.176	-26.195	-0.254	0.528	0.029
60	401.14	17.754	-0.116	-0.357	-12.262	-0.056	0.247	0.025
61	421.25	26.768	-0.252	-0.513	-22.444	-0.177	0.430	0.042
62	423.53	0.518	-0.000	-0.010	-21.079	-0.155	0.401	0.018
63	423.75	-2.495	-0.002	0.047	26.894	-0.253	-0.512	-0.025
64	432.77	0.065	-0.000	-0.001	-26.114	-0.234	0.487	0.022
65	433.39	-2.551	-0.002	0.047	0.077	-0.000	-0.001	-0.002
66	434.07	1.021	-0.000	-0.019	-19.612	-0.131	0.364	0.017
67	438.60	21.382	-0.154	-0.393	62.149	-1.305	-1.143	-0.034
68	440.61	4.357	-0.006	-0.080	17.434	-0.102	-0.319	-0.011
69	441.09	-1.409	-0.001	0.026	28.414	-0.271	-0.520	-0.025
70	457.15	-3.737	-0.005	0.066	1.126	-0.000	-0.020	-0.004
71	458.26	-1.436	-0.001	0.025	2.192	-0.002	-0.039	-0.003
72	458.74	-2.033	-0.001	0.036	5.990	-0.012	-0.105	-0.007
73	466.73	17.881	-0.102	-0.309	2.184	-0.002	-0.038	0.013
74	470.22	-4.410	-0.006	0.076	-10.757	-0.036	0.185	0.005
75	471.57	1.944	-0.001	-0.033	-21.005	-0.139	0.359	0.019
76	524.06	0.303	-0.000	-0.005	-56.976	-0.918	0.877	0.048
77	524.45	0.130	-0.000	-0.002	-138.412	-5.414	2.129	0.117
78	527.57	-4.571	-0.006	0.070	-125.694	-4.438	1.922	0.102
79	549.92	0.209	-0.000	-0.003	15.368	-0.064	-0.225	-0.013
80	550.27	-0.275	-0.000	0.004	15.085	-0.061	-0.221	-0.013
81	552.21	2.430	-0.002	-0.035	-13.208	-0.047	0.193	0.013
82	561.63	-0.007	-0.000	0.000	-103.099	-2.805	1.481	0.087
83	561.88	0.319	-0.000	-0.005	-52.710	-0.733	0.757	0.045
84	566.34	8.417	-0.019	-0.120	149.929	-5.882	-2.135	-0.119
85	568.88	0.408	-0.000	-0.006	-147.996	-5.706	2.098	0.125

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
86	569.06	-0.019	-0.000	0.000	12.189	-0.039	-0.173	-0.010
87	579.70	-1.998	-0.001	0.028	15.319	-0.060	-0.213	-0.015
88	582.59	14.425	-0.053	-0.200	18.264	-0.085	-0.253	-0.003
89	583.44	1.393	-0.000	-0.019	27.528	-0.192	-0.381	-0.022
90	583.55	-0.490	-0.000	0.007	35.416	-0.319	-0.490	-0.030
91	587.01	0.007	-0.000	-0.000	8.117	-0.017	-0.112	-0.007
92	587.21	0.635	-0.000	-0.009	27.551	-0.192	-0.378	-0.023
93	602.16	0.369	-0.000	-0.005	10.198	-0.026	-0.137	-0.008
94	602.50	-0.387	-0.000	0.005	12.092	-0.036	-0.162	-0.011
95	605.02	-3.793	-0.004	0.051	13.568	-0.045	-0.181	-0.015
96	635.75	-1.739	-0.001	0.022	7.172	-0.012	-0.091	-0.008
97	636.58	0.983	-0.000	-0.012	11.612	-0.031	-0.147	-0.009
98	637.27	-5.848	-0.008	0.074	-8.634	-0.017	0.109	0.002
99	650.33	-7.018	-0.011	0.087	-39.048	-0.347	0.484	0.027
100	664.36	0.410	-0.000	-0.005	16.303	-0.059	-0.198	-0.013
101	664.52	-0.061	-0.000	0.001	-40.083	-0.358	0.487	0.034
102	676.77	14.788	-0.048	-0.176	3.346	-0.002	-0.040	0.010
103	687.01	0.468	-0.000	-0.005	20.600	-0.092	-0.242	-0.017
104	687.30	-0.202	-0.000	0.002	-98.980	-2.113	1.162	0.083
105	694.66	0.063	-0.000	-0.001	-1.808	-0.001	0.021	0.002
106	694.99	0.195	-0.000	-0.002	29.029	-0.180	-0.337	-0.024
107	716.02	5.884	-0.007	-0.066	-208.221	-8.974	2.345	0.181
108	722.39	0.025	-0.000	-0.000	-197.780	-8.025	2.208	0.167
109	722.64	0.160	-0.000	-0.002	169.449	-5.889	-1.891	-0.143
110	729.09	-0.940	-0.000	0.010	104.494	-2.219	-1.156	-0.089
111	735.06	12.061	-0.029	-0.132	6.917	-0.010	-0.076	0.004
112	735.40	2.969	-0.002	-0.033	-21.452	-0.093	0.235	0.021
113	735.55	2.043	-0.001	-0.022	-3.387	-0.002	0.037	0.005
114	746.86	-1.807	-0.001	0.020	17.752	-0.063	-0.192	-0.016
115	747.53	-8.394	-0.014	0.091	51.190	-0.520	-0.552	-0.050
116	748.16	2.572	-0.001	-0.028	-28.400	-0.160	0.306	0.026
117	748.59	-0.426	-0.000	0.005	-23.836	-0.112	0.257	0.020
118	751.20	-1.237	-0.000	0.013	54.847	-0.593	-0.589	-0.047
119	751.48	0.780	-0.000	-0.008	121.812	-2.926	-1.307	-0.102
120	763.59	-0.469	-0.000	0.005	-8.289	-0.013	0.088	0.007
121	764.85	0.583	-0.000	-0.006	28.755	-0.160	-0.303	-0.024
122	766.37	-1.553	-0.000	0.016	-26.601	-0.137	0.280	0.021
123	768.16	0.383	-0.000	-0.004	-16.875	-0.055	0.177	0.015
124	768.93	0.450	-0.000	-0.005	11.268	-0.024	-0.118	-0.009
125	773.12	7.529	-0.011	-0.079	25.264	-0.122	-0.264	-0.015
126	779.85	0.747	-0.000	-0.008	2.431	-0.001	-0.025	-0.001
127	780.27	-0.522	-0.000	0.005	1.400	-0.000	-0.014	-0.002
128	780.68	-0.588	-0.000	0.006	7.199	-0.010	-0.074	-0.007
129	791.90	-12.865	-0.031	0.131	-47.565	-0.423	0.484	0.029

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
130	817.63	-1.362	-0.000	0.013	25.409	-0.117	-0.251	-0.023
131	818.00	0.038	-0.000	-0.000	-31.371	-0.178	0.309	0.026
132	822.08	16.175	-0.047	-0.159	72.671	-0.952	-0.713	-0.048
133	841.82	9.431	-0.016	-0.090	-8.344	-0.012	0.080	0.015
134	846.29	-0.198	-0.000	0.002	26.664	-0.125	-0.254	-0.023
135	846.72	0.488	-0.000	-0.005	3.870	-0.003	-0.037	-0.003
136	864.66	0.277	-0.000	-0.003	-14.931	-0.038	0.139	0.013
137	864.77	0.003	-0.000	-0.000	-19.354	-0.064	0.181	0.016
138	870.78	-2.394	-0.001	0.022	-8.878	-0.013	0.082	0.005
139	873.30	-1.898	-0.001	0.018	-1.167	-0.000	0.011	-0.001
140	873.69	1.554	-0.000	-0.014	4.100	-0.003	-0.038	-0.002
141	883.61	0.018	-0.000	-0.000	-6.145	-0.006	0.056	0.005
142	884.81	-1.653	-0.000	0.015	9.598	-0.015	-0.087	-0.009
143	885.54	-2.465	-0.001	0.022	10.419	-0.018	-0.095	-0.011
144	886.51	1.843	-0.001	-0.017	-6.127	-0.006	0.056	0.007
145	903.66	0.033	-0.000	-0.000	8.553	-0.012	-0.076	-0.007
146	907.01	-0.895	-0.000	0.008	-3.371	-0.002	0.030	0.002
147	922.64	5.243	-0.004	-0.046	-10.175	-0.017	0.089	0.013
148	944.10	-0.325	-0.000	0.003	-0.143	-0.000	0.001	-0.000
149	947.35	-0.824	-0.000	0.007	-1.784	-0.000	0.015	0.001
150	947.67	0.874	-0.000	-0.007	-4.464	-0.003	0.038	0.005
151	955.74	-0.593	-0.000	0.005	-1.031	-0.000	0.009	0.000
152	956.71	-0.792	-0.000	0.007	-0.265	-0.000	0.002	-0.000
153	957.63	0.670	-0.000	-0.006	-0.888	-0.000	0.007	0.001
154	966.18	0.397	-0.000	-0.003	2.601	-0.001	-0.022	-0.002
155	966.88	0.948	-0.000	-0.008	-4.987	-0.004	0.042	0.005
156	969.85	-2.977	-0.001	0.025	-5.054	-0.004	0.042	0.002
157	973.07	0.152	-0.000	-0.001	-1.172	-0.000	0.010	0.001
158	973.87	0.863	-0.000	-0.007	-0.988	-0.000	0.008	0.002
159	986.34	-1.084	-0.000	0.009	-1.305	-0.000	0.011	0.000
160	987.22	-2.465	-0.001	0.020	-2.968	-0.001	0.024	0.000
161	989.08	-2.710	-0.001	0.022	-1.444	-0.000	0.012	-0.001
162	991.75	9.104	-0.012	-0.074	13.910	-0.029	-0.113	-0.004
163	1000.97	0.223	-0.000	-0.002	0.044	-0.000	-0.000	0.000
164	1001.29	-0.243	-0.000	0.002	-0.183	-0.000	0.001	-0.000
165	1001.43	0.303	-0.000	-0.002	0.371	-0.000	-0.003	-0.000
166	1021.10	-4.316	-0.003	0.034	-32.622	-0.154	0.258	0.024
167	1041.47	0.634	-0.000	-0.005	53.318	-0.405	-0.413	-0.044
168	1041.70	1.161	-0.000	-0.009	-80.564	-0.923	0.624	0.069
169	1045.35	-19.109	-0.052	0.147	77.279	-0.847	-0.596	-0.081
170	1065.08	2.850	-0.001	-0.022	-6.918	-0.007	0.052	0.008
171	1065.36	3.257	-0.001	-0.025	1.995	-0.001	-0.015	0.001
172	1066.31	-4.539	-0.003	0.034	138.078	-2.650	-1.044	-0.120
173	1069.59	-3.359	-0.002	0.025	114.805	-1.826	-0.866	-0.100

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
174	1070.23	-0.672	-0.000	0.005	43.484	-0.262	-0.328	-0.037
175	1073.13	-18.074	-0.045	0.136	-236.342	-7.714	1.776	0.184
176	1073.45	-2.455	-0.001	0.018	-231.412	-7.393	1.739	0.193
177	1074.18	-0.714	-0.000	0.005	24.796	-0.085	-0.186	-0.022
178	1077.59	-9.424	-0.012	0.071	84.085	-0.972	-0.629	-0.079
179	1105.88	0.927	-0.000	-0.007	146.308	-2.869	-1.067	-0.123
180	1106.40	0.134	-0.000	-0.001	-1.997	-0.001	0.015	0.002
181	1117.87	-6.318	-0.005	0.046	-74.945	-0.745	0.541	0.058
182	1118.34	6.229	-0.005	-0.045	7.537	-0.008	-0.054	-0.001
183	1118.54	-5.933	-0.005	0.043	1.197	-0.000	-0.009	-0.006
184	1152.97	3.165	-0.001	-0.022	21.739	-0.061	-0.152	-0.016
185	1153.11	0.499	-0.000	-0.003	-18.172	-0.042	0.127	0.016
186	1153.95	-10.975	-0.015	0.077	-283.698	-10.337	1.983	0.230
187	1154.44	20.011	-0.051	-0.140	-177.637	-4.051	1.241	0.167
188	1159.31	0.197	-0.000	-0.001	7.834	-0.008	-0.055	-0.006
189	1160.58	0.950	-0.000	-0.007	26.454	-0.089	-0.184	-0.022
190	1170.62	-3.789	-0.002	0.026	-16.219	-0.033	0.112	0.010
191	1172.52	-5.468	-0.004	0.038	250.761	-7.948	-1.725	-0.216
192	1172.95	-9.085	-0.010	0.062	54.037	-0.369	-0.372	-0.053
193	1182.93	11.610	-0.017	-0.079	31.545	-0.125	-0.215	-0.017
194	1183.19	22.205	-0.062	-0.151	48.592	-0.296	-0.331	-0.022
195	1183.97	-24.310	-0.074	0.166	531.887	-35.412	-3.623	-0.469
196	1190.59	-0.441	-0.000	0.003	11.098	-0.015	-0.075	-0.010
197	1191.65	-1.986	-0.000	0.013	-34.042	-0.144	0.230	0.027
198	1193.71	-2.976	-0.001	0.020	-50.815	-0.321	0.343	0.040
199	1196.27	3.495	-0.002	-0.024	5.859	-0.004	-0.040	-0.002
200	1197.77	-4.317	-0.002	0.029	0.718	-0.000	-0.005	-0.004
201	1197.84	-3.350	-0.001	0.023	-67.403	-0.562	0.454	0.054
202	1226.69	8.051	-0.008	-0.053	-7.561	-0.007	0.050	0.013
203	1232.76	1.571	-0.000	-0.010	11.161	-0.015	-0.073	-0.008
204	1233.13	-0.074	-0.000	0.000	-22.238	-0.059	0.145	0.019
205	1263.96	1.898	-0.000	-0.012	37.661	-0.166	-0.240	-0.030
206	1264.11	-2.427	-0.001	0.015	-21.327	-0.053	0.136	0.016
207	1264.50	-2.746	-0.001	0.018	7.609	-0.007	-0.049	-0.009
208	1273.51	-55.839	-0.363	0.354	-56.956	-0.378	0.361	0.001
209	1278.05	5.136	-0.003	-0.032	7.074	-0.006	-0.045	-0.002
210	1279.72	-2.312	-0.001	0.015	19.546	-0.044	-0.123	-0.018
211	1298.93	-4.774	-0.003	0.030	-21.549	-0.053	0.134	0.014
212	1299.78	2.417	-0.001	-0.015	20.903	-0.050	-0.130	-0.016
213	1303.02	28.804	-0.094	-0.178	38.099	-0.165	-0.236	-0.008
214	1320.43	0.404	-0.000	-0.002	-21.905	-0.054	0.134	0.019
215	1321.18	-1.625	-0.000	0.010	-51.796	-0.301	0.316	0.042
216	1329.62	47.606	-0.253	-0.289	-42.115	-0.198	0.255	0.076
217	1340.08	-6.087	-0.004	0.037	-21.094	-0.049	0.127	0.013

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
218	1340.90	3.611	-0.001	-0.022	18.717	-0.039	-0.113	-0.013
219	1345.20	35.427	-0.138	-0.212	46.388	-0.237	-0.278	-0.009
220	1345.97	2.715	-0.001	-0.016	4.376	-0.002	-0.026	-0.001
221	1347.47	-1.234	-0.000	0.007	148.006	-2.409	-0.886	-0.126
222	1348.19	0.117	-0.000	-0.001	0.001	-0.000	-0.000	0.000
223	1363.49	-30.373	-0.100	0.180	-10.860	-0.013	0.064	-0.016
224	1367.79	-3.864	-0.002	0.023	23.182	-0.058	-0.137	-0.023
225	1368.57	-0.884	-0.000	0.005	11.793	-0.015	-0.070	-0.011
226	1374.91	-1.920	-0.000	0.011	-11.366	-0.014	0.067	0.008
227	1377.40	0.189	-0.000	-0.001	-12.469	-0.017	0.073	0.011
228	1377.90	-0.002	-0.000	0.000	41.345	-0.184	-0.242	-0.035
229	1404.14	29.202	-0.090	-0.168	32.113	-0.109	-0.184	-0.002
230	1404.52	13.054	-0.018	-0.075	5.321	-0.003	-0.031	0.007
231	1405.17	-8.080	-0.007	0.046	4.099	-0.002	-0.024	-0.010
232	1405.66	12.616	-0.017	-0.072	3.194	-0.001	-0.018	0.008
233	1419.71	-0.158	-0.000	0.001	-18.686	-0.036	0.106	0.016
234	1420.16	-0.681	-0.000	0.004	4.248	-0.002	-0.024	-0.004
235	1441.10	-28.106	-0.081	0.157	-42.911	-0.189	0.240	0.012
236	1448.95	2.434	-0.001	-0.014	6.674	-0.005	-0.037	-0.004
237	1449.72	-0.689	-0.000	0.004	-23.701	-0.057	0.132	0.019
238	1464.10	-0.729	-0.000	0.004	-13.939	-0.020	0.077	0.011
239	1473.54	15.966	-0.026	-0.087	21.843	-0.048	-0.120	-0.005
240	1476.37	-4.182	-0.002	0.023	-5.816	-0.003	0.032	0.001
241	1477.19	-0.990	-0.000	0.005	4.546	-0.002	-0.025	-0.005
242	1493.29	-18.519	-0.034	0.100	-17.281	-0.030	0.093	-0.001
243	1494.02	15.783	-0.025	-0.085	76.969	-0.588	-0.416	-0.052
244	1495.20	15.273	-0.023	-0.082	-2.616	-0.001	0.014	0.015
245	1511.57	18.247	-0.033	-0.097	20.021	-0.039	-0.107	-0.001
246	1516.07	3.630	-0.001	-0.019	40.288	-0.159	-0.214	-0.031
247	1516.86	0.312	-0.000	-0.002	-1.287	-0.000	0.007	0.001
248	1528.07	2.363	-0.001	-0.012	1.410	-0.000	-0.007	0.001
249	1529.43	1.538	-0.000	-0.008	-28.091	-0.076	0.148	0.025
250	1529.79	-10.802	-0.011	0.057	-11.811	-0.014	0.062	0.001
251	1531.63	-21.074	-0.043	0.111	-5.795	-0.003	0.031	-0.013
252	1532.81	27.556	-0.073	-0.145	34.756	-0.117	-0.183	-0.006
253	1533.15	-12.260	-0.015	0.064	-62.036	-0.372	0.326	0.042
254	1541.53	22.052	-0.047	-0.115	11.701	-0.013	-0.061	0.009
255	1541.85	-27.373	-0.072	0.143	-15.876	-0.024	0.083	-0.010
256	1543.04	27.543	-0.073	-0.144	18.908	-0.034	-0.099	0.007
257	1643.36	0.964	-0.000	-0.005	-91.801	-0.760	0.451	0.078
258	1643.91	0.403	-0.000	-0.002	13.408	-0.016	-0.066	-0.011
259	1651.45	-16.117	-0.023	0.079	-2.038	-0.000	0.010	-0.012
260	1652.33	-11.717	-0.012	0.057	14.201	-0.018	-0.069	-0.022
261	1653.37	-37.076	-0.123	0.181	-31.337	-0.088	0.153	-0.005

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
262	1655.44	13.221	-0.016	-0.064	4.374	-0.002	-0.021	0.007
263	1656.79	-6.095	-0.003	0.030	-14.555	-0.019	0.071	0.007
264	1657.35	-4.101	-0.002	0.020	2.537	-0.001	-0.012	-0.006
265	1666.68	18.240	-0.030	-0.088	-7.974	-0.006	0.039	0.022
266	1667.73	-11.649	-0.012	0.056	-5.634	-0.003	0.027	-0.005
267	1668.39	-9.062	-0.007	0.044	39.211	-0.137	-0.190	-0.041
268	1677.73	-1.040	-0.000	0.005	-23.244	-0.048	0.112	0.019
269	1678.79	-2.838	-0.001	0.014	-105.757	-0.987	0.508	0.087
270	1679.09	-19.675	-0.034	0.095	2.694	-0.001	-0.013	-0.019
271	1679.61	-10.213	-0.009	0.049	52.979	-0.248	-0.254	-0.053
272	1680.06	15.749	-0.022	-0.076	-45.441	-0.182	0.218	0.052
273	1680.87	-14.608	-0.019	0.070	-15.865	-0.022	0.076	0.001
274	1687.64	15.102	-0.020	-0.072	32.143	-0.091	-0.154	-0.014
275	1690.07	-2.553	-0.001	0.012	-28.031	-0.069	0.134	0.021
276	1690.70	-2.321	-0.000	0.011	-38.992	-0.133	0.186	0.031
277	3206.39	0.375	-0.000	-0.001	0.619	-0.000	-0.002	-0.000
278	3206.95	0.286	-0.000	-0.001	0.646	-0.000	-0.002	-0.000
279	3208.69	0.207	-0.000	-0.001	11.900	-0.007	-0.030	-0.010
280	3208.70	0.307	-0.000	-0.001	-2.816	-0.000	0.007	0.003
281	3209.44	0.008	-0.000	-0.000	3.482	-0.001	-0.009	-0.003
282	3210.80	0.285	-0.000	-0.001	-121.751	-0.684	0.306	0.103
283	3218.79	1.006	-0.000	-0.003	-15.080	-0.010	0.038	0.014
284	3220.02	-0.988	-0.000	0.002	-5.779	-0.002	0.014	0.004
285	3220.27	1.039	-0.000	-0.003	-201.245	-1.864	0.504	0.171
286	3220.51	0.952	-0.000	-0.002	-15.486	-0.011	0.039	0.014
287	3222.62	1.469	-0.000	-0.004	3.113	-0.000	-0.008	-0.001
288	3223.76	1.514	-0.000	-0.004	39.720	-0.073	-0.099	-0.032
289	3224.21	1.417	-0.000	-0.004	-0.283	-0.000	0.001	0.001
290	3225.14	1.150	-0.000	-0.003	-15.571	-0.011	0.039	0.014
291	3225.48	1.665	-0.000	-0.004	-97.044	-0.433	0.243	0.083
292	3227.06	0.506	-0.000	-0.001	7.187	-0.002	-0.018	-0.006
293	3227.43	-0.567	-0.000	0.001	-1.292	-0.000	0.003	0.001
294	3229.46	-0.317	-0.000	0.001	-150.385	-1.038	0.376	0.127
295	3229.90	2.306	-0.000	-0.006	-12.881	-0.008	0.032	0.013
296	3230.22	2.396	-0.000	-0.006	-13.541	-0.008	0.034	0.013
297	3232.20	-3.892	-0.001	0.010	2.432	-0.000	-0.006	-0.005
298	3232.93	0.758	-0.000	-0.002	126.617	-0.735	-0.316	-0.106
299	3233.32	4.557	-0.001	-0.011	-151.364	-1.050	0.378	0.132
300	3235.66	-3.097	-0.000	0.008	-12.834	-0.008	0.032	0.008
301	3236.56	0.649	-0.000	-0.002	-22.459	-0.023	0.056	0.019
302	3237.23	0.920	-0.000	-0.002	-8.600	-0.003	0.021	0.008
303	3237.54	-1.659	-0.000	0.004	49.861	-0.114	-0.124	-0.043
304	3237.60	-0.353	-0.000	0.001	319.254	-4.666	-0.795	-0.270
305	3238.62	-0.909	-0.000	0.002	-253.577	-2.942	0.632	0.213

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
306	3238.77	2.257	-0.000	-0.006	16.992	-0.013	-0.042	-0.012
307	3266.38	0.471	-0.000	-0.001	2.266	-0.000	-0.006	-0.002
308	3271.98	-0.939	-0.000	0.002	-12.460	-0.007	0.031	0.010
309	3272.58	1.447	-0.000	-0.004	12.123	-0.007	-0.030	-0.009

Table S16: LVC Analysis for T1 of TAT-3DBTO₂.

α	Freq. /cm ⁻¹	κ_α			κ_α^*			ξ
		κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	
1	7.27	-0.098	-0.000	0.108	0.478	-0.005	-0.530	-0.003
2	8.11	1.116	-0.023	-1.111	0.492	-0.004	-0.489	0.003
3	13.90	-2.647	-0.075	1.535	-2.561	-0.070	1.485	-0.000
4	16.87	-1.329	-0.016	0.635	-0.713	-0.004	0.341	-0.003
5	20.01	-0.041	-0.000	0.016	1.545	-0.018	-0.623	-0.007
6	21.72	-0.609	-0.003	0.226	-2.731	-0.051	1.014	0.010
7	26.17	-0.307	-0.001	0.095	0.178	-0.000	-0.055	-0.002
8	27.20	0.029	-0.000	-0.009	-0.237	-0.000	0.070	0.001
9	27.28	0.235	-0.000	-0.070	0.443	-0.001	-0.131	-0.001
10	52.89	-6.345	-0.113	0.968	-7.487	-0.157	1.142	0.005
11	53.53	-3.536	-0.035	0.533	-7.213	-0.144	1.087	0.017
12	54.84	-1.649	-0.007	0.243	1.688	-0.008	-0.248	-0.015
13	81.36	-4.392	-0.035	0.435	-3.403	-0.021	0.337	-0.004
14	82.52	-0.703	-0.001	0.069	-2.427	-0.011	0.237	0.008
15	83.34	1.019	-0.002	-0.099	3.015	-0.016	-0.292	-0.009
16	92.20	-0.164	-0.000	0.014	-2.601	-0.011	0.227	0.011
17	92.59	0.404	-0.000	-0.035	0.697	-0.001	-0.061	-0.001
18	98.64	2.577	-0.010	-0.211	3.314	-0.016	-0.271	-0.003
19	106.64	-3.715	-0.019	0.281	-4.863	-0.033	0.368	0.005
20	113.36	0.895	-0.001	-0.064	3.462	-0.016	-0.246	-0.012
21	114.43	-0.662	-0.001	0.047	-1.889	-0.005	0.133	0.006
22	122.31	0.377	-0.000	-0.025	4.847	-0.028	-0.320	-0.020
23	123.08	-0.353	-0.000	0.023	2.275	-0.006	-0.149	-0.012
24	124.37	-0.516	-0.000	0.033	0.127	-0.000	-0.008	-0.003
25	135.02	4.423	-0.021	-0.264	7.734	-0.066	-0.462	-0.015
26	144.39	0.038	-0.000	-0.002	2.119	-0.005	-0.118	-0.009
27	144.89	0.143	-0.000	-0.008	-9.088	-0.084	0.506	0.042
28	158.02	-1.327	-0.002	0.068	-2.873	-0.008	0.147	0.007
29	159.46	-0.153	-0.000	0.008	5.085	-0.024	-0.257	-0.024
30	161.93	3.128	-0.009	-0.156	3.426	-0.011	-0.171	-0.001
31	173.08	-0.441	-0.000	0.021	1.069	-0.001	-0.050	-0.007
32	173.40	-0.534	-0.000	0.025	-1.603	-0.002	0.075	0.005
33	174.49	-3.783	-0.012	0.175	-2.068	-0.004	0.096	-0.008
34	190.80	-0.327	-0.000	0.014	-3.263	-0.008	0.138	0.013
35	191.18	0.130	-0.000	-0.005	-3.720	-0.011	0.157	0.017

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
36	236.90	0.252	-0.000	-0.009	-2.528	-0.004	0.086	0.013
37	237.25	1.284	-0.001	-0.044	-0.061	-0.000	0.002	0.006
38	238.02	3.647	-0.008	-0.124	2.590	-0.004	-0.088	0.005
39	239.23	2.332	-0.003	-0.079	3.881	-0.009	-0.131	-0.007
40	246.13	0.023	-0.000	-0.001	1.881	-0.002	-0.062	-0.008
41	246.29	0.551	-0.000	-0.018	-6.069	-0.022	0.199	0.030
42	257.54	-2.433	-0.003	0.076	-6.955	-0.028	0.218	0.020
43	282.13	0.033	-0.000	-0.001	-2.082	-0.002	0.060	0.010
44	282.85	0.370	-0.000	-0.011	-10.666	-0.060	0.304	0.050
45	296.86	7.875	-0.031	-0.214	12.547	-0.079	-0.341	-0.021
46	302.95	11.203	-0.061	-0.298	14.405	-0.102	-0.384	-0.014
47	314.98	0.092	-0.000	-0.002	0.615	-0.000	-0.016	-0.002
48	315.29	0.389	-0.000	-0.010	-1.438	-0.001	0.037	0.008
49	316.37	-2.780	-0.004	0.071	-1.920	-0.002	0.049	-0.004
50	330.08	0.394	-0.000	-0.010	14.847	-0.099	-0.363	-0.065
51	330.19	0.113	-0.000	-0.003	10.410	-0.049	-0.254	-0.047
52	355.94	6.122	-0.016	-0.139	15.462	-0.100	-0.350	-0.042
53	376.88	-0.316	-0.000	0.007	8.167	-0.026	-0.175	-0.038
54	377.11	-0.004	-0.000	0.000	-5.144	-0.010	0.110	0.023
55	387.54	5.884	-0.013	-0.122	5.144	-0.010	-0.107	0.003
56	388.06	1.449	-0.001	-0.030	12.838	-0.063	-0.267	-0.051
57	388.36	-0.816	-0.000	0.017	0.039	-0.000	-0.001	-0.004
58	399.76	-1.637	-0.001	0.033	0.037	-0.000	-0.001	-0.008
59	400.25	4.822	-0.009	-0.097	16.557	-0.102	-0.334	-0.053
60	401.14	9.778	-0.035	-0.197	4.122	-0.006	-0.083	0.026
61	421.25	4.364	-0.007	-0.084	4.848	-0.008	-0.093	-0.002
62	423.53	-0.233	-0.000	0.004	2.590	-0.002	-0.049	-0.013
63	423.75	-0.393	-0.000	0.007	0.682	-0.000	-0.013	-0.005
64	432.77	2.477	-0.002	-0.046	-1.162	-0.000	0.022	0.016
65	433.39	-0.798	-0.000	0.015	-4.514	-0.007	0.084	0.017
66	434.07	-0.002	-0.000	0.000	-0.271	-0.000	0.005	0.001
67	438.60	7.157	-0.017	-0.132	12.883	-0.056	-0.237	-0.026
68	440.61	1.593	-0.001	-0.029	-10.517	-0.037	0.193	0.055
69	441.09	-0.469	-0.000	0.009	11.087	-0.041	-0.203	-0.052
70	457.15	-7.292	-0.017	0.129	-6.778	-0.015	0.120	-0.002
71	458.26	-2.403	-0.002	0.042	-5.173	-0.009	0.091	0.013
72	458.74	-2.222	-0.002	0.039	-4.455	-0.006	0.078	0.010
73	466.73	10.753	-0.037	-0.186	15.052	-0.072	-0.260	-0.019
74	470.22	-3.014	-0.003	0.052	5.824	-0.011	-0.100	-0.040
75	471.57	1.307	-0.001	-0.022	-2.223	-0.002	0.038	0.016
76	524.06	-0.155	-0.000	0.002	0.722	-0.000	-0.011	-0.004
77	524.45	-0.032	-0.000	0.000	5.704	-0.009	-0.088	-0.026
78	527.57	1.248	-0.000	-0.019	-6.958	-0.014	0.106	0.037
79	549.92	0.424	-0.000	-0.006	-0.953	-0.000	0.014	0.006

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
80	550.27	-0.125	-0.000	0.002	-1.093	-0.000	0.016	0.004
81	552.21	-0.346	-0.000	0.005	-1.643	-0.001	0.024	0.006
82	561.63	0.035	-0.000	-0.001	-0.579	-0.000	0.008	0.003
83	561.88	0.199	-0.000	-0.003	2.362	-0.001	-0.034	-0.010
84	566.34	4.355	-0.005	-0.062	4.705	-0.006	-0.067	-0.002
85	568.88	0.151	-0.000	-0.002	-5.566	-0.008	0.079	0.026
86	569.06	0.148	-0.000	-0.002	8.892	-0.021	-0.126	-0.040
87	579.70	3.811	-0.004	-0.053	3.026	-0.002	-0.042	0.004
88	582.59	6.849	-0.012	-0.095	6.529	-0.011	-0.090	0.001
89	583.44	0.663	-0.000	-0.009	3.411	-0.003	-0.047	-0.012
90	583.55	-0.202	-0.000	0.003	-3.438	-0.003	0.048	0.015
91	587.01	0.096	-0.000	-0.001	-12.895	-0.042	0.177	0.059
92	587.21	0.592	-0.000	-0.008	0.601	-0.000	-0.008	-0.000
93	602.16	-0.375	-0.000	0.005	-4.500	-0.005	0.060	0.019
94	602.50	-0.132	-0.000	0.002	6.697	-0.011	-0.090	-0.031
95	605.02	4.054	-0.004	-0.054	4.786	-0.006	-0.064	-0.003
96	635.75	-1.169	-0.000	0.015	0.032	-0.000	-0.000	-0.005
97	636.58	0.754	-0.000	-0.010	2.941	-0.002	-0.037	-0.010
98	637.27	-4.568	-0.005	0.058	-3.028	-0.002	0.038	-0.007
99	650.33	4.518	-0.005	-0.056	3.520	-0.003	-0.044	0.005
100	664.36	0.311	-0.000	-0.004	-2.059	-0.001	0.025	0.011
101	664.52	-0.237	-0.000	0.003	0.867	-0.000	-0.011	-0.005
102	676.77	13.346	-0.039	-0.159	16.019	-0.056	-0.191	-0.012
103	687.01	0.383	-0.000	-0.004	15.825	-0.054	-0.186	-0.070
104	687.30	-0.284	-0.000	0.003	-8.298	-0.015	0.097	0.036
105	694.66	-0.090	-0.000	0.001	-0.008	-0.000	0.000	-0.000
106	694.99	0.154	-0.000	-0.002	-4.028	-0.003	0.047	0.019
107	716.02	9.435	-0.018	-0.106	0.699	-0.000	-0.008	0.039
108	722.39	0.130	-0.000	-0.001	8.746	-0.016	-0.098	-0.039
109	722.64	0.309	-0.000	-0.003	3.551	-0.003	-0.040	-0.015
110	729.09	4.532	-0.004	-0.050	9.797	-0.020	-0.108	-0.024
111	735.06	-1.776	-0.001	0.019	-8.440	-0.014	0.093	0.030
112	735.40	-0.510	-0.000	0.006	-8.738	-0.015	0.096	0.037
113	735.55	-0.283	-0.000	0.003	-0.033	-0.000	0.000	-0.001
114	746.86	-2.576	-0.001	0.028	-0.947	-0.000	0.010	-0.007
115	747.53	-4.440	-0.004	0.048	1.298	-0.000	-0.014	-0.026
116	748.16	-0.136	-0.000	0.001	-3.386	-0.002	0.037	0.015
117	748.59	0.713	-0.000	-0.008	0.868	-0.000	-0.009	-0.001
118	751.20	-0.757	-0.000	0.008	-6.839	-0.009	0.073	0.027
119	751.48	0.808	-0.000	-0.009	3.360	-0.002	-0.036	-0.012
120	763.59	1.039	-0.000	-0.011	3.439	-0.002	-0.036	-0.011
121	764.85	-1.456	-0.000	0.015	2.608	-0.001	-0.028	-0.018
122	766.37	0.791	-0.000	-0.008	-2.008	-0.001	0.021	0.013
123	768.16	0.319	-0.000	-0.003	3.448	-0.002	-0.036	-0.014

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
124	768.93	-0.449	-0.000	0.005	0.800	-0.000	-0.008	-0.006
125	773.12	1.082	-0.000	-0.011	-0.504	-0.000	0.005	0.007
126	779.85	0.217	-0.000	-0.002	0.138	-0.000	-0.001	0.000
127	780.27	-0.067	-0.000	0.001	-0.341	-0.000	0.004	0.001
128	780.68	-0.295	-0.000	0.003	-0.701	-0.000	0.007	0.002
129	791.90	-15.870	-0.047	0.162	-18.861	-0.067	0.192	0.014
130	817.63	-0.250	-0.000	0.002	-14.121	-0.036	0.139	0.063
131	818.00	0.041	-0.000	-0.000	6.488	-0.008	-0.064	-0.029
132	822.08	4.411	-0.004	-0.043	9.429	-0.016	-0.093	-0.023
133	841.82	1.857	-0.001	-0.018	-3.309	-0.002	0.032	0.023
134	846.29	0.051	-0.000	-0.000	1.985	-0.001	-0.019	-0.009
135	846.72	0.475	-0.000	-0.005	-6.535	-0.007	0.062	0.032
136	864.66	0.080	-0.000	-0.001	-0.802	-0.000	0.007	0.004
137	864.77	0.051	-0.000	-0.000	-16.179	-0.045	0.151	0.073
138	870.78	-1.046	-0.000	0.010	0.285	-0.000	-0.003	-0.006
139	873.30	-0.662	-0.000	0.006	-4.729	-0.004	0.044	0.018
140	873.69	0.609	-0.000	-0.006	-2.295	-0.001	0.021	0.013
141	883.61	-2.021	-0.001	0.018	-4.852	-0.004	0.044	0.013
142	884.81	3.585	-0.002	-0.033	10.191	-0.017	-0.093	-0.030
143	885.54	2.855	-0.001	-0.026	8.598	-0.012	-0.078	-0.026
144	886.51	-1.550	-0.000	0.014	-4.662	-0.004	0.042	0.014
145	903.66	0.046	-0.000	-0.000	6.454	-0.007	-0.058	-0.029
146	907.01	0.503	-0.000	-0.004	-1.284	-0.000	0.011	0.008
147	922.64	-1.981	-0.001	0.017	-13.079	-0.027	0.114	0.050
148	944.10	-1.278	-0.000	0.011	-6.672	-0.007	0.057	0.024
149	947.35	-1.387	-0.000	0.012	-1.691	-0.000	0.014	0.001
150	947.67	2.192	-0.001	-0.019	0.452	-0.000	-0.004	0.008
151	955.74	-0.155	-0.000	0.001	0.040	-0.000	-0.000	-0.001
152	956.71	-0.335	-0.000	0.003	-0.164	-0.000	0.001	-0.001
153	957.63	0.218	-0.000	-0.002	0.284	-0.000	-0.002	-0.000
154	966.18	0.332	-0.000	-0.003	12.567	-0.024	-0.105	-0.055
155	966.88	0.753	-0.000	-0.006	9.423	-0.014	-0.079	-0.039
156	969.85	-2.315	-0.001	0.019	0.741	-0.000	-0.006	-0.014
157	973.07	0.094	-0.000	-0.001	13.594	-0.028	-0.113	-0.061
158	973.87	0.705	-0.000	-0.006	5.873	-0.005	-0.049	-0.023
159	986.34	-2.025	-0.001	0.017	-3.734	-0.002	0.031	0.008
160	987.22	-3.796	-0.002	0.031	-4.076	-0.002	0.033	0.001
161	989.08	-4.308	-0.003	0.035	-6.597	-0.007	0.054	0.010
162	991.75	11.720	-0.021	-0.095	21.734	-0.071	-0.177	-0.045
163	1000.97	0.008	-0.000	-0.000	-0.067	-0.000	0.001	0.000
164	1001.29	-0.015	-0.000	0.000	0.154	-0.000	-0.001	-0.001
165	1001.43	0.093	-0.000	-0.001	-0.066	-0.000	0.001	0.001
166	1021.10	-6.415	-0.006	0.051	-12.843	-0.024	0.101	0.029
167	1041.47	0.214	-0.000	-0.002	-9.911	-0.014	0.077	0.046

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
168	1041.70	0.784	-0.000	-0.006	2.522	-0.001	-0.020	-0.008
169	1045.35	-7.227	-0.007	0.056	5.916	-0.005	-0.046	-0.059
170	1065.08	1.804	-0.000	-0.014	0.101	-0.000	-0.001	0.008
171	1065.36	1.925	-0.001	-0.015	-4.930	-0.003	0.037	0.031
172	1066.31	-2.716	-0.001	0.021	1.673	-0.000	-0.013	-0.020
173	1069.59	-2.899	-0.001	0.022	-8.828	-0.011	0.067	0.027
174	1070.23	-0.581	-0.000	0.004	-4.697	-0.003	0.035	0.019
175	1073.13	-13.662	-0.026	0.103	-11.185	-0.017	0.084	-0.011
176	1073.45	-2.687	-0.001	0.020	-6.815	-0.006	0.051	0.019
177	1074.18	-0.794	-0.000	0.006	3.043	-0.001	-0.023	-0.017
178	1077.59	-11.260	-0.017	0.084	-9.513	-0.012	0.071	-0.008
179	1105.88	0.703	-0.000	-0.005	8.703	-0.010	-0.063	-0.036
180	1106.40	0.026	-0.000	-0.000	20.043	-0.054	-0.146	-0.090
181	1117.87	-4.282	-0.002	0.031	-0.106	-0.000	0.001	-0.019
182	1118.34	4.468	-0.003	-0.032	2.186	-0.001	-0.016	0.010
183	1118.54	-4.288	-0.002	0.031	-0.999	-0.000	0.007	-0.015
184	1152.97	2.519	-0.001	-0.018	0.493	-0.000	-0.003	0.009
185	1153.11	-2.305	-0.001	0.016	-7.432	-0.007	0.052	0.023
186	1153.95	-12.040	-0.019	0.084	-15.573	-0.031	0.109	0.016
187	1154.44	17.331	-0.039	-0.121	19.260	-0.048	-0.135	-0.009
188	1159.31	-0.185	-0.000	0.001	-7.651	-0.007	0.053	0.034
189	1160.58	0.985	-0.000	-0.007	-5.441	-0.004	0.038	0.029
190	1170.62	-2.173	-0.001	0.015	8.065	-0.008	-0.056	-0.046
191	1172.52	-3.480	-0.002	0.024	-1.510	-0.000	0.010	-0.009
192	1172.95	-4.671	-0.003	0.032	1.616	-0.000	-0.011	-0.028
193	1182.93	5.714	-0.004	-0.039	-1.383	-0.000	0.009	0.032
194	1183.19	10.876	-0.015	-0.074	3.262	-0.001	-0.022	0.034
195	1183.97	-11.740	-0.017	0.080	-3.216	-0.001	0.022	-0.039
196	1190.59	-0.590	-0.000	0.004	-8.297	-0.009	0.056	0.035
197	1191.65	-1.607	-0.000	0.011	13.849	-0.024	-0.094	-0.070
198	1193.71	-1.472	-0.000	0.010	-12.900	-0.021	0.087	0.052
199	1196.27	0.794	-0.000	-0.005	3.974	-0.002	-0.027	-0.014
200	1197.77	-1.128	-0.000	0.008	1.148	-0.000	-0.008	-0.010
201	1197.84	-0.764	-0.000	0.005	-0.513	-0.000	0.003	-0.001
202	1226.69	-16.284	-0.032	0.107	-25.473	-0.078	0.167	0.042
203	1232.76	1.208	-0.000	-0.008	-8.092	-0.008	0.053	0.042
204	1233.13	-0.333	-0.000	0.002	11.866	-0.017	-0.078	-0.055
205	1263.96	5.735	-0.004	-0.037	20.916	-0.051	-0.133	-0.069
206	1264.11	-5.418	-0.003	0.035	-1.648	-0.000	0.011	-0.017
207	1264.50	-9.460	-0.010	0.060	-21.469	-0.054	0.137	0.054
208	1273.51	-56.370	-0.370	0.357	-60.328	-0.424	0.382	0.018
209	1278.05	5.417	-0.003	-0.034	6.166	-0.004	-0.039	-0.003
210	1279.72	-2.435	-0.001	0.015	-35.041	-0.142	0.221	0.147
211	1298.93	-5.015	-0.003	0.031	-0.587	-0.000	0.004	-0.020

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
212	1299.78	2.574	-0.001	-0.016	-16.653	-0.032	0.103	0.087
213	1303.02	29.581	-0.100	-0.183	34.367	-0.134	-0.213	-0.022
214	1320.43	0.661	-0.000	-0.004	0.679	-0.000	-0.004	-0.000
215	1321.18	-1.273	-0.000	0.008	-5.223	-0.003	0.032	0.018
216	1329.62	40.242	-0.181	-0.244	32.450	-0.117	-0.197	0.035
217	1340.08	-6.924	-0.005	0.042	-11.039	-0.013	0.066	0.019
218	1340.90	3.418	-0.001	-0.021	19.216	-0.041	-0.116	-0.071
219	1345.20	38.972	-0.167	-0.234	37.368	-0.154	-0.224	0.007
220	1345.97	4.568	-0.002	-0.027	4.705	-0.002	-0.028	-0.001
221	1347.47	-2.742	-0.001	0.016	1.066	-0.000	-0.006	-0.017
222	1348.19	1.324	-0.000	-0.008	3.020	-0.001	-0.018	-0.008
223	1363.49	-38.480	-0.161	0.228	-48.842	-0.259	0.289	0.047
224	1367.79	-5.309	-0.003	0.031	-18.381	-0.037	0.108	0.059
225	1368.57	-1.840	-0.000	0.011	-9.930	-0.011	0.059	0.037
226	1374.91	-14.725	-0.023	0.086	-16.943	-0.031	0.099	0.010
227	1377.40	-4.022	-0.002	0.024	-24.958	-0.067	0.146	0.095
228	1377.90	-0.485	-0.000	0.003	-23.369	-0.059	0.137	0.103
229	1404.14	8.226	-0.007	-0.047	13.672	-0.020	-0.079	-0.025
230	1404.52	10.981	-0.013	-0.063	6.275	-0.004	-0.036	0.021
231	1405.17	-8.263	-0.007	0.047	6.505	-0.004	-0.037	-0.067
232	1405.66	8.507	-0.008	-0.049	16.852	-0.030	-0.097	-0.038
233	1419.71	0.024	-0.000	-0.000	2.937	-0.001	-0.017	-0.013
234	1420.16	-0.581	-0.000	0.003	15.004	-0.023	-0.085	-0.070
235	1441.10	-12.158	-0.015	0.068	-14.665	-0.022	0.082	0.011
236	1448.95	0.865	-0.000	-0.005	-37.675	-0.145	0.210	0.174
237	1449.72	-0.507	-0.000	0.003	8.922	-0.008	-0.050	-0.043
238	1464.10	0.852	-0.000	-0.005	-4.946	-0.002	0.027	0.026
239	1473.54	6.710	-0.005	-0.037	12.961	-0.017	-0.071	-0.028
240	1476.37	-1.739	-0.000	0.009	9.174	-0.008	-0.050	-0.049
241	1477.19	-0.149	-0.000	0.001	3.848	-0.001	-0.021	-0.018
242	1493.29	-6.181	-0.004	0.033	-2.351	-0.001	0.013	-0.017
243	1494.02	5.273	-0.003	-0.028	0.611	-0.000	-0.003	0.021
244	1495.20	5.288	-0.003	-0.029	-1.347	-0.000	0.007	0.030
245	1511.57	4.462	-0.002	-0.024	14.710	-0.021	-0.078	-0.046
246	1516.07	0.189	-0.000	-0.001	-0.331	-0.000	0.002	0.002
247	1516.86	0.175	-0.000	-0.001	-12.473	-0.015	0.066	0.057
248	1528.07	20.724	-0.042	-0.109	33.374	-0.108	-0.176	-0.057
249	1529.43	-1.175	-0.000	0.006	-8.744	-0.007	0.046	0.034
250	1529.79	-10.476	-0.011	0.055	-1.589	-0.000	0.008	-0.040
251	1531.63	-16.344	-0.026	0.086	-23.089	-0.052	0.122	0.030
252	1532.81	19.138	-0.035	-0.101	3.173	-0.001	-0.017	0.072
253	1533.15	-7.141	-0.005	0.038	-6.688	-0.004	0.035	-0.002
254	1541.53	6.766	-0.004	-0.035	8.740	-0.007	-0.046	-0.009
255	1541.85	-6.903	-0.005	0.036	-5.653	-0.003	0.030	-0.006

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
256	1543.04	8.188	-0.006	-0.043	6.729	-0.004	-0.035	0.007
257	1643.36	0.416	-0.000	-0.002	-4.055	-0.001	0.020	0.020
258	1643.91	0.630	-0.000	-0.003	-133.887	-1.616	0.657	0.608
259	1651.45	-10.183	-0.009	0.050	-19.238	-0.033	0.094	0.041
260	1652.33	-7.883	-0.006	0.038	2.831	-0.001	-0.014	-0.048
261	1653.37	-21.320	-0.041	0.104	-13.886	-0.017	0.068	-0.034
262	1655.44	26.140	-0.061	-0.127	36.697	-0.121	-0.179	-0.048
263	1656.79	-6.671	-0.004	0.032	61.137	-0.334	-0.298	-0.306
264	1657.35	-4.116	-0.002	0.020	-4.680	-0.002	0.023	0.003
265	1666.68	8.519	-0.006	-0.041	21.636	-0.042	-0.105	-0.059
266	1667.73	-5.408	-0.003	0.026	18.437	-0.030	-0.089	-0.108
267	1668.39	-3.910	-0.001	0.019	9.209	-0.008	-0.045	-0.059
268	1677.73	-9.355	-0.008	0.045	-22.301	-0.044	0.107	0.058
269	1678.79	10.482	-0.010	-0.050	13.089	-0.015	-0.063	-0.012
270	1679.09	-6.218	-0.003	0.030	10.204	-0.009	-0.049	-0.074
271	1679.61	-21.460	-0.041	0.103	-16.454	-0.024	0.079	-0.023
272	1680.06	1.956	-0.000	-0.009	-2.821	-0.001	0.014	0.022
273	1680.87	23.545	-0.049	-0.113	22.237	-0.044	-0.107	0.006
274	1687.64	33.130	-0.096	-0.158	67.937	-0.405	-0.325	-0.157
275	1690.07	-5.708	-0.003	0.027	89.902	-0.709	-0.429	-0.432
276	1690.70	-3.776	-0.001	0.018	-11.242	-0.011	0.054	0.034
277	3206.39	-0.954	-0.000	0.002	0.425	-0.000	-0.001	-0.006
278	3206.95	-0.961	-0.000	0.002	-2.346	-0.000	0.006	0.006
279	3208.69	-1.028	-0.000	0.003	0.432	-0.000	-0.001	-0.007
280	3208.70	0.167	-0.000	-0.000	-5.913	-0.002	0.015	0.027
281	3209.44	0.034	-0.000	-0.000	-0.269	-0.000	0.001	0.001
282	3210.80	0.180	-0.000	-0.000	-0.896	-0.000	0.002	0.005
283	3218.79	0.148	-0.000	-0.000	-0.202	-0.000	0.001	0.002
284	3220.02	-0.155	-0.000	0.000	-0.313	-0.000	0.001	0.001
285	3220.27	0.163	-0.000	-0.000	2.400	-0.000	-0.006	-0.010
286	3220.51	0.529	-0.000	-0.001	1.202	-0.000	-0.003	-0.003
287	3222.62	0.565	-0.000	-0.001	-1.414	-0.000	0.004	0.009
288	3223.76	0.682	-0.000	-0.002	1.150	-0.000	-0.003	-0.002
289	3224.21	0.417	-0.000	-0.001	-2.375	-0.000	0.006	0.013
290	3225.14	0.142	-0.000	-0.000	-1.036	-0.000	0.003	0.005
291	3225.48	0.347	-0.000	-0.001	1.707	-0.000	-0.004	-0.006
292	3227.06	0.176	-0.000	-0.000	3.486	-0.001	-0.009	-0.015
293	3227.43	-0.085	-0.000	0.000	0.125	-0.000	-0.000	-0.001
294	3229.46	-0.156	-0.000	0.000	-1.358	-0.000	0.003	0.005
295	3229.90	-0.014	-0.000	0.000	-0.361	-0.000	0.001	0.002
296	3230.22	0.035	-0.000	-0.000	-10.169	-0.005	0.025	0.046
297	3232.20	-2.006	-0.000	0.005	-5.782	-0.002	0.014	0.017
298	3232.93	1.315	-0.000	-0.003	3.779	-0.001	-0.009	-0.011
299	3233.32	1.729	-0.000	-0.004	-1.531	-0.000	0.004	0.015

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α	Freq. /cm ⁻¹	κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	ξ
300	3235.66	-1.531	-0.000	0.004	-3.589	-0.001	0.009	0.009
301	3236.56	-0.084	-0.000	0.000	-0.161	-0.000	0.000	0.000
302	3237.23	0.279	-0.000	-0.001	-2.172	-0.000	0.005	0.011
303	3237.54	-1.263	-0.000	0.003	-12.015	-0.007	0.030	0.049
304	3237.60	0.306	-0.000	-0.001	5.607	-0.001	-0.014	-0.024
305	3238.62	-0.939	-0.000	0.002	-7.854	-0.003	0.020	0.031
306	3238.77	1.567	-0.000	-0.004	1.570	-0.000	-0.004	-0.000
307	3266.38	1.860	-0.000	-0.005	10.312	-0.005	-0.025	-0.038
308	3271.98	-2.267	-0.000	0.006	-3.956	-0.001	0.010	0.008
309	3272.58	2.883	-0.000	-0.007	2.718	-0.000	-0.007	0.001

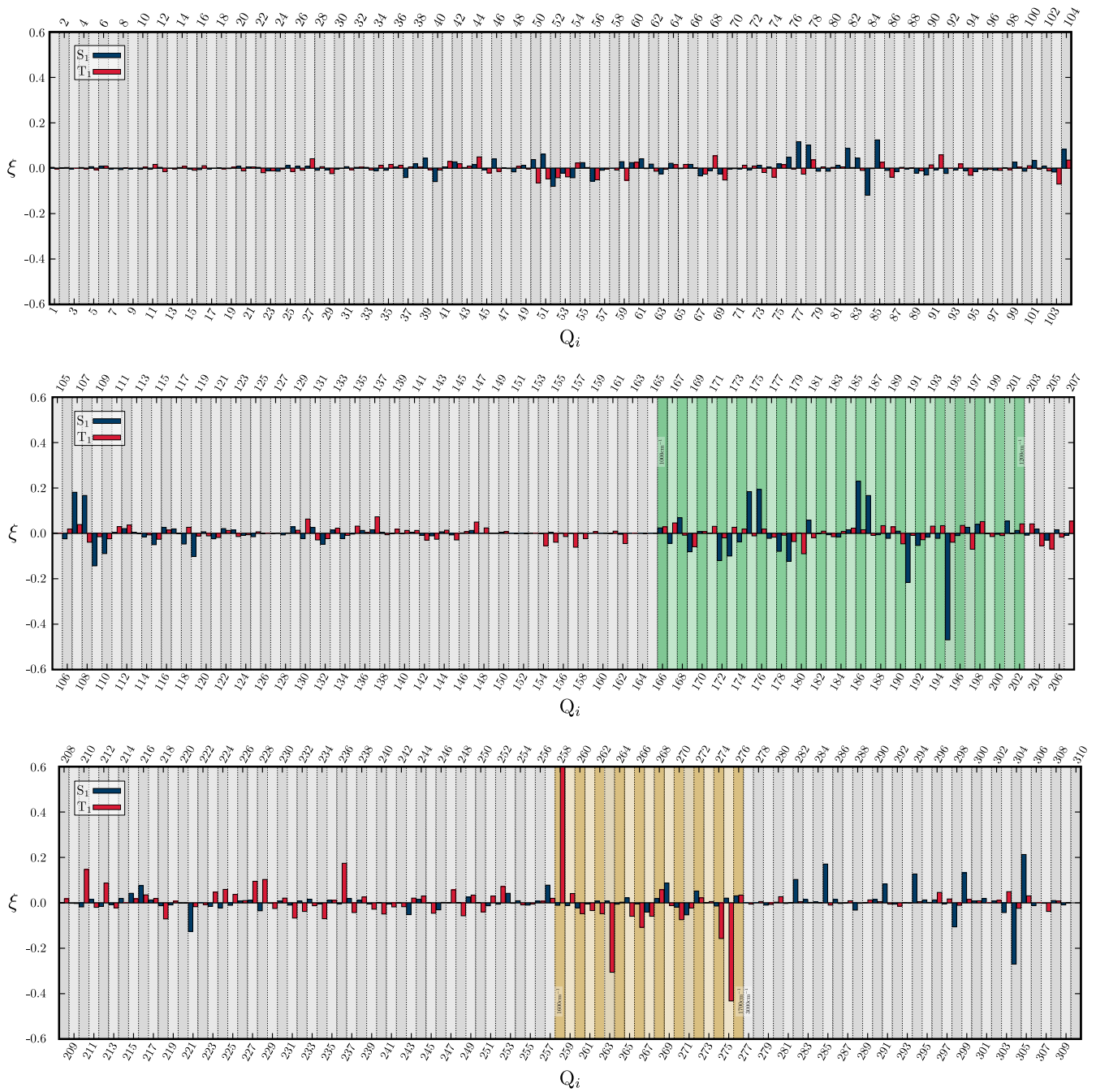


Figure S4: RSMA for all the normal modes of TAT-3DBTO₂ for S_1 and T_1 as a function of their index. The range of frequencies mentioned in the main text are emphasized in colours.

S3 Maleimide

S3-1 Geometry

Table S17: Cartesian coordinates different minima of Maleimide.

GS				S1				S2			
At	x	y	z	At	x	y	z	At	x	y	z
C	1.0895	-1.9669	-0.0163	C	1.1089	-1.9661	-0.0175	C	1.1163	-1.9345	-0.0166
C	-0.2581	-1.9317	0.0190	C	-0.2773	-1.9300	0.0198	C	-0.2831	-1.8979	0.0202
N	0.4744	0.2624	0.0335	N	0.4734	0.2303	0.0323	N	0.4742	0.2544	0.0336
H	1.7572	-2.8303	-0.0466	H	1.7681	-2.8330	-0.0447	H	1.7646	-2.8106	-0.0466
C	1.6147	-0.5474	-0.0086	C	1.6093	-0.6053	-0.0120	C	1.5932	-0.5687	-0.0082
O	-1.8355	-0.0527	0.0883	O	-1.8158	0.0211	0.0901	O	-1.8707	-0.0542	0.0892
C	-0.7073	-0.4867	0.0527	C	-0.7049	-0.5450	0.0506	C	-0.6869	-0.5091	0.0517
O	2.7643	-0.1729	-0.0324	O	2.7486	-0.0980	-0.0325	O	2.7994	-0.1762	-0.0336
H	-0.9706	-2.7591	0.0249	H	-0.9813	-2.7614	0.0253	H	-0.9769	-2.7390	0.0253
H	0.5012	1.2755	0.0482	H	0.5002	1.2442	0.0506	H	0.5010	1.2652	0.0478

Table S18: Cartesian coordinates different minima of Maleimide.

S3				S4			
At	x	y	z	At	x	y	z
C	1.1255	-1.9283	-0.0168	C	1.1334	-1.9550	-0.0174
C	-0.2920	-1.8913	0.0206	C	-0.3012	-1.9175	0.0204
N	0.4739	0.2431	0.0332	N	0.4736	0.2321	0.0330
H	1.7384	-2.8306	-0.0466	H	1.7890	-2.8265	-0.0475
C	1.7047	-0.6229	-0.0115	C	1.6146	-0.5770	-0.0090
O	-1.8771	0.0143	0.0905	O	-1.8640	-0.0271	0.0895
C	-0.8012	-0.5574	0.0532	C	-0.7088	-0.5163	0.0521
O	2.8094	-0.1082	-0.0327	O	2.7941	-0.1489	-0.0329
H	-0.9518	-2.7603	0.0249	H	-1.0022	-2.7536	0.0258
H	0.5011	1.2710	0.0481	H	0.5005	1.2466	0.0478

S3-2 Electronic Structure

State	Nature	ΔE /eV
S ₀	GS	0.00
S ₁	$n_2 \rightarrow \pi^*$	4.07
S ₂	$n_1 \rightarrow \pi^*$	4.84
S ₃	$\pi_2 \rightarrow \pi^*$	5.23
S ₄	$\pi_1 \rightarrow \pi^*$	6.70

Table S19: Electronic structure at the ground state optimised geometry. GS stands for the ground state electronic structure: $(\pi_1)^2(\pi_2)^2(n_1)^2(n_2)^2(\pi^*)^0$. Molecular orbitals are shown in figure S5.

$S_{n_2}^{\text{MIN}}$			$S_{n_1}^{\text{MIN}}$		
State	Nature	$\Delta E / \text{eV}$	State	Nature	$\Delta E / \text{eV}$
S ₀	GS	0.27	S ₀	GS	0.37
S ₁	$n_2 \rightarrow \pi^*$	3.76	S ₁	$n_2 \rightarrow \pi^*$	3.89
S ₂	$n_1 \rightarrow \pi^*$	4.55	S ₂	$n_1 \rightarrow \pi^*$	4.44
S ₃	$\pi_2 \rightarrow \pi^*$	4.79	S ₃	$\pi_2 \rightarrow \pi^*$	5.03
S ₄	$\pi_1 \rightarrow \pi^*$	6.42	S ₄	$\pi_1 \rightarrow \pi^*$	6.36

$S_{\pi_2}^{\text{MIN}}$			$S_{\pi_1}^{\text{MIN}}$		
State	Nature	$\Delta E / \text{eV}$	State	Nature	$\Delta E / \text{eV}$
S ₀	GS	0.74	S ₀	GS	0.36
S ₁	$n_2 \rightarrow \pi^*$	3.95	S ₁	$n_2 \rightarrow \pi^*$	3.88
S ₂	$\pi_2 \rightarrow \pi^*$	4.45	S ₂	$n_1 \rightarrow \pi^*$	4.50
S ₃	$n_1 \rightarrow \pi^*$	4.93	S ₃	$\pi_1 \rightarrow \pi^*$	4.46
S ₄	$\pi_1 \rightarrow \pi^*$	6.65	S ₄	$\pi_2 \rightarrow \pi^*$	6.30

Table S20: Electronic structure at the excited states optimised geometries. GS stands for the ground state electronic structure: $(\pi_1)^2(\pi_2)^2(n_1)^2(n_2)^2(\pi^*)^0$. Molecular orbitals are shown in figure S5.

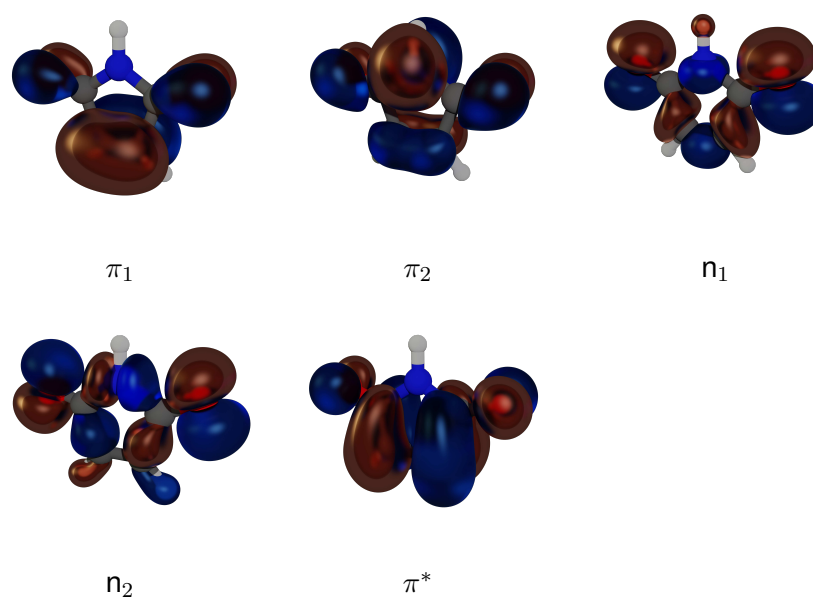


Figure S5: Orbitals involved in the four lowest excited singlet states of **Maleimide**.

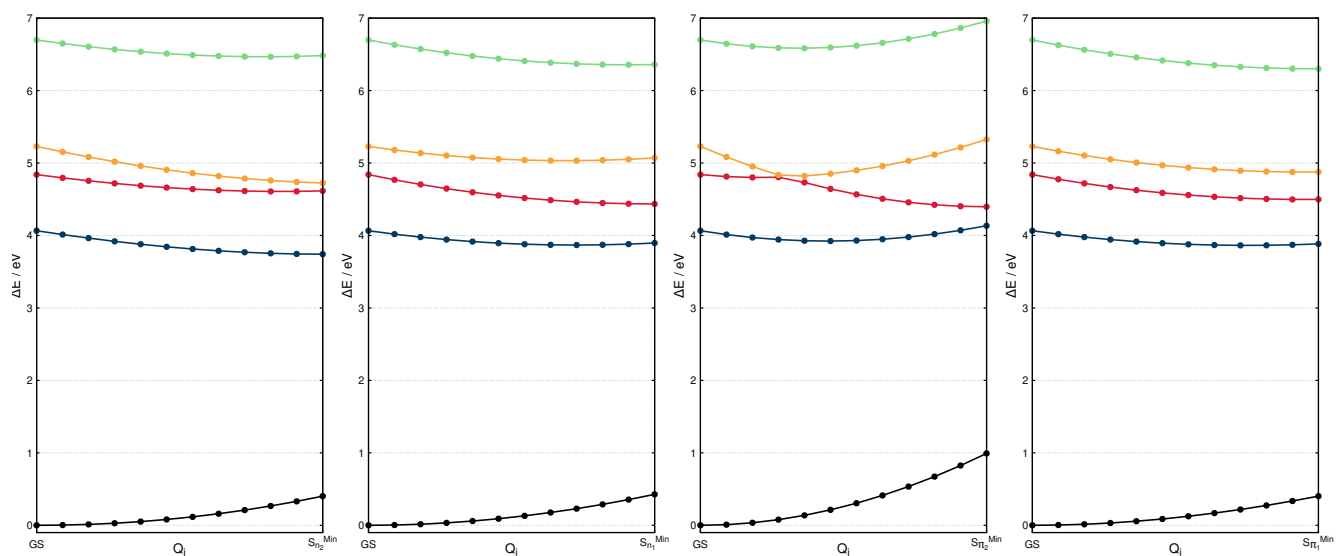


Figure S6: EOM-CCSD Path between Franck-Condon and the minimum of each of the four lowest excited states.

S3-3 LVC parameters

Table S21: LVC Analysis for S1 of Maleimide.

α	Freq. /cm ⁻¹	κ_{α}			κ_{α}^*			ξ
		κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	
1	112.79	0.014	0.000	-0.001	0.067	0.000	-0.005	-0.001
2	288.75	0.066	0.000	-0.002	-0.076	0.000	0.002	0.002
3	396.51	44.668	-0.746	-0.909	76.328	-2.178	-1.553	-0.362
4	498.39	-0.009	0.000	0.000	0.419	0.000	-0.007	-0.005
5	540.97	-0.006	0.000	0.000	0.074	0.000	-0.001	-0.001
6	638.81	-0.153	0.000	0.002	2.283	-0.001	-0.029	-0.028
7	641.93	29.268	-0.198	-0.368	15.163	-0.053	-0.191	0.161
8	679.27	-0.018	0.000	0.000	0.103	0.000	-0.001	-0.001
9	778.30	0.181	0.000	-0.002	-0.271	0.000	0.003	0.005
10	848.65	-0.085	0.000	0.001	1.597	0.000	-0.015	-0.019
11	922.62	-68.779	-0.760	0.601	-72.741	-0.850	0.636	0.045
12	931.40	0.002	0.000	0.000	0.077	0.000	-0.001	-0.001
13	958.55	-0.052	0.000	0.000	-1.609	0.000	0.014	0.018
14	1070.20	-46.143	-0.295	0.348	-33.550	-0.156	0.253	-0.144
15	1168.61	-0.011	0.000	0.000	-0.190	0.000	0.001	0.002
16	1344.99	0.023	0.000	0.000	0.177	0.000	-0.001	-0.002
17	1367.17	-0.078	0.000	0.000	-0.084	0.000	0.000	0.000
18	1387.29	171.623	-3.147	-0.998	243.160	-6.316	-1.414	-0.817
19	1663.40	-49.647	-0.220	0.241	-81.986	-0.599	0.398	0.369
20	1870.47	0.012	0.000	0.000	-0.458	0.000	0.002	0.005
21	1907.74	-228.863	-4.069	0.968	-219.644	-3.748	0.929	-0.105
22	3265.71	0.008	0.000	0.000	-0.067	0.000	0.000	0.001
23	3288.38	11.883	-0.006	-0.029	13.503	-0.008	-0.033	-0.018
24	3692.77	-5.709	-0.001	0.012	-0.222	0.000	0.000	-0.063

Table S22: LVC Analysis for S2 of Maleimide.

α	Freq. /cm ⁻¹	κ_{α}			κ_{α}^*			ξ
		κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	
1	112.79	-0.016	0.000	0.001	-0.032	0.000	0.002	0.000
2	288.75	0.049	0.000	-0.001	-0.022	0.000	0.001	0.001
3	396.51	-22.843	-0.195	0.465	-17.500	-0.114	0.356	-0.102
4	498.39	-0.032	0.000	0.001	-0.020	0.000	0.000	0.000
5	540.97	-0.007	0.000	0.000	-0.010	0.000	0.000	0.000
6	638.81	-0.160	0.000	0.002	-0.086	0.000	0.001	-0.001
7	641.93	33.574	-0.260	-0.422	35.347	-0.288	-0.444	-0.034
8	679.27	-0.014	0.000	0.000	-0.012	0.000	0.000	0.000
9	778.30	0.201	0.000	-0.002	0.286	0.000	-0.003	-0.002
10	848.65	-0.077	0.000	0.001	-0.077	0.000	0.001	0.000
11	922.62	-89.165	-1.277	0.779	-74.511	-0.892	0.651	-0.279

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α	Freq. /cm ⁻¹	κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	ξ
12	931.40	0.005	0.000	0.000	0.004	0.000	0.000	0.000
13	958.55	-0.027	0.000	0.000	-0.028	0.000	0.000	0.000
14	1070.20	-37.682	-0.197	0.284	-42.193	-0.247	0.318	0.086
15	1168.61	-0.009	0.000	0.000	-0.012	0.000	0.000	0.000
16	1344.99	0.027	0.000	0.000	0.020	0.000	0.000	0.000
17	1367.17	-0.025	0.000	0.000	-0.027	0.000	0.000	0.000
18	1387.29	69.308	-0.513	-0.403	72.635	-0.564	-0.422	-0.063
19	1663.40	-130.588	-1.519	0.633	-136.437	-1.659	0.662	0.111
20	1870.47	0.021	0.000	0.000	0.035	0.000	0.000	0.000
21	1907.74	-359.289	-10.028	1.519	-408.708	-12.977	1.728	0.941
22	3265.71	0.004	0.000	0.000	0.002	0.000	0.000	0.000
23	3288.38	13.468	-0.008	-0.033	15.534	-0.011	-0.038	-0.039
24	3692.77	7.223	-0.002	-0.016	5.819	-0.001	-0.013	0.027

Table S23: LVC Analysis for S3 of Maleimide.

α	Freq. /cm ⁻¹	κ_α			κ_α^*			ξ
		κ_α / meV	dE / meV	dQ	κ_α / meV	dE / meV	dQ	
1	112.79	0.115	0.000	-0.008	0.007	0.000	0.000	0.001
2	288.75	0.035	0.000	-0.001	-0.031	0.000	0.001	0.000
3	396.51	52.225	-1.019	-1.062	37.456	-0.524	-0.762	0.070
4	498.39	0.164	0.000	-0.003	0.003	0.000	0.000	0.001
5	540.97	-0.007	0.000	0.000	-0.009	0.000	0.000	0.000
6	638.81	-0.221	0.000	0.003	-0.019	0.000	0.000	-0.001
7	641.93	162.755	-6.115	-2.045	191.876	-8.500	-2.411	-0.138
8	679.27	-0.030	0.000	0.000	-0.032	0.000	0.000	0.000
9	778.30	0.169	0.000	-0.002	1.539	0.000	-0.016	-0.007
10	848.65	-0.096	0.000	0.001	0.052	0.000	0.000	-0.001
11	922.62	-127.267	-2.602	1.113	-91.200	-1.336	0.797	-0.171
12	931.40	0.005	0.000	0.000	-0.004	0.000	0.000	0.000
13	958.55	-0.034	0.000	0.000	0.187	0.000	-0.002	-0.001
14	1070.20	-47.579	-0.313	0.359	-31.831	-0.140	0.240	-0.075
15	1168.61	-0.007	0.000	0.000	-0.010	0.000	0.000	0.000
16	1344.99	0.036	0.000	0.000	0.049	0.000	0.000	0.000
17	1367.17	-0.201	0.000	0.001	-0.281	0.000	0.002	0.000
18	1387.29	351.904	-13.229	-2.046	486.258	-25.259	-2.827	-0.638
19	1663.40	-169.241	-2.552	0.821	-196.667	-3.446	0.954	0.130
20	1870.47	0.000	0.000	0.000	-0.067	0.000	0.000	0.000
21	1907.74	-99.559	-0.770	0.421	51.194	-0.204	-0.216	-0.716
22	3265.71	0.005	0.000	0.000	0.020	0.000	0.000	0.000
23	3288.38	13.292	-0.008	-0.033	28.114	-0.036	-0.069	-0.070
24	3692.77	-43.547	-0.076	0.095	-41.051	-0.068	0.090	-0.012

Table S24: LVC Analysis for S4 of Maleimide.

α	Freq. /cm ⁻¹	κ_{α}			κ_{α}^*			ξ
		κ_{α} / meV	dE / meV	dQ	κ_{α} / meV	dE / meV	dQ	
1	112.79	0.035	0.000	-0.003	0.007	0.000	0.000	0.001
2	288.75	0.021	0.000	-0.001	0.002	0.000	0.000	0.001
3	396.51	7.174	-0.019	-0.146	16.914	-0.107	-0.344	-0.267
4	498.39	0.022	0.000	0.000	0.029	0.000	0.000	0.000
5	540.97	-0.005	0.000	0.000	-0.008	0.000	0.000	0.000
6	638.81	-0.197	0.000	0.002	-0.071	0.000	0.001	-0.003
7	641.93	69.043	-1.101	-0.867	66.421	-1.019	-0.835	0.072
8	679.27	-0.018	0.000	0.000	-0.017	0.000	0.000	0.000
9	778.30	0.124	0.000	-0.001	0.364	0.000	-0.004	-0.007
10	848.65	-0.096	0.000	0.001	-0.040	0.000	0.000	-0.002
11	922.62	-64.619	-0.671	0.565	-53.773	-0.464	0.470	-0.297
12	931.40	0.000	0.000	0.000	0.002	0.000	0.000	0.000
13	958.55	-0.171	0.000	0.001	-0.041	0.000	0.000	-0.004
14	1070.20	-78.423	-0.852	0.591	-85.513	-1.013	0.644	0.194
15	1168.61	-0.001	0.000	0.000	-0.009	0.000	0.000	0.000
16	1344.99	0.015	0.000	0.000	0.020	0.000	0.000	0.000
17	1367.17	-0.042	0.000	0.000	-0.044	0.000	0.000	0.000
18	1387.29	91.931	-0.903	-0.534	96.808	-1.001	-0.563	-0.134
19	1663.40	-229.182	-4.680	1.111	-242.490	-5.239	1.176	0.365
20	1870.47	0.035	0.000	0.000	0.031	0.000	0.000	0.000
21	1907.74	-278.474	-6.024	1.177	-307.323	-7.337	1.299	0.790
22	3265.71	0.008	0.000	0.000	0.007	0.000	0.000	0.000
23	3288.38	27.002	-0.033	-0.066	31.775	-0.046	-0.078	-0.131
24	3692.77	-10.163	-0.004	0.022	-7.659	-0.002	0.017	-0.069

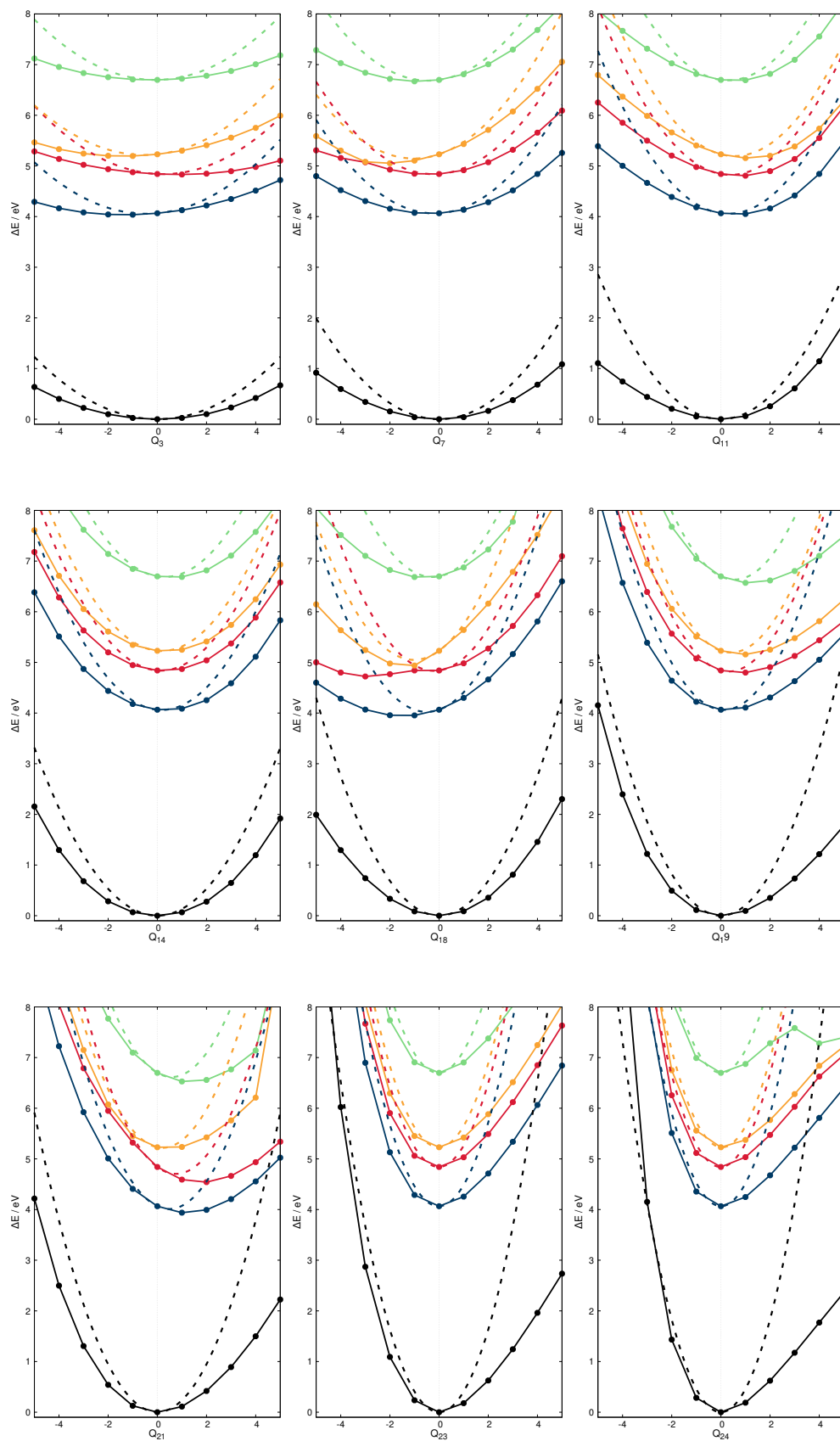


Figure S7: Comparison between the computed adiabatic (full lines) and LVC diabatic (dashed lines) PES along a_1 normal modes.

S3-4 Excited-states Dynamics

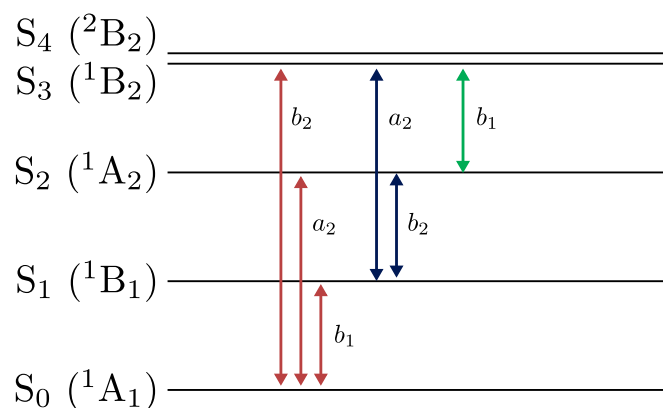


Figure S8: Schematic representation of the coupling selection rules at the C_{2v} ground state minimum of **Maleimide**. Arrows represent possible vibronic coupling and lowercase irreps correspond to the irreps of the normal modes that enable the coupling.

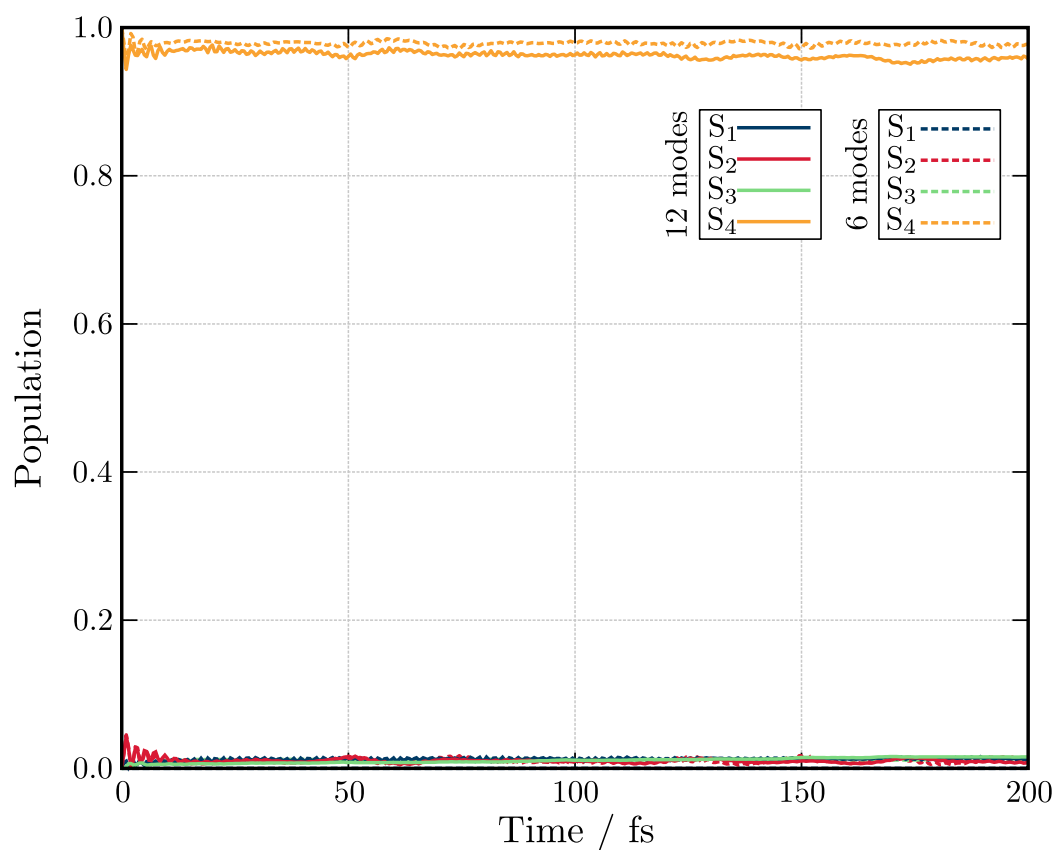


Figure S9: Population kinetics of the lowest excited singlet states of **Maleimide** using a model Hamiltonian along 12 (full lines) and 6 (dashed lines) normal modes. The initial wavepacket is position at Q_0 in S_4 .

S3-4.1 6-modes Hamiltonian parameters

Q_α	ω_α	$K_\alpha^{S_1}$	$K_\alpha^{S_2}$	$K_\alpha^{S_3}$	$K_\alpha^{S_4}$
7 (a ₁)	641.9	0.029	0.034	0.163	0.069
11 (a ₁)	922.6	-0.069	-0.089	-0.127	-0.065
18 (a ₁)	1387.3	0.172	0.069	0.352	0.092
19 (a ₁)	1663.4	-0.050	-0.131	-0.169	-0.229

Table S25: Intrastate coupling parameters for the 6-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.

Q_α	ω_α	$\lambda_\alpha^{S_0/S_1}$	$\lambda_\alpha^{S_2/S_3}$	$\lambda_\alpha^{S_2/S_4}$
1 (b ₁)	112.8	-0.167	0.117	0.216
4 (b ₁)	498.4	-0.151	0.092	0.208

Table S26: Intrastate coupling parameters for the 6-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.

Modes	Primitive basis	SPF basis
Initial wavepacket in $1B_2$		
(m7 m18)	(21 31)	(2 2 35 32 5)
(m1 m11)	(16 16)	(2 2 35 32 5)
(m4 m19)	(16 16)	(2 2 18 18 4)
Initial wavepacket in $2B_2$		
(m7 m18)	(21 31)	(2 2 2 12 7)
(m1 m11)	(16 16)	(2 2 2 11 7)
(m4 m19)	(16 16)	(2 2 2 11 7)

Table S27: Computational details of the 6-modes MCTDH propagations with wavepackets with an initial wavepacket in $1B_2$ or $2B_2$. The number of primitive basis and Single Particule Functions are given for each set of combined modes.

S3-4.2 12-modes Hamiltonian parameters

Q_α	ω_α	$\kappa_\alpha^{S_1}$	$\kappa_\alpha^{S_2}$	$\kappa_\alpha^{S_3}$	$\kappa_\alpha^{S_4}$
3 (a ₁)	396.5	0.045	-0.023	0.052	0.007
7 (a ₁)	641.9	0.029	0.034	0.163	0.069
11 (a ₁)	922.6	-0.069	-0.089	-0.127	-0.065
18 (a ₁)	1387.3	0.172	0.069	0.352	0.092
19 (a ₁)	1663.4	-0.050	-0.131	-0.169	-0.229
21 (a ₁)	1907.7	-0.229	-0.359	-0.100	-0.278

Table S28: Intrastate coupling parameters for the 12-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.

Q_α	ω_α	$\lambda_\alpha^{S_0/S_1}$	$\lambda_\alpha^{S_0/S_2}$	$\lambda_\alpha^{S_0/S_3}$	$\lambda_\alpha^{S_0/S_4}$	$\lambda_\alpha^{S_1/S_2}$
1 (b ₁)	112.8	-0.167	0.000	0.000	0.000	0.000
2 (a ₂)	288.9	0.000	-0.217	0.000	0.000	0.000
4 (b ₁)	498.4	-0.151	0.000	0.000	0.000	0.000
9 (a ₂)	778.6	0.000	-0.221	0.000	0.000	0.000
13 (a ₂)	958.7	0.000	-0.186	0.000	0.000	0.000
20 (b ₂)	1871.1	0.000	0.000	-0.332	-0.375	0.128

Q_α	ω_α	$\lambda_\alpha^{S_1/S_3}$	$\lambda_\alpha^{S_1/S_4}$	$\lambda_\alpha^{S_2/S_3}$	$\lambda_\alpha^{S_2/S_4}$
1 (b ₁)	112.8	0.000	0.000	0.117	0.216
2 (a ₂)	288.9	-0.038	-0.049	0.000	0.000
4 (b ₁)	498.4	0.000	0.000	0.092	0.208
9 (a ₂)	778.6	0.019	-0.071	0.000	0.000
13 (a ₂)	958.7	0.119	0.180	0.000	0.000
20 (b ₂)	1871.1	0.000	0.000	0.000	0.000

Table S29: Intrastate coupling parameters for the 12-modes model Hamiltonian. Frequencies are given in cm^{-1} and couplings in eV.

Modes	Primitive basis	SPF basis
Initial wavepacket in 1B_2		
(m3 m4 m7 m11)	(21 16 21 16)	(2 22 19 22 5)
(m1 m9 m13 m18)	(16 21 11 31)	(2 26 22 22 7)
(m2 m19 m20 m21)	(11 16 11 16)	(2 20 15 15 4)
Initial wavepacket in 2B_2		
(m3 m4 m7 m11)	(21 16 21 16)	(2 6 4 13 5)
(m1 m9 m13 m18)	(16 21 11 31)	(2 9 4 14 9)
(m2 m19 m20 m21)	(11 16 11 16)	(2 9 3 13 8)

Table S30: Computational details of the 12-modes MCTDH propagations with wavepackets with an initial wavepacket in 1B_2 or 2B_2 . The number of primitive basis and Single Particle Functions are given for each set of combined modes.