Pressure induced emission enhancement (PIEE) in solid-state 2,3,4,5-Tetraphenylthiophene: a QM/MM study

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Table S 1 Geometry parameters of S_0 states for TPT in solid phase. Dihedral angles (θ_1, θ_2, θ_3, and θ_4) are shown in Fig. 1

Pressure/GPa	**θ_1**	**θ_2**	**θ_3**	**θ_4**
0	146.07	113.19	66.84	38.21
0.93	146.56	114.24	66.71	37.72
2.12	146.91	115.29	66.07	36.23
3.41	146.81	116.29	66.49	35.14
5.06	146.71	117.93	66.56	32.23
6.63	146.73	119.50	66.74	30.26
7.46	145.89	119.65	67.16	28.87
8.5	146.81	121.30	67.17	28.04

Table S 2 Geometry parameters of S_1 states for TPT in solid phase. Dihedral angles (θ_1, θ_2, θ_3, and θ_4) are shown in Fig. 1.

Pressure/GPa	**θ_1**	**θ_2**	**θ_3**	**θ_4**
0	158.93	122.18	58.30	24.08
0.93	158.44	123.06	58.53	24.76
2.12	158.53	123.81	58.05	23.82
3.41	158.62	124.64	58.55	22.84
5.06	158.97	125.61	58.79	20.39
6.63	159.56	126.88	58.89	18.49
7.46	159.72	126.79	59.08	17.19
8.5	161.72	128.37	58.85	16.07

Table S 3 Energy levels of HOMO, LUMO, the corresponding energy gaps (ΔE_{gap}) and S_1 energy level of TPT in solid state at different pressures.

Pressure/GPa	**HOMO/eV**	**LUMO/eV**	ΔE_{gap} **/eV**	**S_1/eV**
0	-5.41289	-1.23458	4.17831	3.0649
0.93	-5.38241	-1.23023	4.15218	3.0572
2.12	-5.36282	-1.22995	4.13286	3.0516
3.41	-5.34214	-1.22669	4.11545	3.0456
5.06	-5.29316	-1.22832	4.06484	2.9962
6.63	-5.26622	-1.23376	4.03245	2.9667
7.46	-5.22976	-1.22125	4.00851	2.9308
8.50	-5.21316	-1.22533	3.98783	2.8977

Table S 4 The calculated k_r, k_{ic} and Φ_F at different pressure.

Pressure/GPa	**0**	**0.93**	**2.12**	**3.41**	**5.06**	**6.63**	**7.46**	**8.50**
k_r**(10^8 s^{-1})**	2.384	2.348	2.350	2.386	2.260	2.169	2.111	2.100
k_{ic}**(10^8 s^{-1})**	5.803	2.242	2.060	2.488	2.979	3.208	5.224	7.884
Φ_F**(%)**	29.11	51.16	53.29	48.96	43.14	40.34	28.78	21.64

Table S 5 Adiabatic excitation energy (v_{fi}) and the oscillator strength (f) at different pressure.

Pressure/GPa	**0**	**0.93**	**2.12**	**3.41**	**5.06**	**6.63**	**7.46**	**8.50**
v_{fi}**/a.u.**	0.1260	0.1262	0.1262	0.1261	0.1252	0.1243	0.1237	0.1234
f	0.5887	0.5882	0.5815	0.5754	0.5489	0.5332	0.5100	0.5025

Table S 6 Contributions of low-frequency modes (λ_{LF}) and high frequency modes (λ_{HF}) to the total λ_e for TPT in solid state at different pressures.

Pressure/GPa	**0**	**0.93**	**2.12**	**3.41**	**5.06**	**6.63**	**7.46**	**8.50**
λ_{LF}/λ_e	0.50	0.51	0.52	0.54	0.60	0.63	0.69	0.72
λ_{HF}/λ_e	0.50	0.49	0.48	0.47	0.48	0.48	0.46	0.44

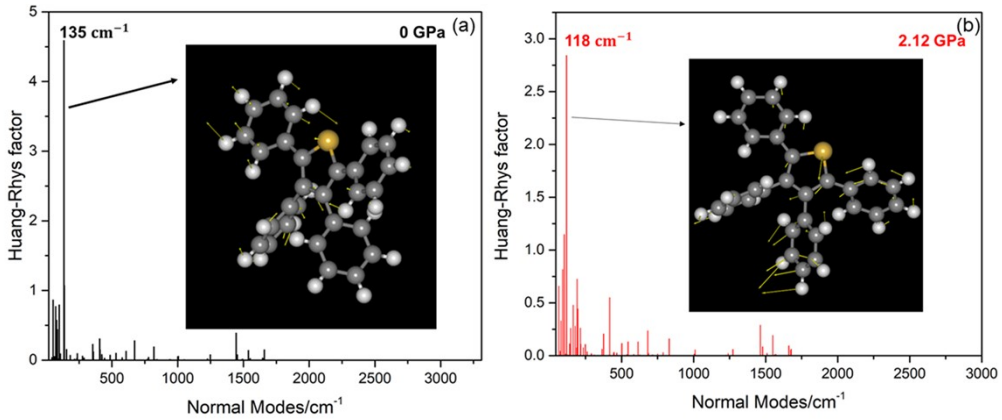

Fig. S 1 Calculated HR factors versus the normal mode frequencies at 0 GPa (a) and 2.12 GPa(b). Representative vibration modes are shown in the insets.

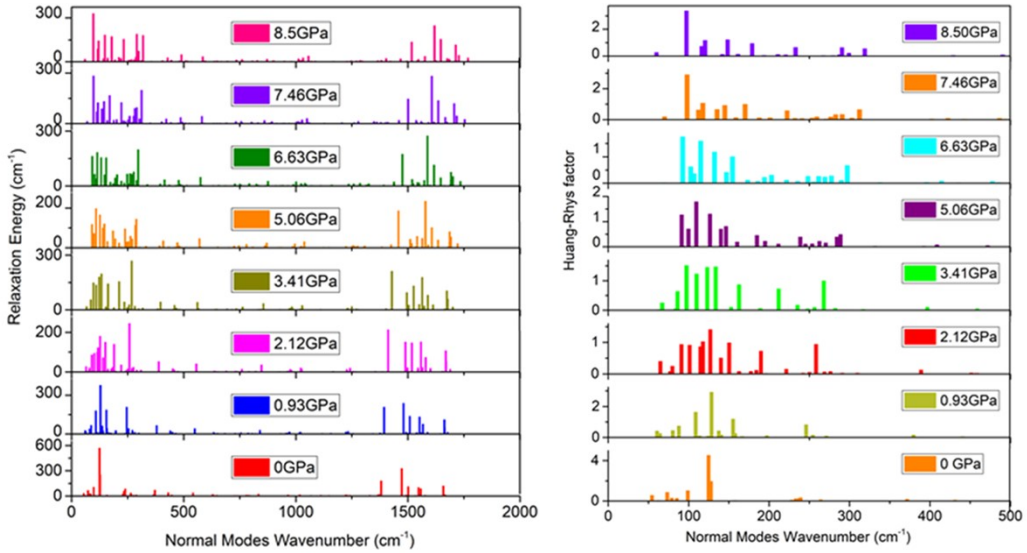

Fig. S 2 Calculated Huang-Rhys factor HR_k (right) and reorganization energies $\lambda_{j,g}$ (left) versus the normal mode frequencies for TPT molecules in solid state at different pressure.

Table S7 Reorganization energy λ_e contributions (meV) from the bond lengths, bond angles, and dihedral angles for TPT in the solid phase at different pressure.

Pressure/GPa	Bond length	Bond angle	Dihedral angle	Total
0	235.03	7.56	150.89	384.48
0.93	220.92	2.81	150.18	373.91
2.12	215.26	2.55	156.00	373.81
3.41	211.07	7.70	162.34	381.11
5.06	203.50	18.10	157.04	378.64
6.63	199.60	23.56	159.99	383.15
7.46	195.63	36.11	176.47	408.21
8.50	194.53	50.30	205.92	450.75