Exploring the Intriguing Terpyridine World: Synthesis, Structural, Optical, and Theoretical Insights Into Bis(p-phenyl-2,2':6',2'')terpyridine

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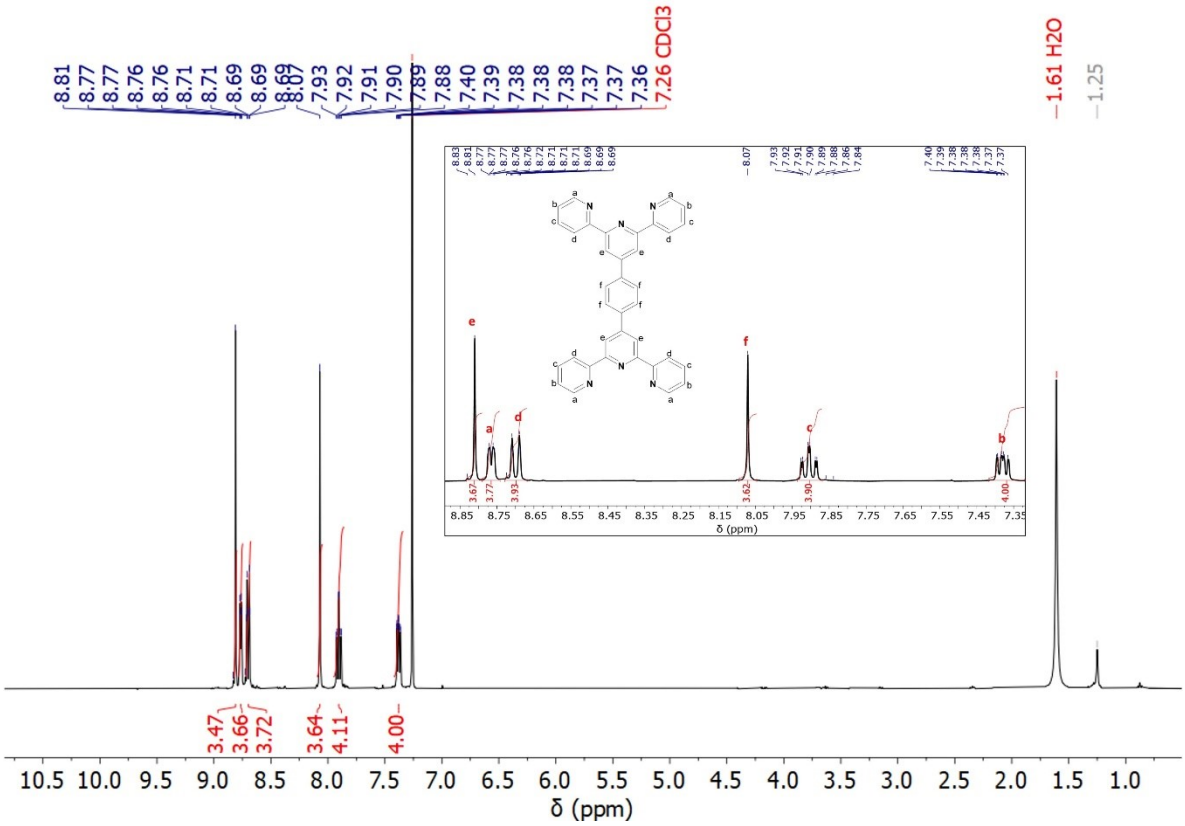
Supp. Inf. S1. 1H-NMR spectrum of **Bis-TPY-Bulk**

Supp. Inf. S2. FT-IR spectra, table of bands assignement and analysis of **Bis-TPY-Bulk** and **Bis-TPY-Crys**

Supp. Inf. S3. HOMO and LUMO orbitals of *anti-anti*, *syn-syn-A*, and *syn-syn-B* conformers

Supp. Inf. S4. Experimental and calculated UV-Vis spectra of **Bis-TPY-Bulk** and **Bis-TPY-Crys** in DMSO

Supp. Inf. S1. 1H-NMR spectrum of **Bis-TPY-Bulk**



Supp. Inf. S2. FT-IR spectra, table of bands assignement and analysis of **Bis-TPY-Bulk** and **Bis-TPY-Crys**

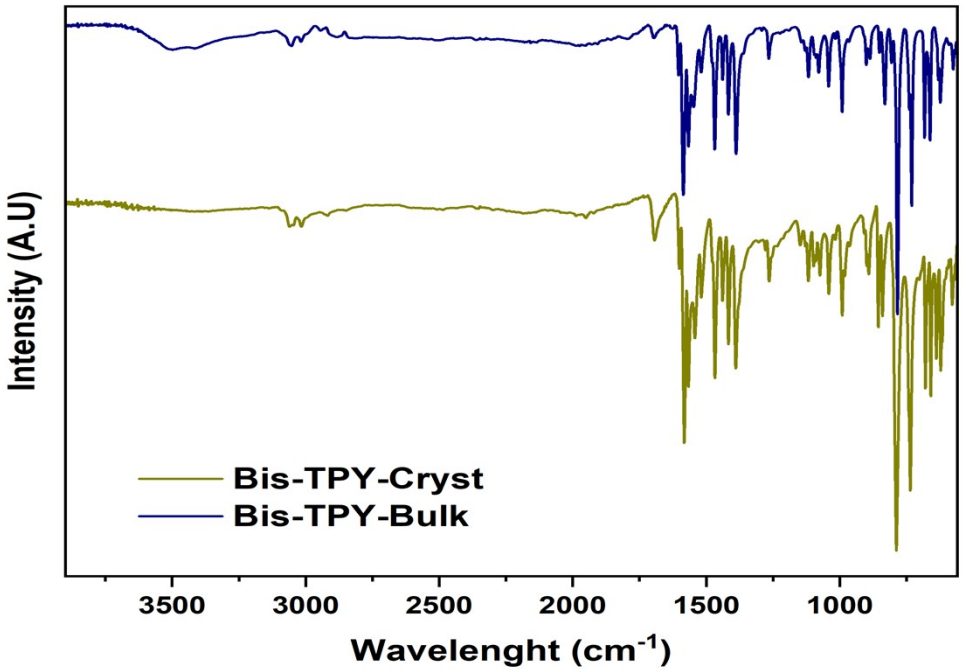
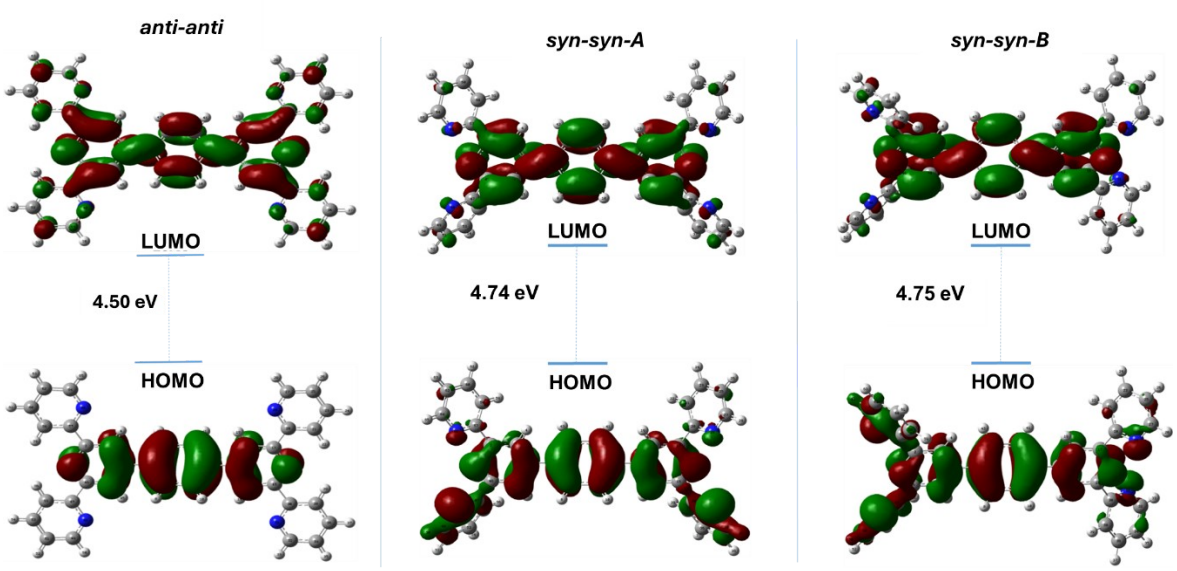


Table 1. Bands assignment for **Bis-TPY-Bulk** and **Bis-TPY-Crys.**

Band assignment	**Bis-TPY-Bulk wavenumber (cm^{-1})**	**Bis-TPY-Crys wavenumber (cm^{-1})**
ν(O-H) stretching	3510-3410	Not observed
ν(C–H) aromatic	3052, 3016, 2944	3061, 3043, 3016, 2918
ν(C=N) + ν(C=C) stretching	1603, 1585	1600, 1582
ν(C=C) internal vibration	1567, 1547	1567, 1542
δ(C–H) + ν(C=C) deformation	1468, 1438	1466, 1439
δ(C–H) deformation	1388	1389
ν(C–N) stretching	1265	1264
γ(C–H) out-plane	783	788

FT-IR analysis revealed slight differences in the spectra of the two solids. In Supp. Inf. S2, the band assignment and FT-IR spectra for both compounds are present. **Bis-TPY-Bulk** exhibits a broad band at 3510-3410 cm^{-1} that is attributed to the O-H vibration of residual adsorbed water in the sample. This band is not present in **Bis-TPY-Crys**. The C-H bands around 3000 cm^{-1} show a slight shift towards higher wavenumbers due to the presence of hydrogen bonds in **Bis-TPY-Crys**. Intramolecular hydrogen bonds polarize the C=C bond, as evidenced by an increased intensity of the bands around 1600-1580 cm^{-1} (see Supp. Inf. S2). This evidence indicates that the molecule has two different structural arrangements, suggesting the possibility of isomerization. The weak band observed around 1690 cm^{-1} is attributed to the δ(H–O–H) bending vibration of adsorbed water, which is consistent with the presence of a broad band in the 3200–3600 cm^{-1} region corresponding to the stretching vibration of the O–H bond in water.

Supp. Inf. S3. HOMO and LUMO orbitals of *anti-anti*, *syn-syn-A*, and *syn-syn-B* conformers



Supp. Inf. S4. Experimental and calculated UV-Vis spectra of **Bis-TPY-Bulk** and **Bis-TPY-Crys** in DMSO