

CrystEngComm - Supporting Information for

Acidochromic Spiropyran-Merocyanine stabilization in the solid-state

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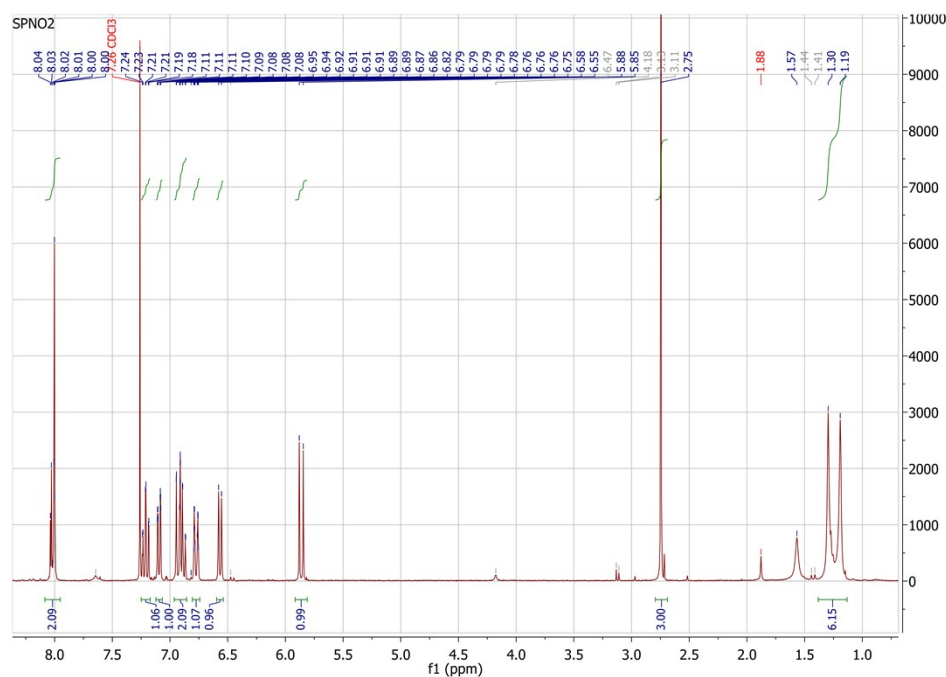


Figure A 1: ^1H -NMR of **SPNO2**. Traces of H_2O (δ (ppm): 1.88) present.

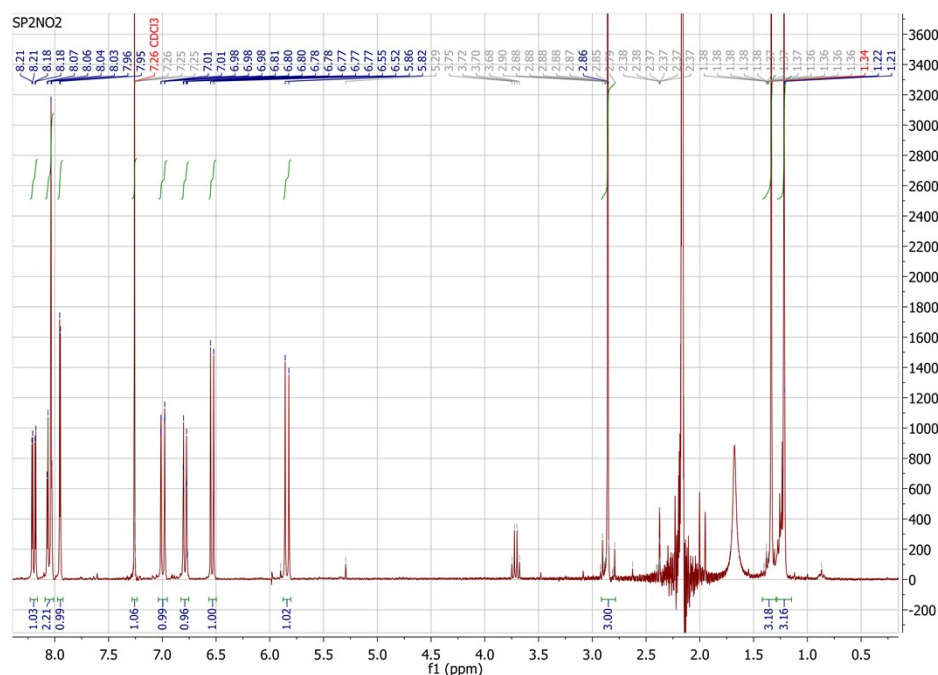


Figure A 2: ¹H-NMR of **SP2NO2**. Traces of H₂O (δ (ppm): 1.34) and ACN (δ (ppm): 2.2) present. High resolution mass spectra (HRMS; APCI, m/z): calcd for C₁₉H₁₈O₅N₃; 368.12410; found: 368.12392.

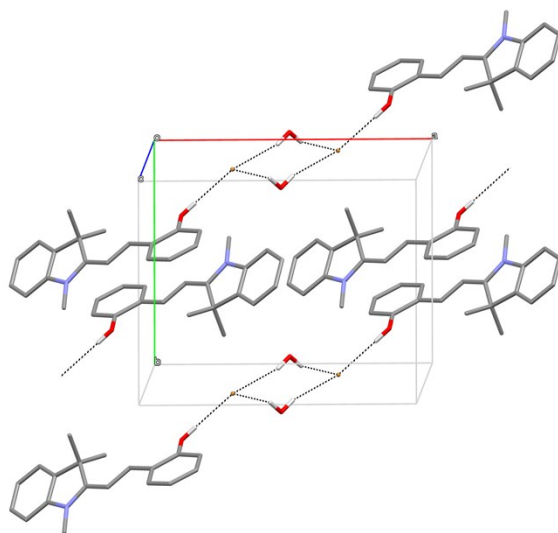


Figure A 3: A partial packing diagram for (Ib'). Hydrogen bonds are indicated as dashed lines.

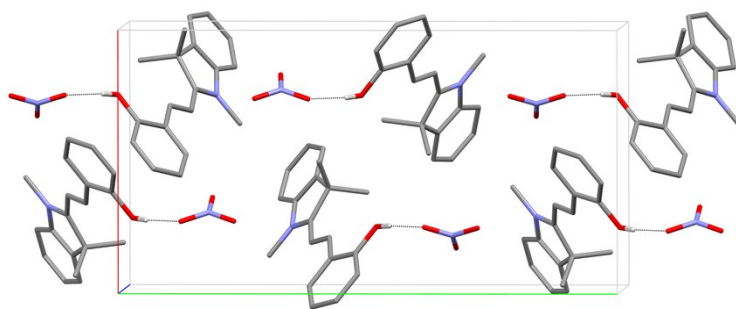


Figure A 4: A partial packing diagram for (Ic). Hydrogen bonds are indicated as dashed lines.

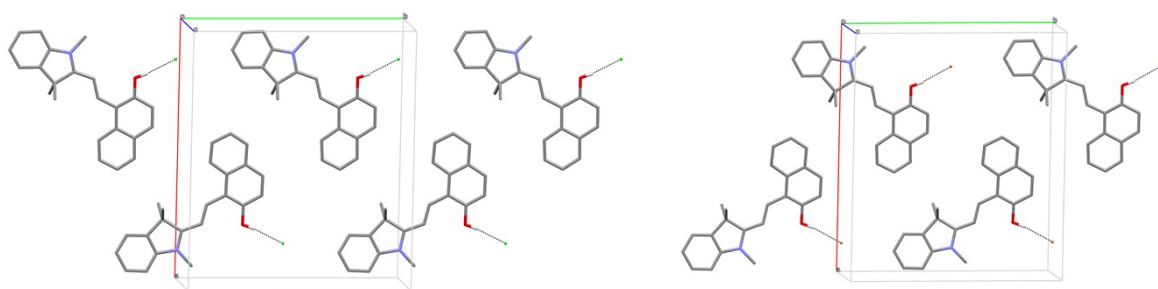


Figure A 5: A partial packing diagram for (IIa; left) and (IIb; right). Hydrogen bonds are indicated as dashed lines.

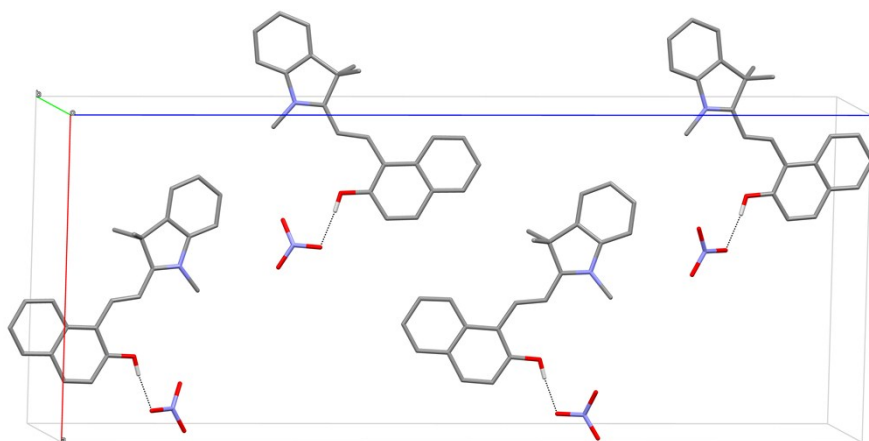


Figure A 6: A partial packing diagram for (IIc). Hydrogen bonds are indicated as dashed lines.

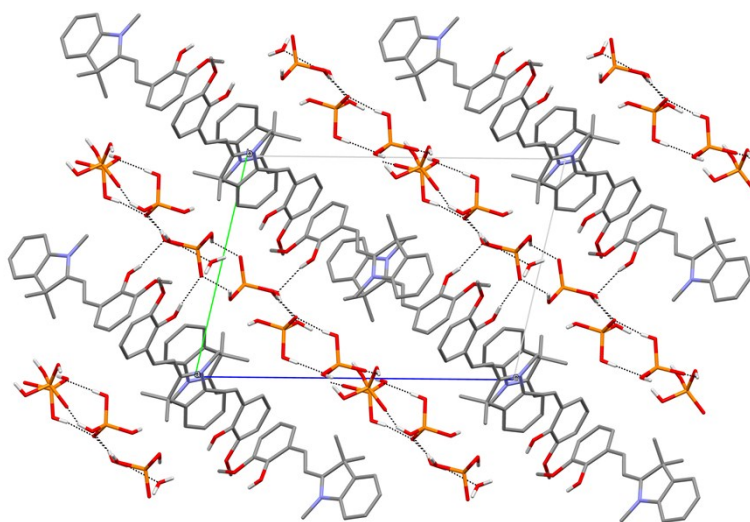


Figure A 7: A partial packing diagram for (IIle). Hydrogen bonds are indicated as dashed lines. Only the major occupied sites of the disordered parts are shown.

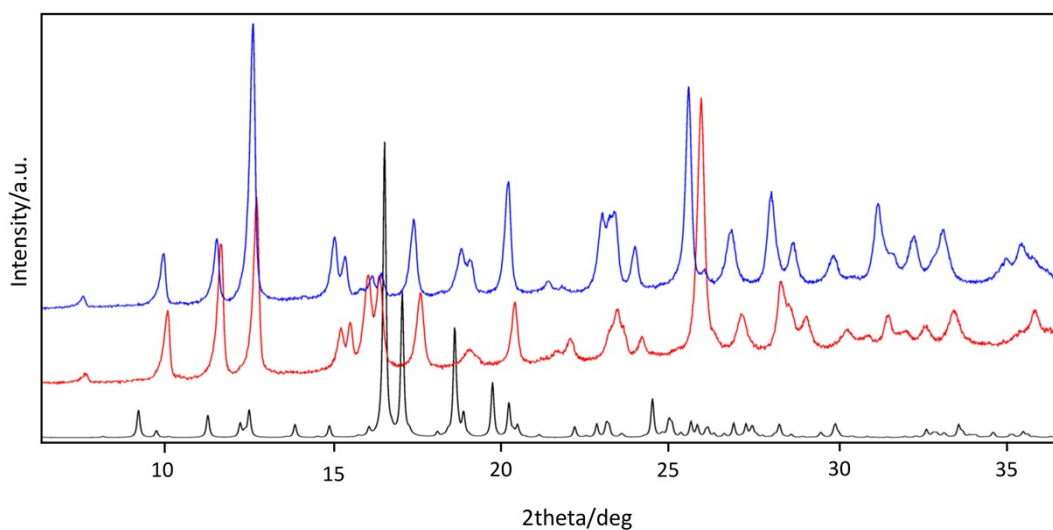


Figure A 8: X-Ray powder diffraction measurement of **SPNO2** (black, simulated powder patterns from single crystal data) in comparison with (IVa; red) and (IVb; blue); measured at room temperature.

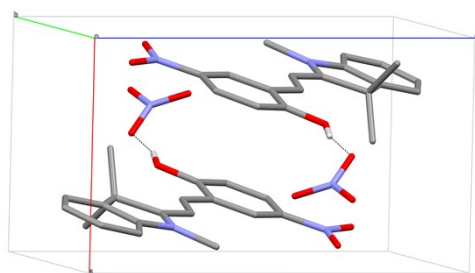


Figure A 9: A partial packing diagram for (IVc). Hydrogen bonds are indicated as dashed lines.

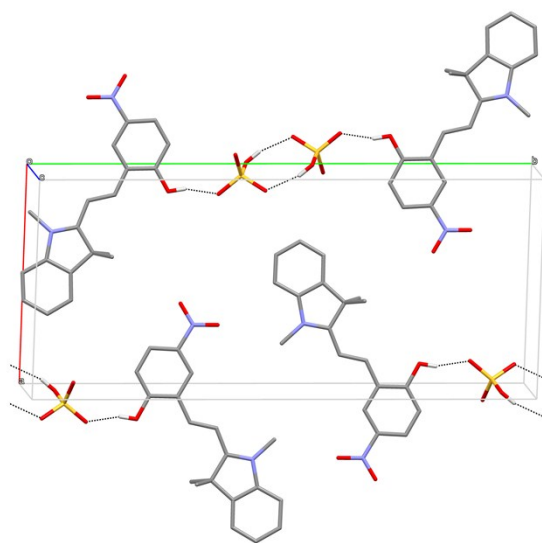


Figure A 10: A partial packing diagram for (IVd). Hydrogen bonds are indicated as dashed lines.

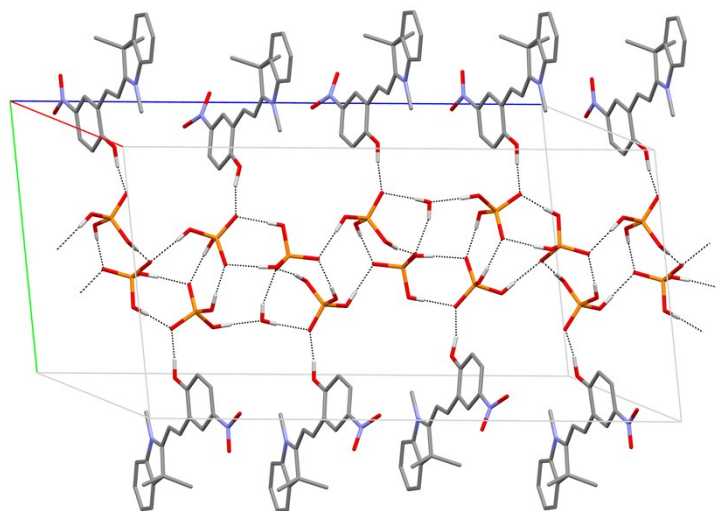


Figure A 11: A partial packing diagram for (IVe). Hydrogen bonds are indicated as dashed lines. Only the major occupied sites of the disordered parts are shown. Solvent molecules are not displayed.

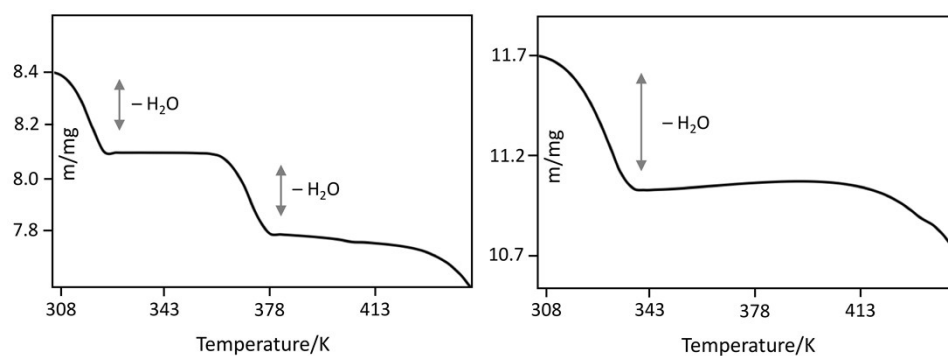


Figure A 12: TGA of (IIIb; left) and (IIIc; right).

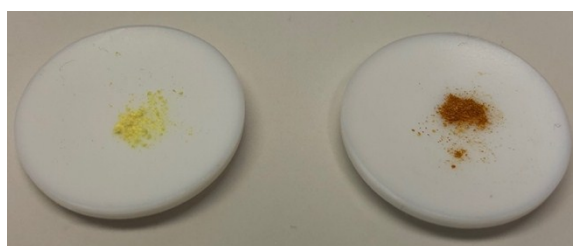


Figure A 13: Visible colour change of **SPNO2** (left) under irradiation at 360 nm for 30 min (left).

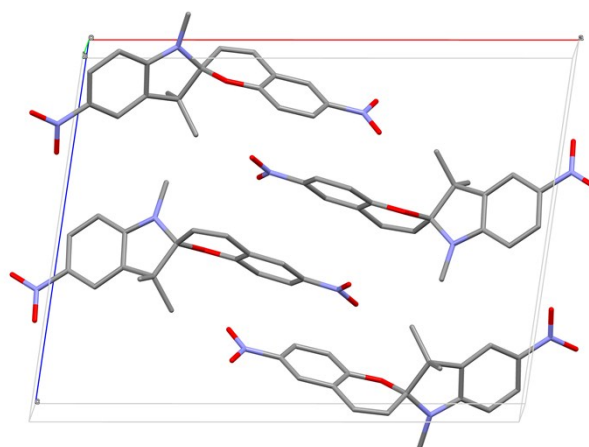


Figure A 14: A partial packing diagram for (V).