(Perylene)$_3$-(TCNQF$_1$)$_2$: Yet Another Member in the Series of Perylene–TCNQF$_x$ Polymorphic Charge Transfer Crystals

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1. Quantum Chemical Calculations

DFT calculations of the harmonic vibrational normal modes have been performed with the GAMESS code[1], using the 6-31G(d,p) basis set and the B3LYP hybrid functionals for both neutral and ionic TCNQF$_1$

2. Full Analysis and the Assignment of the IR Spectra

Table S1. Frequencies, eigenvectors and infrared intensities of the most important vibrational modes.

	TCNQF$_1^0$		**TCNQF$_1^{-1}$**	
	[a]Calc. ω/cm^{-1} & (IR$_{int}$ Debye^2/amu Å^2)	**Exp.**	**[a]Calc. ω**/cm^{-1} & (IR$_{int}$ Debye^2/amu Å^2)	**Exp.**
ν_{CN} asym.	2245 (0.6)	2223 (s)	2209 (0.3)	-
ν_{CN} sym.	2243 (0.3)	2215 (sh)	2206 (13.2)	2201 (vs)
ν_{CN}	2229 (0.1)	-	2175 (4.3)	2189 (sh)
ν_{CN}	2227 (0.0)	-	2174 (1.6)	2180 (sh)
ν_1 (C=C)	1621 (0.6)	1618 (m)	1599 (0.5)	1591 (m)
ν_2 (C=C)	1550 (1.6)	1557 (m)	1491 (2.5)	1515 (m)
ν_3 (C=C)	1521 (1.5)	1549 (s)	1329 (0.7)	1361 (m)
ν_R (C=C)	1442 (0,0)	1459	1360 (0.2)	1407
ν (C-F)	1204 (1.0)	1210 (m)	1190 (1.5)	1194 (m)

a Harmonic frequencies scaled by the 0.9614 factor[2].

3. TCNQF$_1$: Charge Sensitive Modes

4. Raman Spectra of the Neutral Donor and Acceptor Molecules, the Full Ionized Acceptor and of the Charge Transfer Complex TCNQF$_1$-Perylene

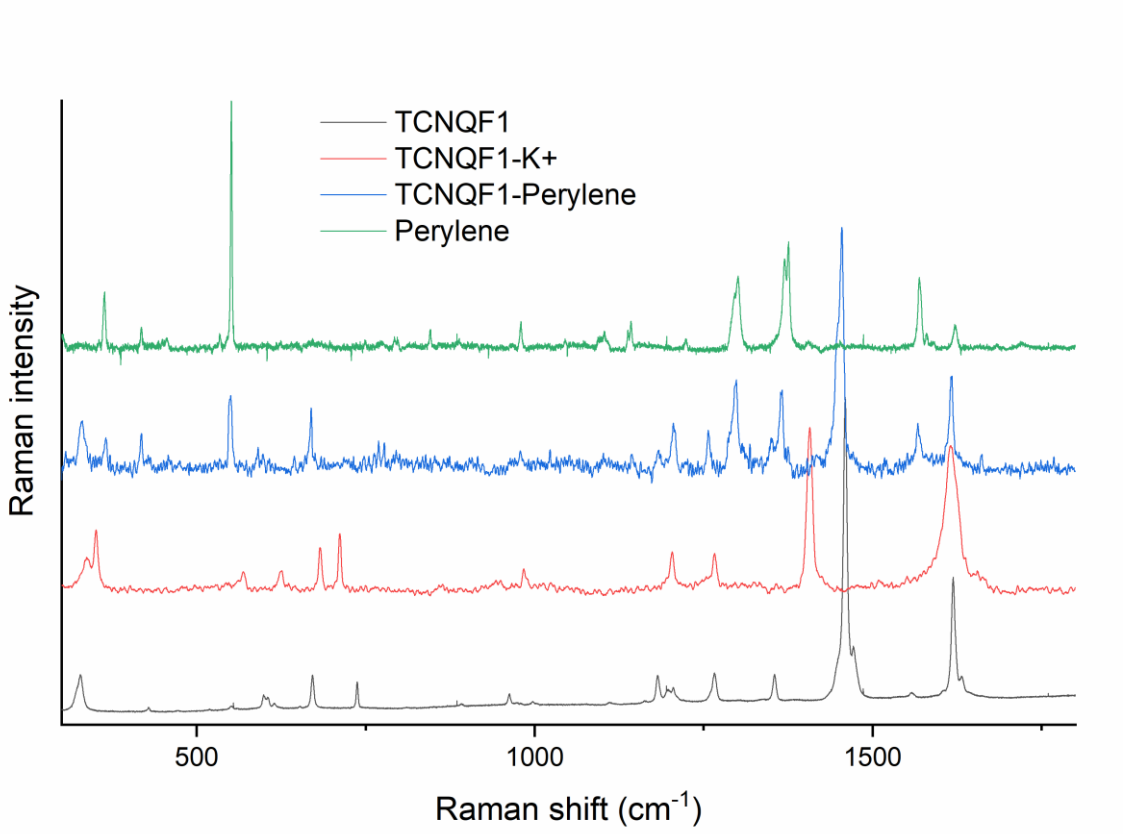

Figure S1. Raman spectra of the neutral $TCNQF_1$(black), Perylene (green), potassium $TCNQF_1$ salt (red) and of the charge transfer complex $TCNQF_1$-Perylene (blue).

References

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