Structural, Cyclic Voltammetric and IR-Spectral Evidences for Preorientation in PET-Active Phthalimido Carboxylic Acids

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SUPPORTING INFORMATION:

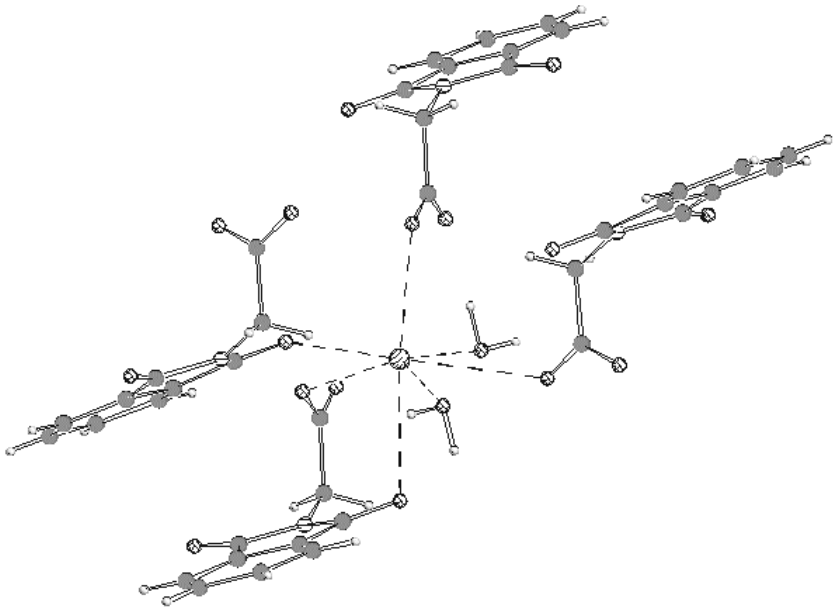
X-RAY DATA for compound **1-K**

IR-SPECTRA for compounds **1**, **1-K** and **2**

CV DETAILS

Crystal data and structure refinement for 1-K:

Structure



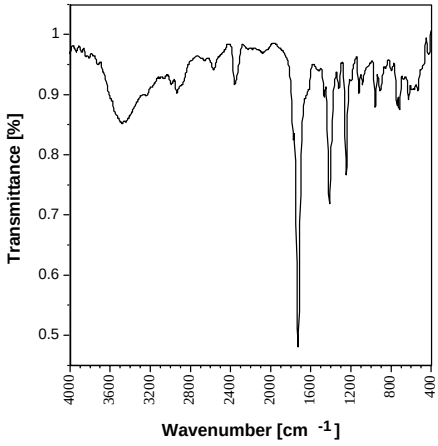
Empirical formula	C10 H8 K N O5
Formula weight	261.27
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	P 21/c
Unit cell dimensions	a = 15.528(1) A alpha = 90 deg.
	b = 9.075(1) A beta = 94.16(1) deg.
	c = 8.218(1) A gamma = 90 deg.
Volume	1155.0(2) A^3
Z	4
Density (calculated)	1.503 g/cm^3
Absorption coefficient	0.468 mm^-1
F(000)	536
Crystal size	0.20 x 0.20 x 0.20 mm
Theta range for data collection	1.31 to 27.00 deg.
Index ranges	-19<=h<=19, -11<=k<=11, -10<=l<=10
Reflections collected	4863

Independent reflections	2518 [R(int) = 0.0337]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2518 / 0 / 186
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1463
Reflection observed [I>2sigma(I)]	1854
R indices (all data)	R1 = 0.0798, wR2 = 0.1618
Largest diff. peak and hole	0.419 and -0.356 e.A^-3

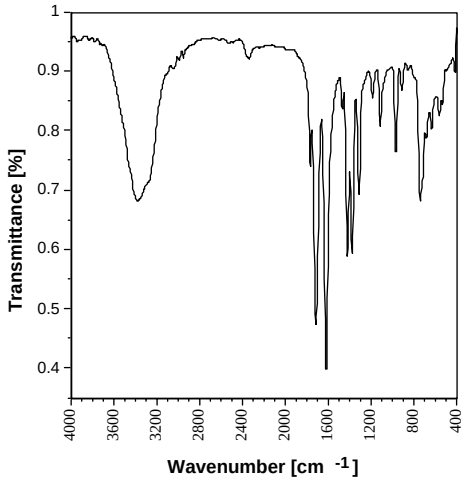
IR Data:

IR: Perkin-Elmer 1600, FT-IR spectrometer; $\tilde{\nu}$ in cm-1.

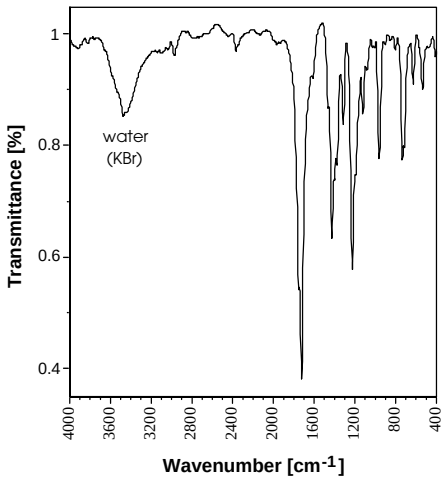
IR data for **1** (KBr disc): $\tilde{\nu}$ = 3479, 2931, 2564, 2357, 1770, 1724, 1415, 1246.



IR data for **1-K** (KBr disc): $\tilde{\nu}$ = 3379, 2333, 1766, 1712, 1616, 1419, 1376, 1311, 740.



IR data for **2** (KBr disc): $\tilde{\nu}$ = 2970, 1724, 1423, 1311, 1223, 960, 732.



Cyclic Voltammetry:

In a glove box *n*-tetrabutylammonium hexafluorophosphate (232 mg, 600 µmol) and the electroactive species (6 µmol) were placed into a thoroughly dried CV cell. At a high purity argon line acetonitrile or DMF (6.0 ml) was added through a gastight syringe, a 1 mm platinum disc electrode as working electrode and a Pt wire counter electrode as well as an Ag reference electrode were placed into the solution. The CVs were recorded at various scan rates using various starting and switching potentials. For determination of the oxidation potentials ferrocene (6 µmol) was added as the internal standard. CVs were recorded using a Princeton Applied Research Model 362

potentiostat with a Philips model PM 8271 XYt-recorder for scan rates <1 V s-1. The ratios Ipc/Ipa were determined according to the equation of Nicholson [R. S. Nicholson, *Anal. Chem.* **1966**, 1406.].