Vibrational Structure of Molecular Charge Transfer Bands in Hydrocarbon-Tetrahalo p-Benzoquinone Complexes

Molecular charge transfer bands in solution are usually broad and diffuse showing no vibrational structures. Some preliminary measurements with a Beckman Spectrophotometer Model DU at ·1 position of the selector switch showed that the charge transfer bands in anthracene-tetrahalo p-benzoquinone complexes in chloroform are structured. Measurements were therefore made using a large glass prism monochromator (manufactured by Hilger & Co.) having a dispersion of 5 Å, in the range 5000 to 7000 Å, in conjunction with a 1P21 Photomultiplier tube and a Phymale-Hansen type D.C.Amplifier. The spectra were found to be quite complicated. The prominent peaks are listed below. (Anth.- = Anthracene-.)

Anth.-chloranil			Anth.-bromanil			Anth.-iodanil		
λ, Å	ν, cm^{-1}	$\Delta\nu$	λ, Å	ν, cm^{-1}	$\Delta\nu$	λ, Å	ν, cm^{-1}	$\Delta\nu$
6520	15340		6450	15511		6425	15590	
6470	15470	130	6400	15620	129	6360	15720	150
6420	15580	110	6340	15770	150	6300	15870	160
6360	15720	140	6280	15920	160	6240	16030	160
6300	15870	150	6220	16080	160	6185	16190	200

The charge transfer bands for naphthalene, phenanthrene and pyrene complexes with tetrahalo p-benzoquinone were also found to be structured, but the vibrational structures were not as sharp or as well resolved as is the case with anthracene complexes. A detailed paper will be published elsewhere.

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