Supplementary Material for PCCP

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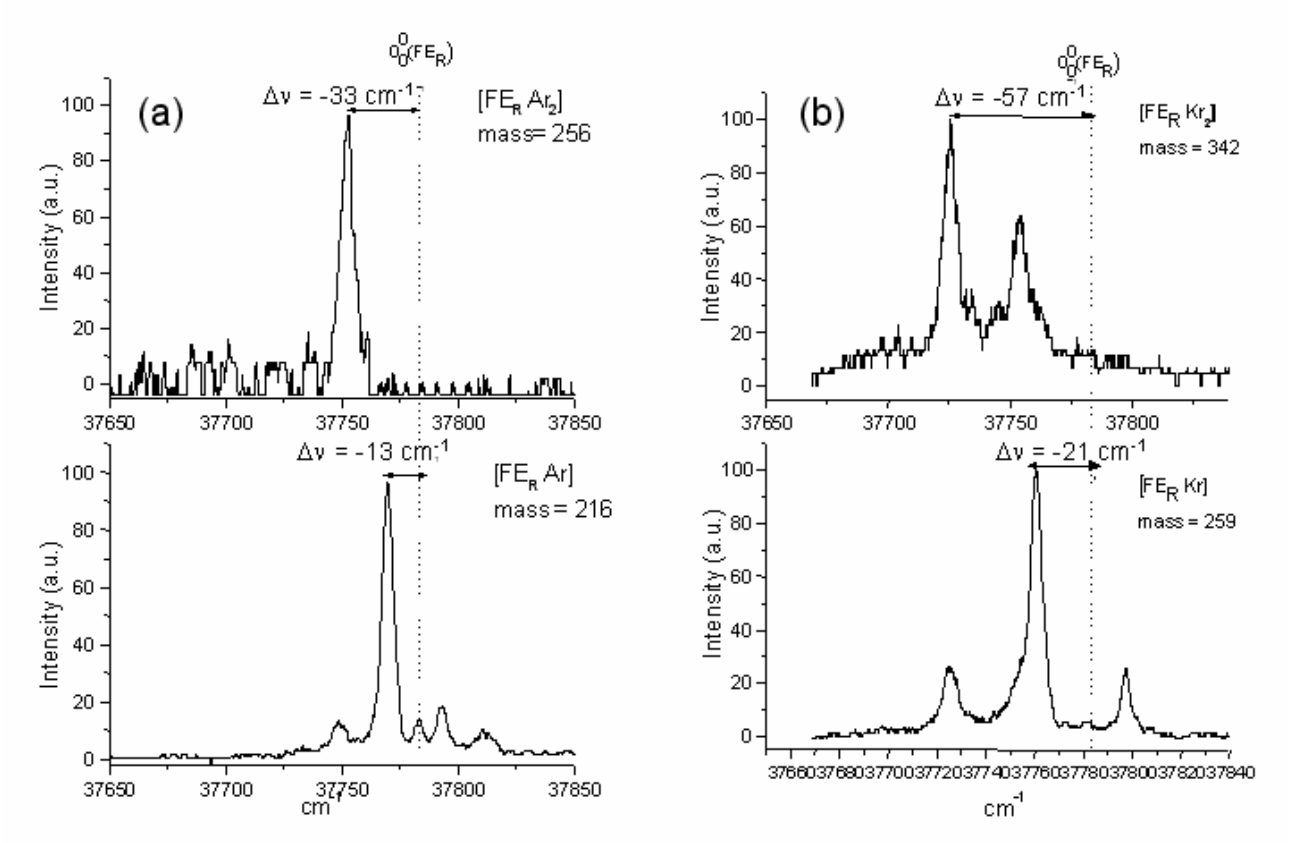
Dissymmetry Effects on the Laser Spectroscopy of Supersonically Expanded Rare Gas/Chiral Arene Heteroclusters.

Electronic Supporting Information

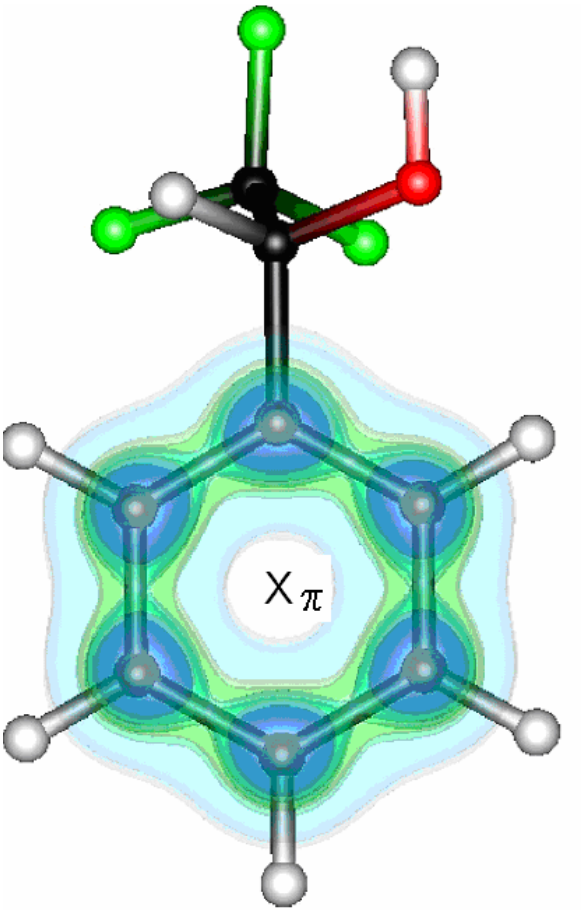
R2PI-TOF Spectroscopy

Electronic spectra of the [$\mathbf{FE_R}$•$(Rg)_n$] (n=1,2; Rg=Ar (a), Kr (b)) clusters. The dotted line indicates the 0_0^0 electronic transition of the bare $\mathbf{FE_R}$ molecule. The signals at 37749 cm^{-1} (bottom of Fig. a) and at 37725 cm^{-1} (bottom of Fig. b), measured at the mass corresponding to [$\mathbf{FE_R}$•Rg], arise from fragmentation of the corresponding [$\mathbf{FE_R}$•$(Rg)_2$] clusters.

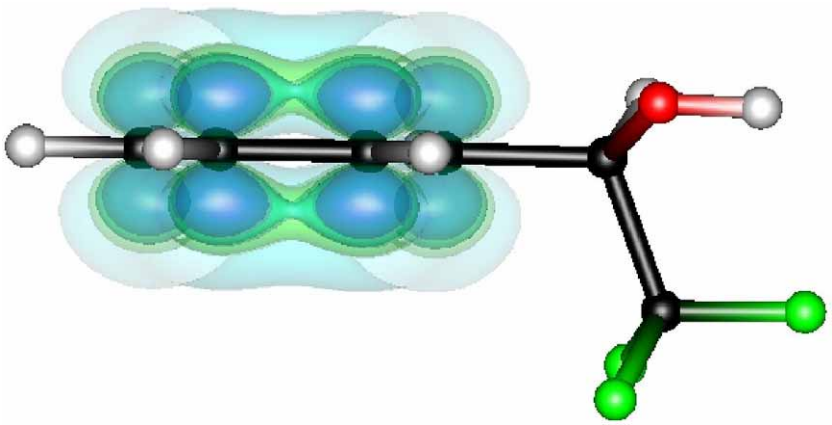


CAS(6,6)/Slater^{+}-calculated π-electron density of ground-state FE_R

Bottom view



Side view



Geometrical parameters of the [FE_R•$(Ar)_n$] (n=0-2 clusters].

Geometric parameters of [$\mathbf{FE_R}$•$(Ar)_n$] (n=1,2) have been calculated at the MP2/6-31G(d,p) ($\mathbf{FE_R}$) and AUG-cc-pVQZ (Ar) levels of theory (GAUSSIAN 03).

	[FER•Ar]			**[FER•$(Ar)_2$]**		
	[1,0]	**[0,1]**	**$[1,0]_{side}$**	**[1,1]**	**[2,0]**	**$[2,0]_{side}$**
R(Ar-π) (Å)	3.53	3.51	6.55	3.52	3.52	3.52
				3.50	4.65	6.56
R(Ar-CF_3) (Å)	4.03	5.91	4.08	4.05	4.04	4.08
				5.87	4.79	4.10
R(Ar-OH) (Å)	5.56	4.39	3.51	5.57	5.53	5.61
				4.35	6.54	3.55
α(Ar-$X_π$-C_1) (degrees)	90.05	86.04	35.34	90.20	90.65	90.29
				85.28	82.46	35.81