

*Article*

# Supplementary Materials: Local Vibrational Mode Analysis of $\pi$ -Hole Interactions between Aryl Donors and Small Molecule Acceptors

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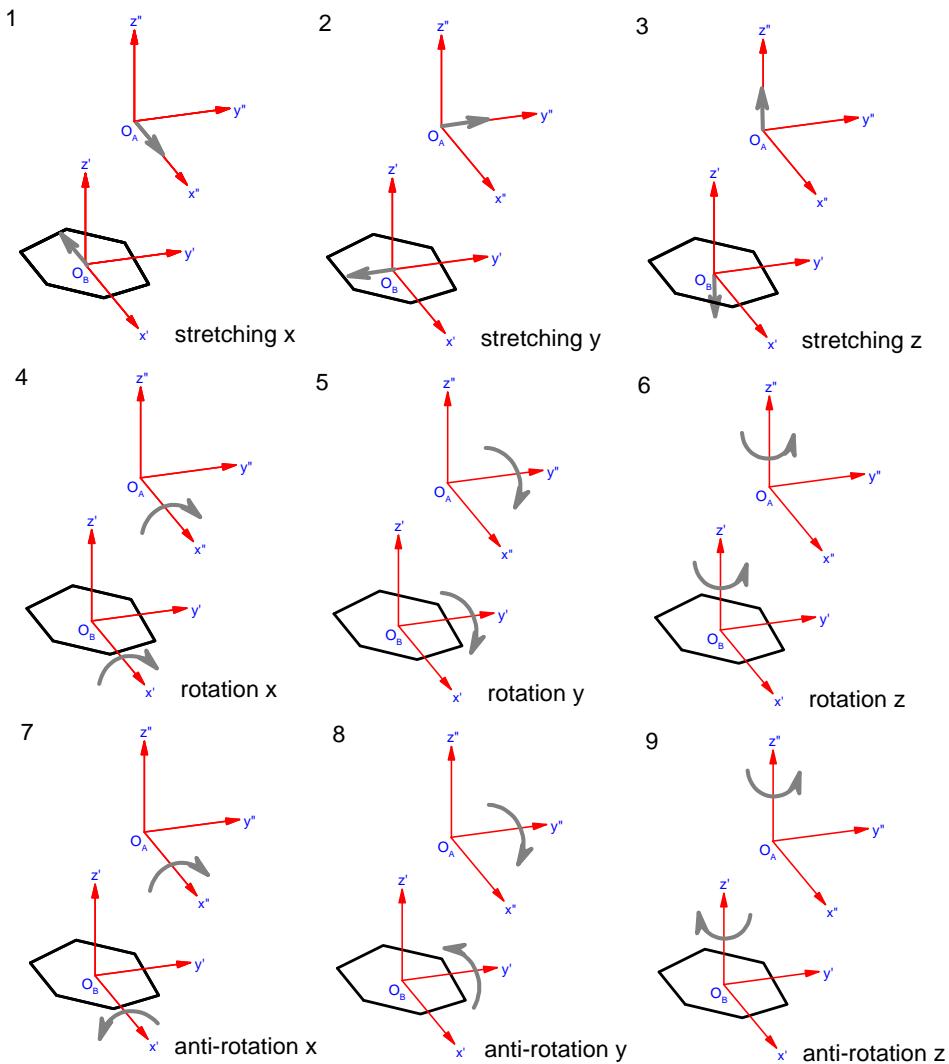
Version June 4, 2020 submitted to Crystals

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### 1. Description of local vibrational modes between two monomers forming a complex.



**Figure S1.** Description of local vibrational modes between two monomers forming a complex.

**2. Overview of movies (uploaded as separate files) describing the normal vibrational modes with predominant  $\pi$ -hole interaction character for the  $\text{Ar}\cdots\text{C}_6\text{H}_6$  and the  $\text{H}_2\text{O}\cdots\text{C}_6\text{F}_6$  complex.****Table S1.** Overview of movies (uploaded as separate files) describing the normal vibrational modes with predominant  $\pi$ -hole interaction character for the  $\text{Ar}\cdots\text{C}_6\text{H}_6$  and the  $\text{H}_2\text{O}\cdots\text{C}_6\text{F}_6$  complex.

Normal Mode	File name
$\text{Ar}\cdots\text{C}_6\text{H}_6$	
$\omega_3$	ar-v3.gif
$\omega_8$	ar-v8.gif
$\text{H}_2\text{O}\cdots\text{C}_6\text{F}_6$	
$\omega_1$	h2o-v1.gif
$\omega_4$	h2o-v4.gif
$\omega_7$	h2o-v7.gif
$\omega_{10}$	h2o-v10.gif
$\omega_{17}$	h2o-v17.gif

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