

Electronic Supplementary Information for:

A 2-D dimer model system to investigate structure-charge transfer relationships in rubrene

Sherlyn C. Jing,^a Callum J. McHugh^{b} and Jesus Calvo-Castro^{a*}*

^a School of Life and Medical Sciences, University of Hertfordshire, Hatfield, AL10 9AB, UK.

^b School of Computing, Engineering and Physical Sciences, University of the West of Scotland, Paisley, PA1 2BE, UK.

*Corresponding author: j.calvo-castro@herts.ac.uk, callum.mchugh@uws.ac.uk.

	Page
SI.1 Chemical structures and space-filled representation for π-π dimer pairs of reported PDPP crystal structures	2-9

SI.1 Chemical structures and space-filled representation for the investigated π - π dimer pairs of reported rubrene-based crystal structures

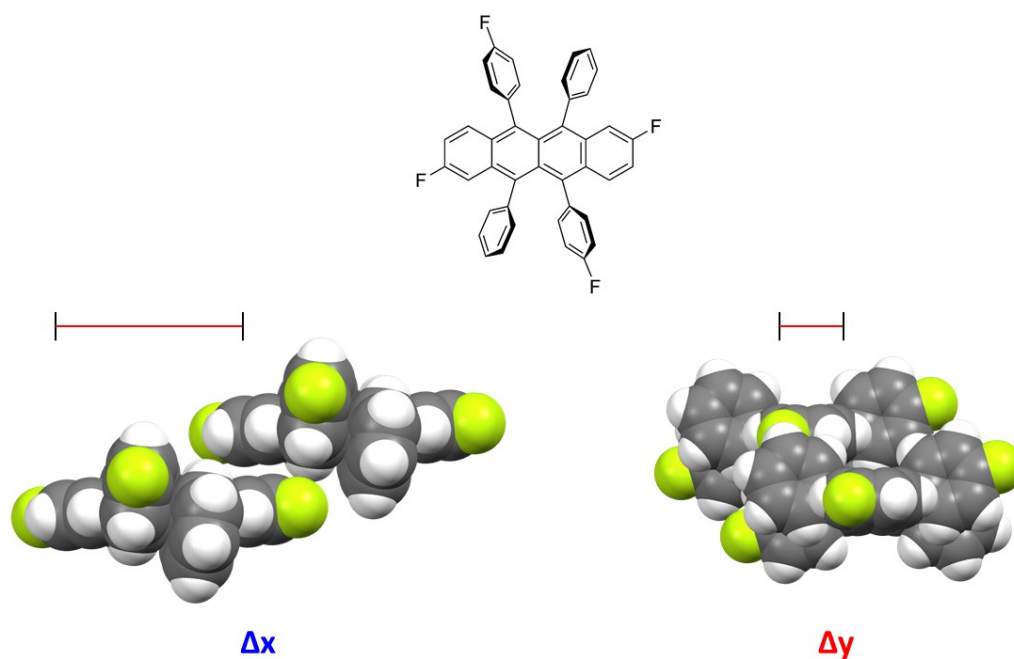


Figure SI.1.1 Chemical structure and space-filled illustration of π - π dimer pair of **AXIDER**.

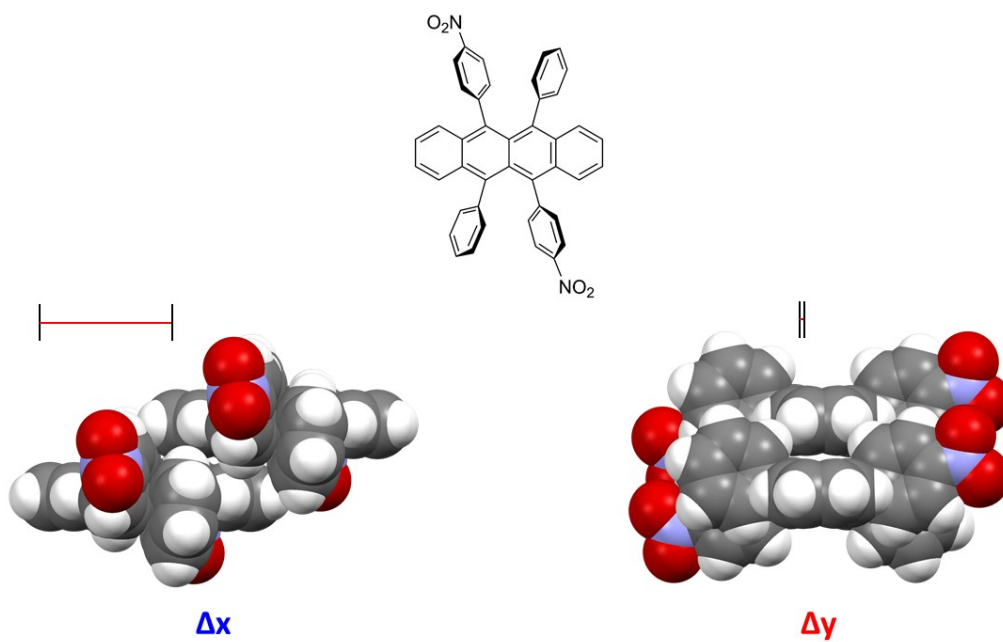


Figure SI.1.2 Chemical structure and space-filled illustration of π - π dimer pair of **CIYNAB**.

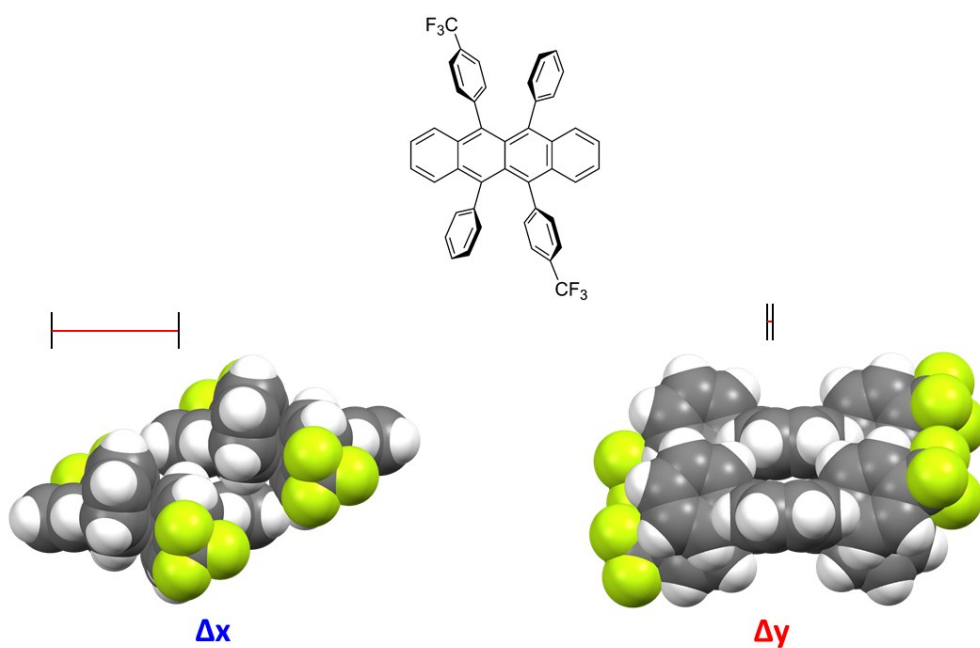


Figure SI.1.3 Chemical structure and space-filled illustration of π - π dimer pair of **CIYXUF**.

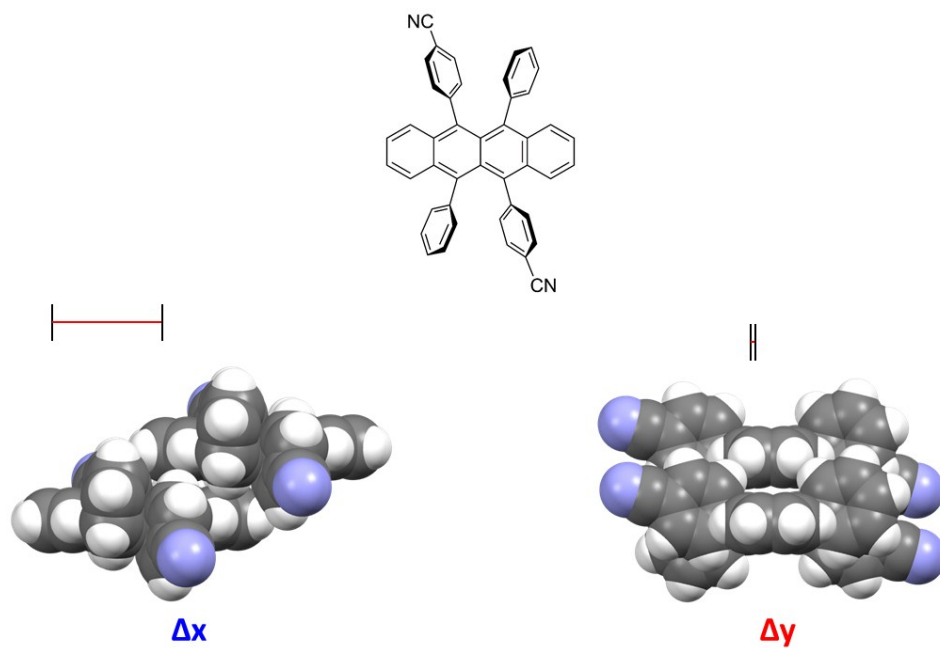


Figure SI.1.4 Chemical structure and space-filled illustration of π - π dimer pair of **CIYYAM**.

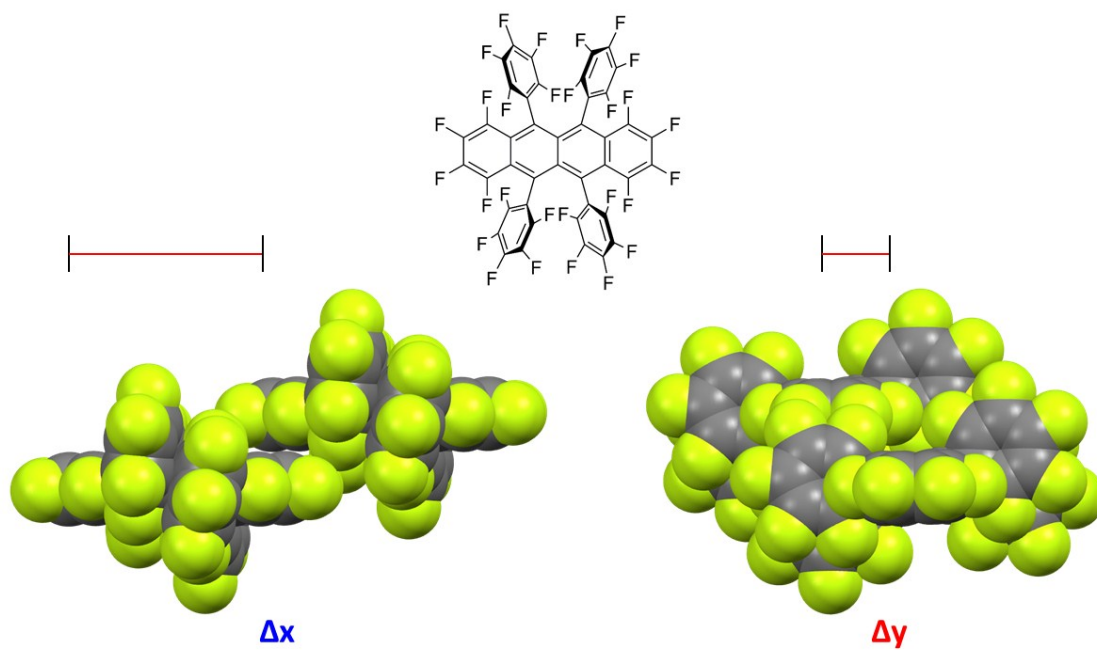


Figure SI.1.5 Chemical structure and space-filled illustration of π - π dimer pair of **INELUK02**.

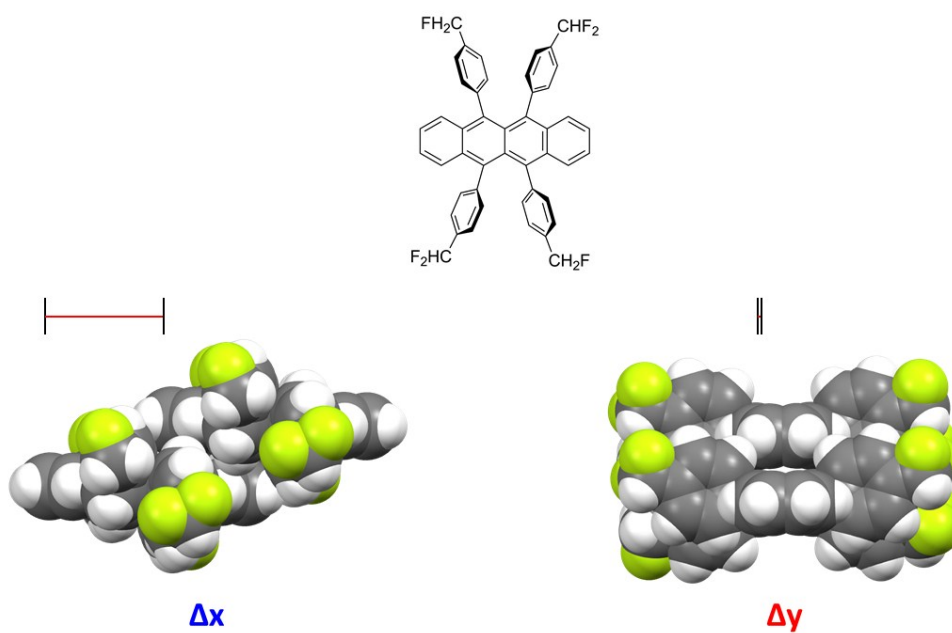


Figure SI.1.6 Chemical structure and space-filled illustration of π - π dimer pair of **KUSDEJ**.

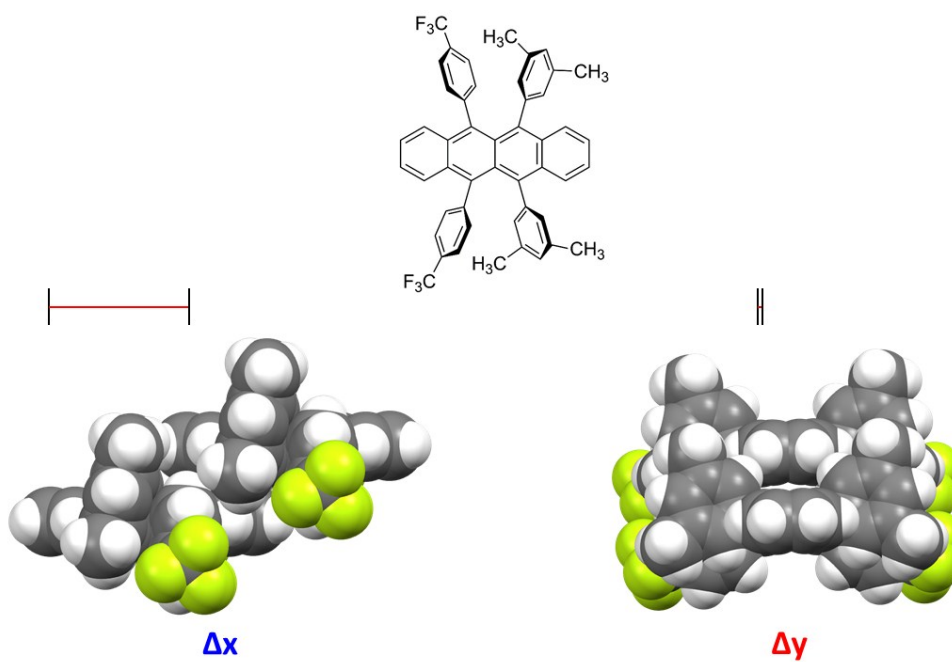


Figure SI.1.7 Chemical structure and space-filled illustration of π - π dimer pair of **MIVDOM**.

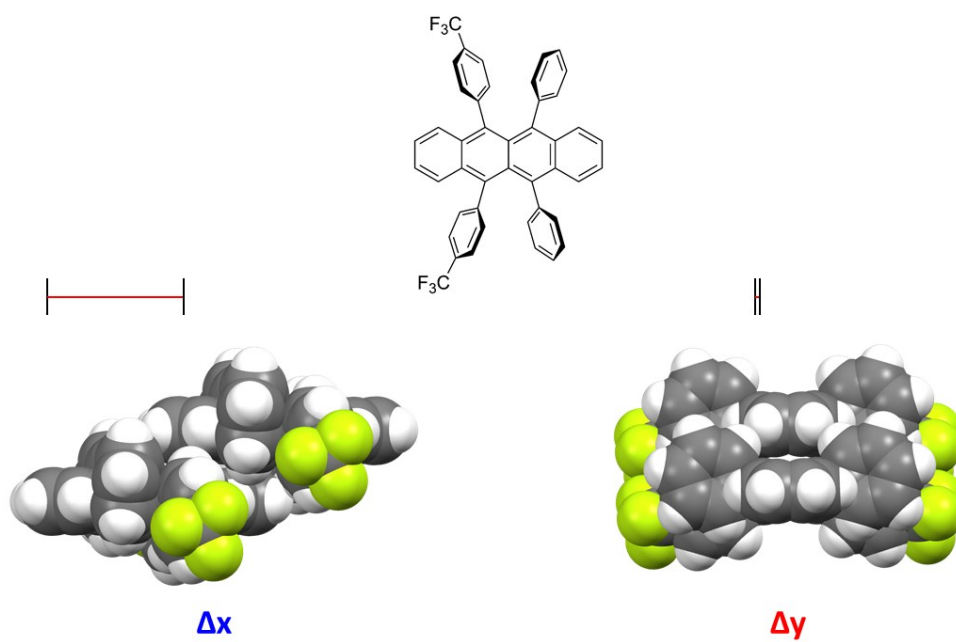


Figure SI.1.8 Chemical structure and space-filled illustration of π - π dimer pair of **MIVDUS**.

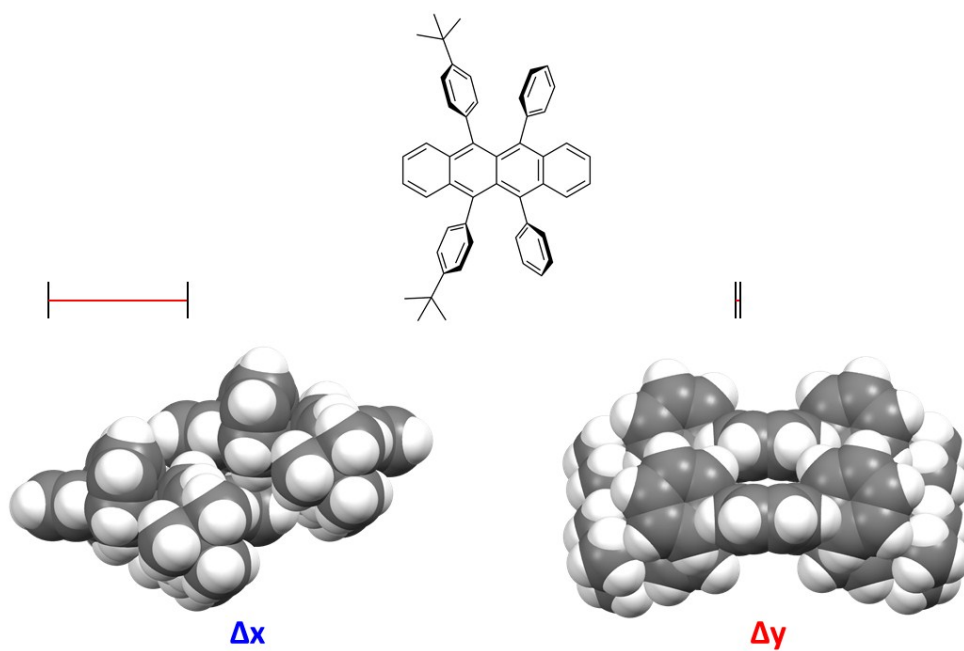


Figure SI.1.9 Chemical structure and space-filled illustration of π - π dimer pair of **PIFHIW**.

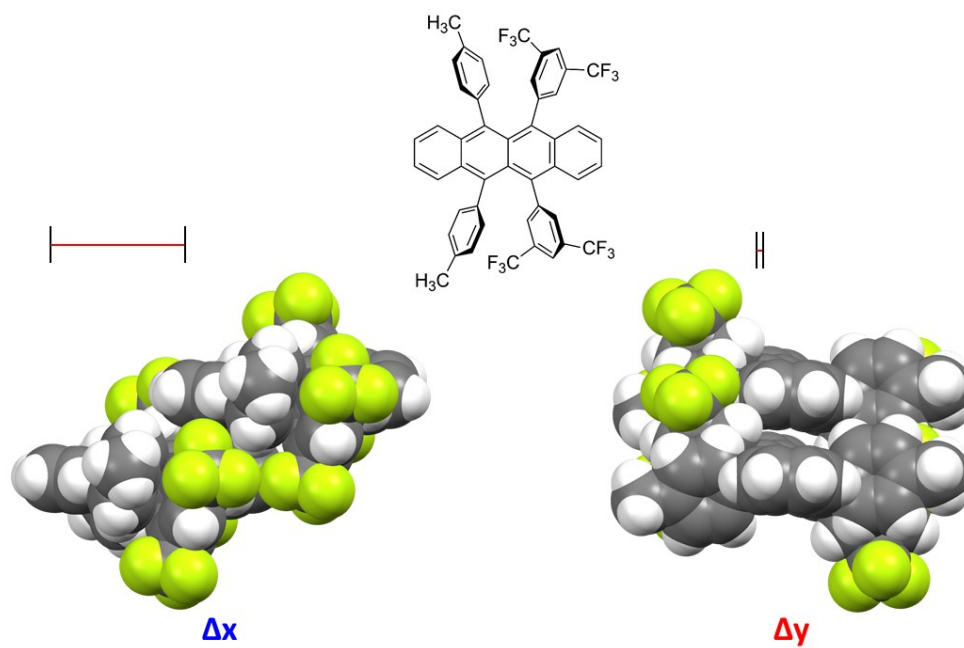


Figure SI.1.10 Chemical structure and space-filled illustration of π - π dimer pair of **RAGCEK**.

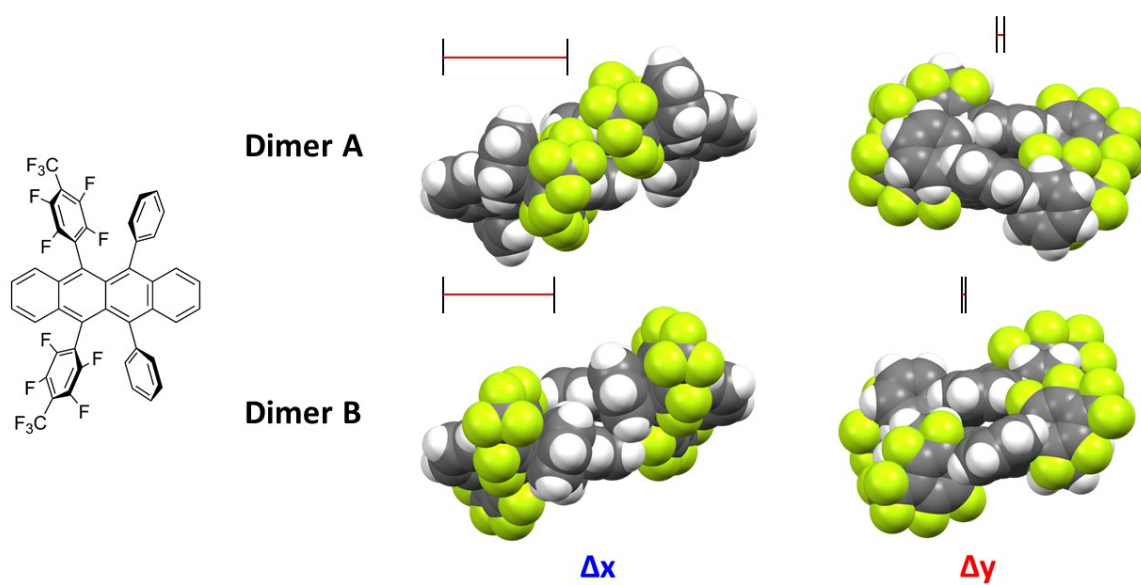


Figure SI.1.11 Chemical structure and space-filled illustration of π - π dimer pair of **RAGCUA**.

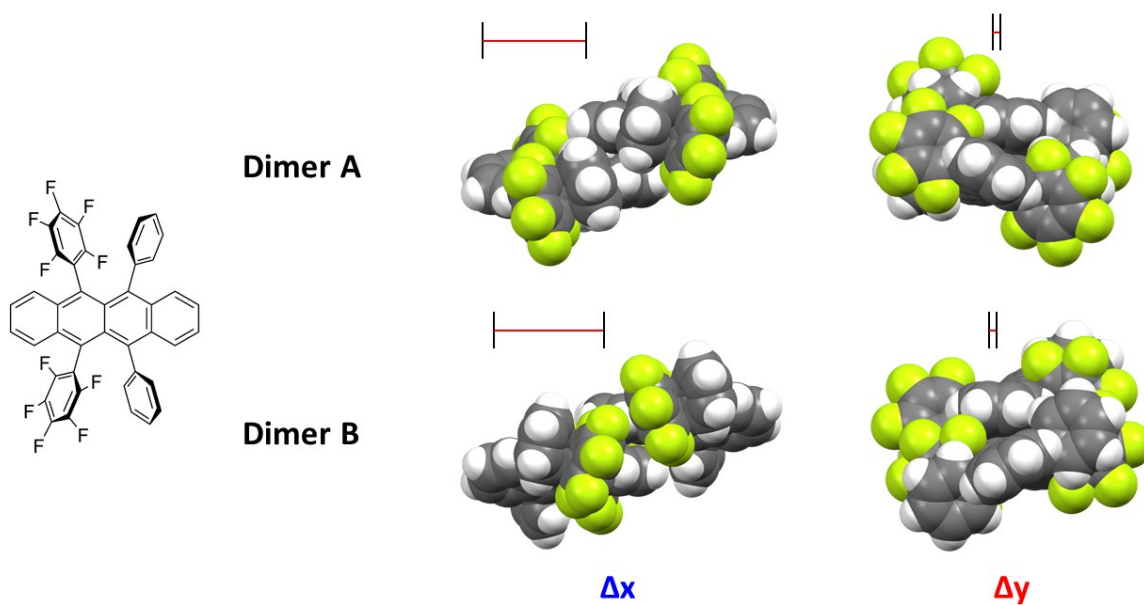


Figure SI.1.12 Chemical structure and space-filled illustration of π - π dimer pair of **RAGDEL**.

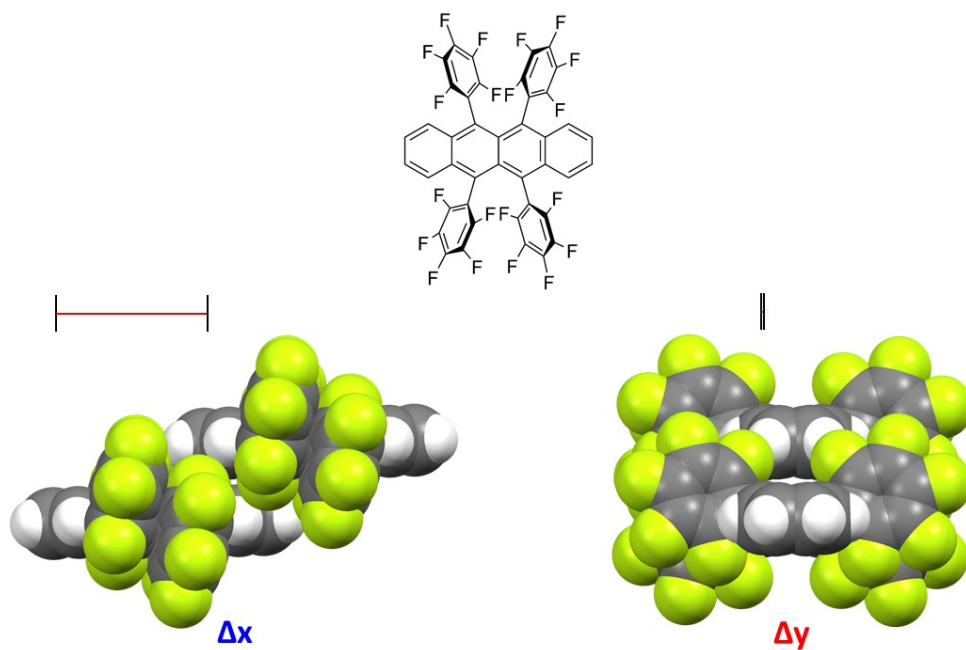


Figure SI.1.13 Chemical structure and space-filled illustration of π - π dimer pair of **RAGDIP**.

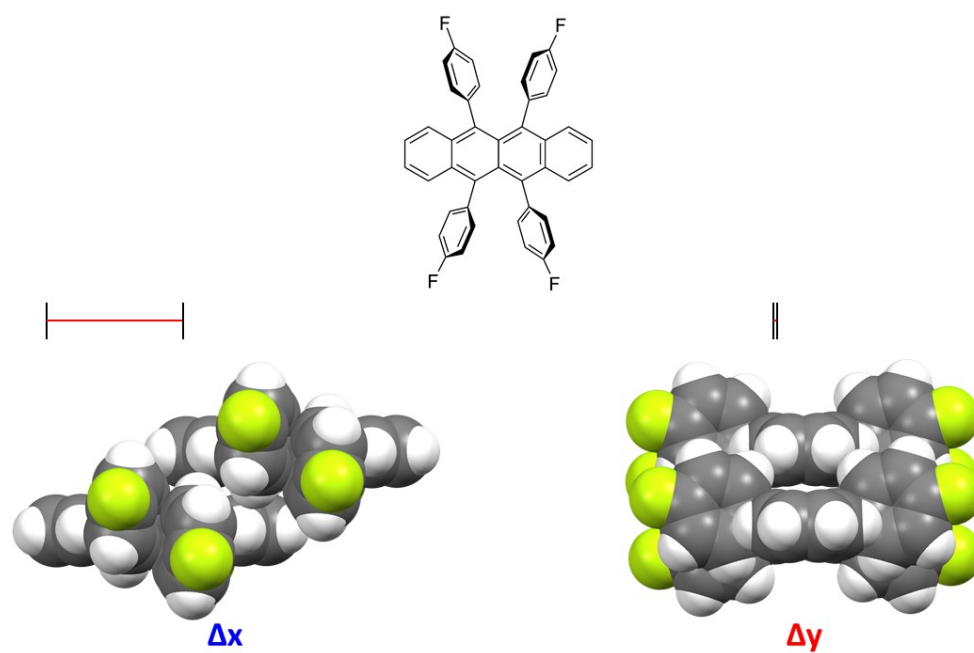


Figure SI.1.14 Chemical structure and space-filled illustration of π - π dimer pair of **TOMVUM**.