

MS36-05 | CHARGE TRANSFER DONOR-ACCEPTOR COMPLEXES OF SEVERAL POLYCYCLIC AROMATIC MOLECULES

Rigin, Sergei (New Mexico Highlands University, LAS VEGAS, USA); Lesse, Daniel (Department of Chemistry, New Mexico Highlands University, Las Vegas, USA); Timofeeva, Tatiana (Department of Chemistry, New Mexico Highlands University, Las Vegas, USA)

For donor-acceptor pairs of 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, acceptor) and triphenylene, chrysene, dibenz[a,c]anthracene, and benzo[a]pyrene HOMO-LUMO energy levels have been calculated using DFT approach. Calculations demonstrated overlap of HOMO-LUMO gaps of acceptor and donors that suggested possibility of existence of charge transfer complexes for their adducts. Crystals of four adducts have been grown and their structures have been elucidated using X-ray diffraction analysis. It appears that all crystals are built of molecular stacks with alternating donor-acceptor positions (..D..A..D..A..). Degree of charge transfer was estimated using obtained molecular geometries. According to this approach, chrysene-DDQ complex has the highest charge-transfer degree among the other complexes with DDQ acceptor. The appearance of the chrysene-DDQ co-crystal is consistent with this result since a darker crystal usually indicates a stronger charge-transfer.