Crystal Growth and Design 2016 vol.16 N1, pages 331-338

Crystal Growth, Dynamic and Charge Transfer Properties of New Coronene Charge Transfer Complexes

Kataeva O., Khrizanforov M., Budnikova Y., Islamov D., Burganov T., Vandyukov A., Lyssenko K., Mahns B., Nohr M., Hampel S., Knupfer M.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 American Chemical Society.Two new coronene charge transfer complexes with F4-TCNQ of 2:1 and 1:1:1 (solvate with acetonitrile, MeCN) stoichiometry were obtained using crystal growth procedures from the solution and vapor phase. It was shown that mobility of coronene molecules in crystals is more affected by the asymmetry of its surrounding than by the composition and degree of charge transfer and interstack interactions. The combination of X-ray diffraction and electrochemistry in the solid state and a time-resolved one in solution allowed us to clarify the nucleation in solution showing that the formation of 2:1 coronene/F4-TCNQ complexes is thermodynamically preferable. The X-ray single crystal data for pristine coronene showed the crystal structure to be the same as at ambient temperature, raising doubt about the previously reported phase transitions at 140-180 K.

http://dx.doi.org/10.1021/acs.cgd.5b01301