Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Helical inversion reaction pathway for π/π stacking in aromatic compounds AZUSA MURAOKA, Meiji University, CREST, HIROSHI USHIYAMA, KOICHI YAMASHITA, University of Tokyo, CREST — Polyaromatics have the π/π stacking interaction, which shows that two aromatic units preferentially interact in a parallel-displaced orientation, such as the crystal packing of organic molecules. Recently, π/π stacking compounds have become of interest in the photocatalysis solor energy transformational materials. In particular, the stable configurations of neutral and cationic *o*-phenylenes have helical tightly packed *n*-phenylenes with π/π stacking interactions. To investigate helical inversion pathways, we have studied theoretically the stable and transition-state geometries of neutral and cationic *o*-phenylenes using the density functional theory method. We have found that *o*-phenylenes follow an inversion reaction pathway with three transition-states in which the configuration of each phenylene is inverted. This means that *o*-phenylenes cannot convert from right- to left-handed geometry at once; however, we suggest a step-by-step reaction pathway through the three transition-state structures.

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Date submitted: 27 Nov 2012

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