Electronical supporting information

The crystallographic observation for mesitylene-mesitylene and mesitylene-CH_2Cl_2-mesitylene adducts trapped in irregular cavity

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Materials and measurements

Complex **1** is prepared according to the method reported previously.[1] Crystal **1**•mesitylene and **1**•mesitylene•CH_2Cl_2 were picked for X-ray structural analysis on a Bruker SMART CCD diffractometer with a Mo-K_α radiation source (λ = 0.71073 Å). The structures were solved and refined by full matrix least-squares on F^2 values (SHELXL-97).[2] Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were fixed at calculated positions and were refined using a riding mode. TEM observations were performed on a JEOL JEM-1011 transmission electron microscope operated at an acceleration voltage of 100 kV. Samples were prepared by wiping a small amount of gel samples onto carbon-coated copper grid followed by naturally evaporating the solvent. SEM pictures were taken using an XL 30 ESEM FEG field emission scanning electron microscope with 20 kV operating voltage. PXRD patterns were recorded by Rigaku D/max 2000 X-ray diffractometer with CuK_α1 radiation source.

Computations

The geometrical structures of mesitylene-mesitylene and mesitylene-CH_2Cl_2-mesitylene cluster were optimized at the B3LYP/6-31G(d) level. The CH/π interaction energies were calculated at the MP2/aug-cc-pVDZ level.[3] All the calculations were completed by employing Gaussian 09 program.

References

1 a) L. Ma, R. Jin, Z. Bian, C. Kang, Y. Chen, J. Xu and L. Gao, *Chem. Eur. J.*, 2012, **18**, 13168; b) L. Ma, R. Z. Jin, G. H. Lv, Z. Bian, M. X. Ding and L. X. Gao, *Synthesis*, 2007, **16**, 2461.

2 A. L. Spek, *J. Appl. Crystallogr.*, 2003, **36**, 7.

3 A. Fujii, K. Shibasaki, T. Kazama, R. Itaya, N. Mikami and S. Tsuzuki, *Phys. Chem. Chem. Phys.*, 2008, **10**, 2836.