SUPPLMENTARY INFORMATIONS

The interplay of secondary Hg…S, Hg…N and Hg…π bonding interactions in supramolecular structures of phenylmercury(II) dithiocarbamates

Vikram Singh,[†] Abhinav Kumar, [‡] Rajendra Prasad,[§] Gunjan Rajput,[†] M. G. B. Drew,[±] and

Nanhai Singh,* [†]

[†] Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi-221005, India

 [‡] Department of Chemistry, Faculty of Science, Lucknow University, Lucknow-226007, India
[§]Department of Chemistry, S. G. B. Amravati University, Amravati-444602, India
[±] Department of Chemistry, University of Reading, Whiteknight, Reading, RG6 6AD, UK. nsinghbhu@gmail.com

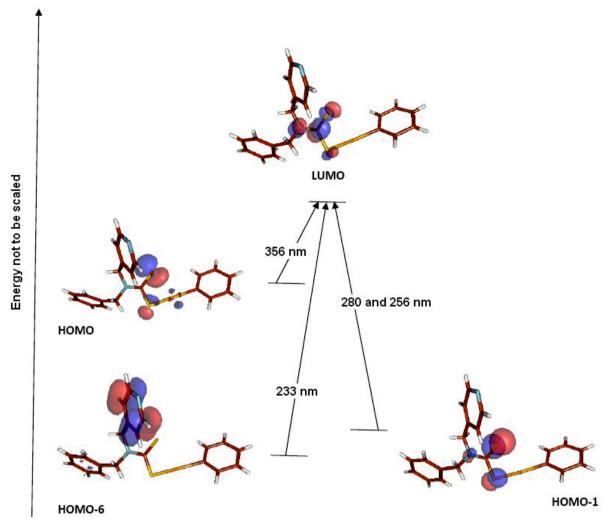


Fig. S1 Selected orbital transitions for complex 1 (orbital contour value 0.05).

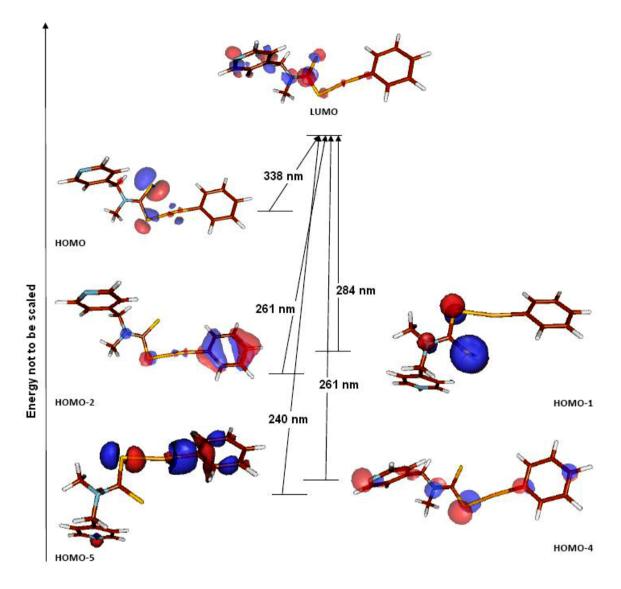


Fig. S2 Selected orbital transitions for 2 (orbital contour value 0.05).

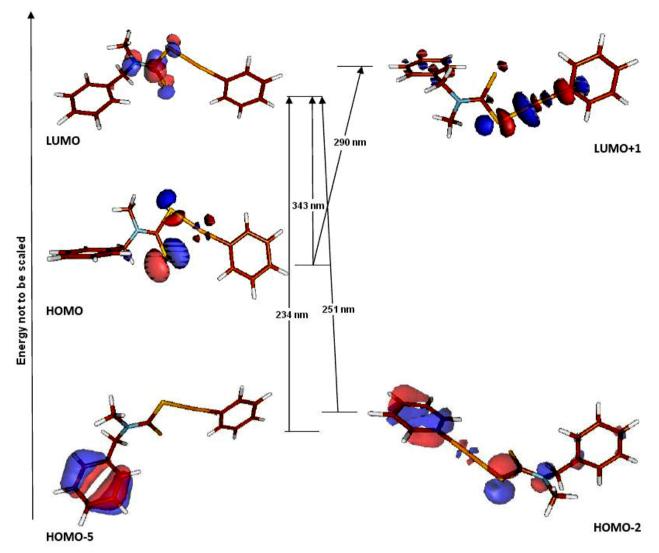


Fig. S3 Selected orbital transitions for complex 3 (orbital contour value 0.05).