

Molecular and supramolecular structures of Cd(II) complexes with hydralazine-based ligands; A new example for cyclization of hydrazonophthalazine to triazolophthalazine

Saied M. Soliman^{1,*}, Raghdaa A. Massoud¹, Hessa H. Al-Rasheed^{2,*} and Ayman El-Faham^{1,2}

¹Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia, Alexandria 21321, Egypt; saied1soliman@yahoo.com (S.M.S.); raghdaamassoud@yahoo.com (R. A. M); aymanel_faham@hotmail.com

²Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia; halbahli@ksu.edu.sa (H.H. A.); aelfaham@ksu.edu.sa (A.E-F.)

* Correspondence: Saied M. Soliman: saied1soliman@yahoo.com (S.M.S), Tel.: +201111361059; and Ayman El-Faham: aymanel_faham@hotmail.com (A.E-F.), Tel.: +966114673195

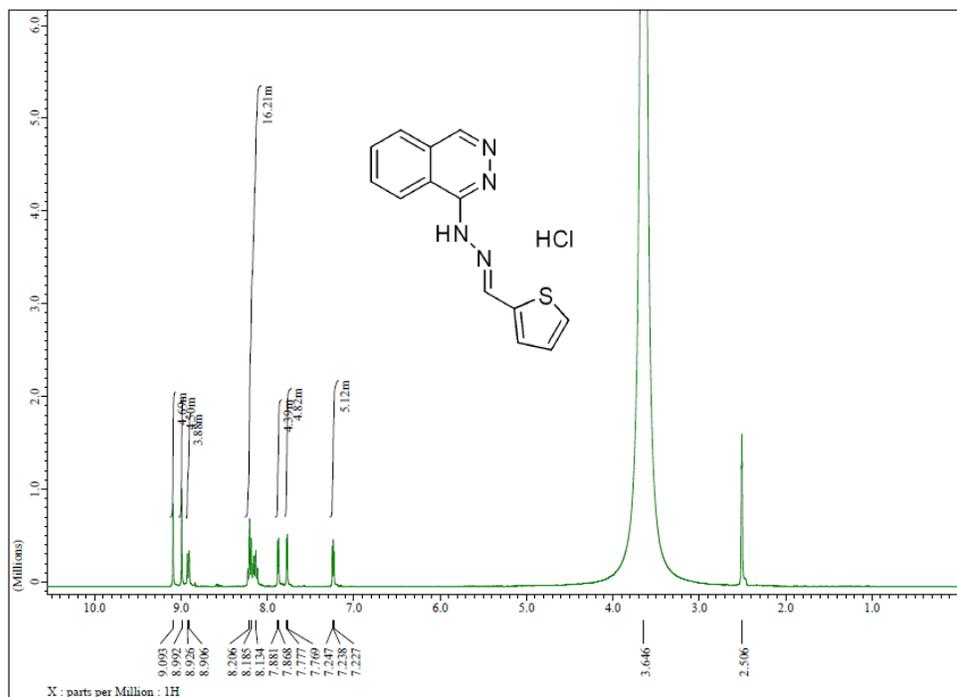


Figure S1. ¹H-NMR spectra of HL.

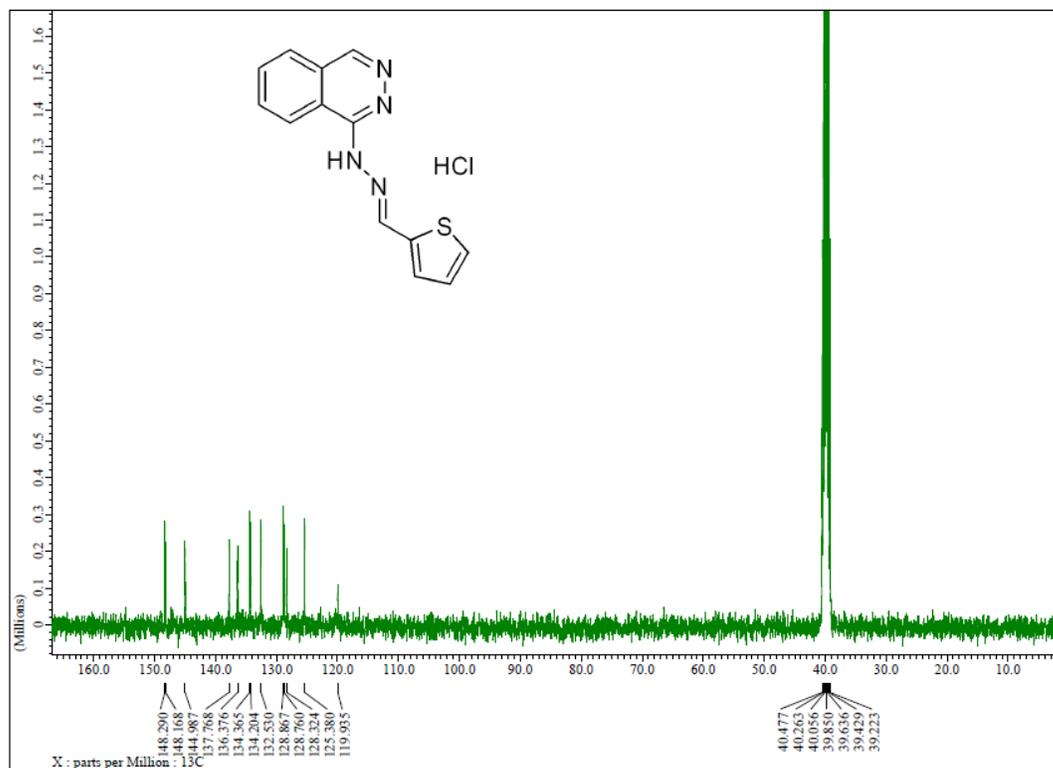


Figure S2. ^{13}C -NMR spectra of HL.

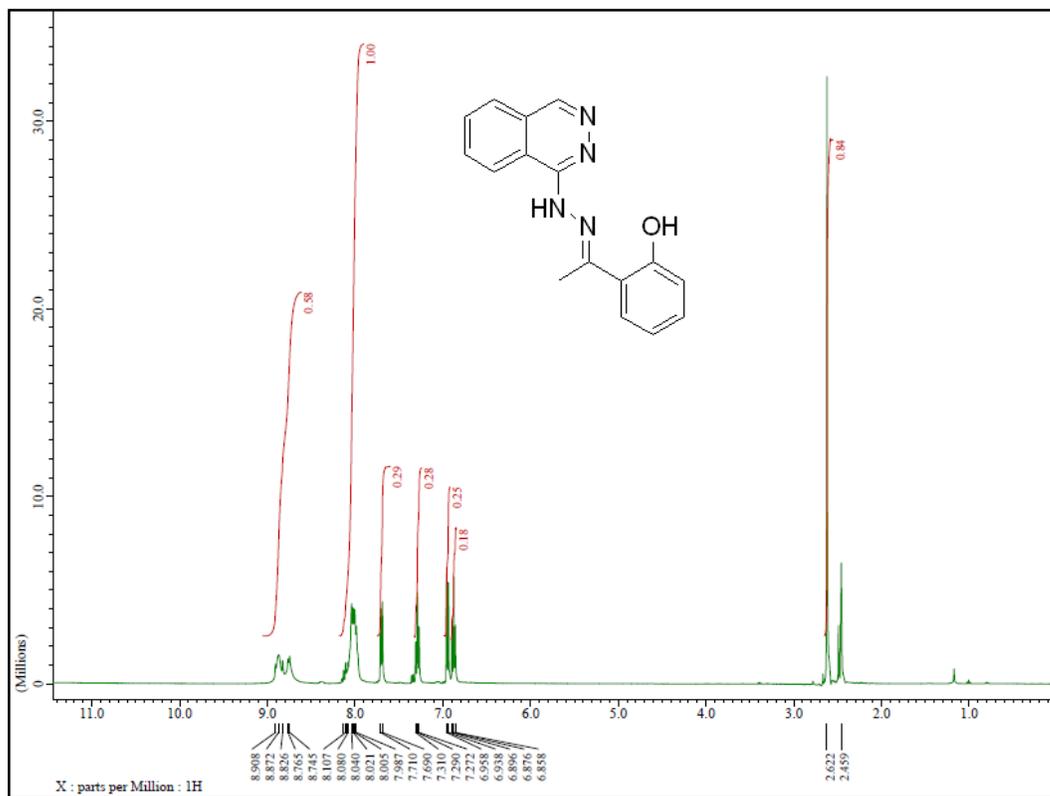


Figure S3. ¹H-NMR spectra of HL^{OH}.

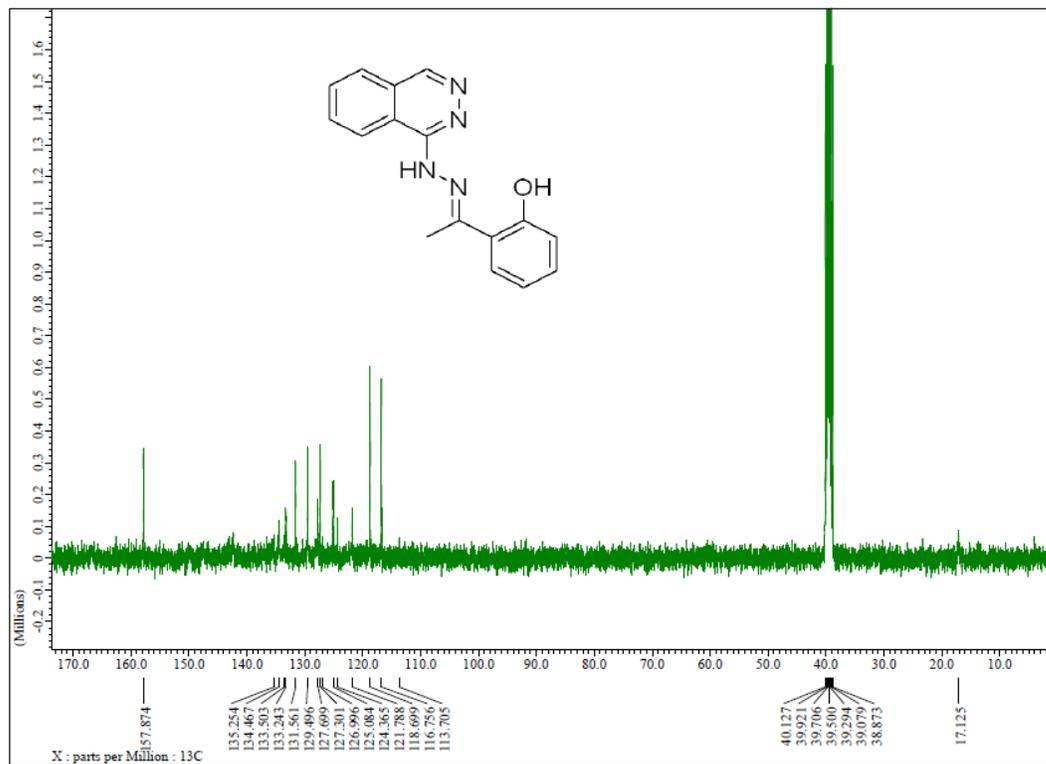


Figure S4. ^{13}C -NMR spectra of HL^{OH} .

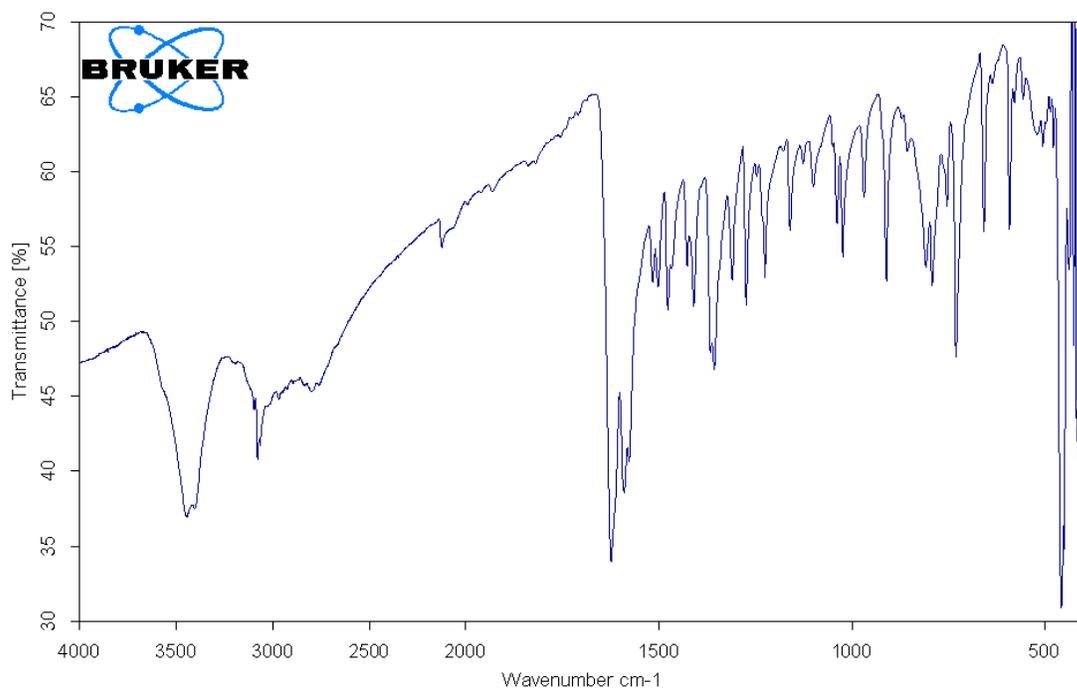


Figure S5. FTIR spectra of $[\text{Cd}(\text{H}_2\text{L})\text{Cl}_3]_n \cdot \text{H}_2\text{O}$; **1**.

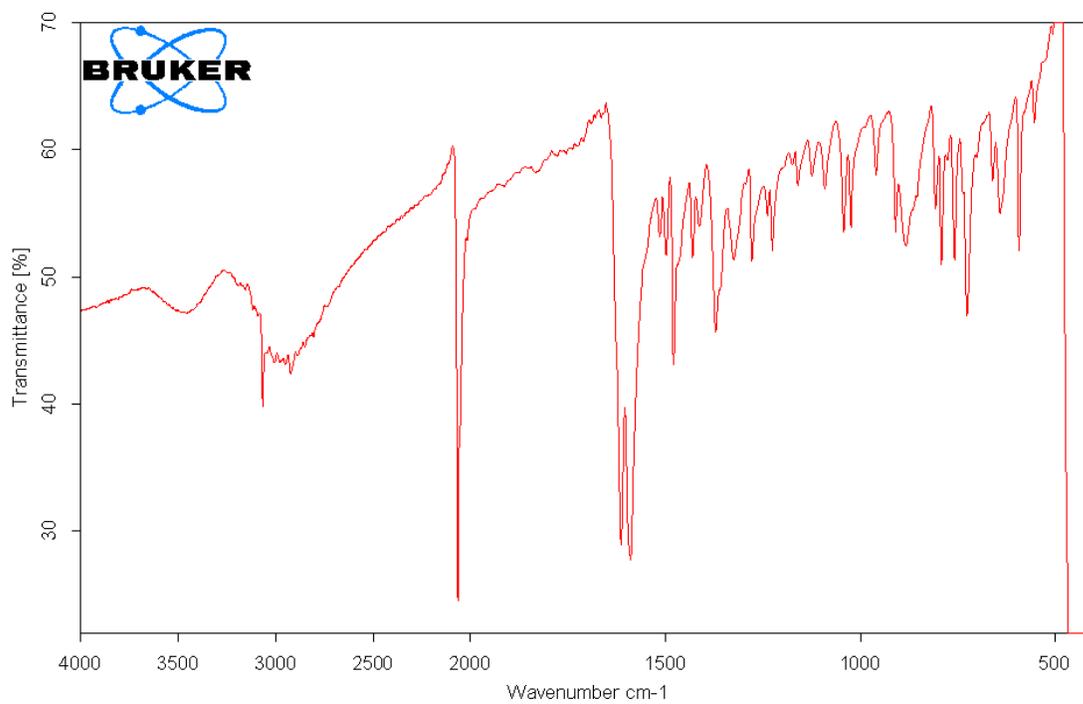


Figure S6. FTIR spectra of $[\text{Cd}(\text{TPT})(\text{SCN})_2]_n \cdot \text{H}_2\text{O}$; **2**.

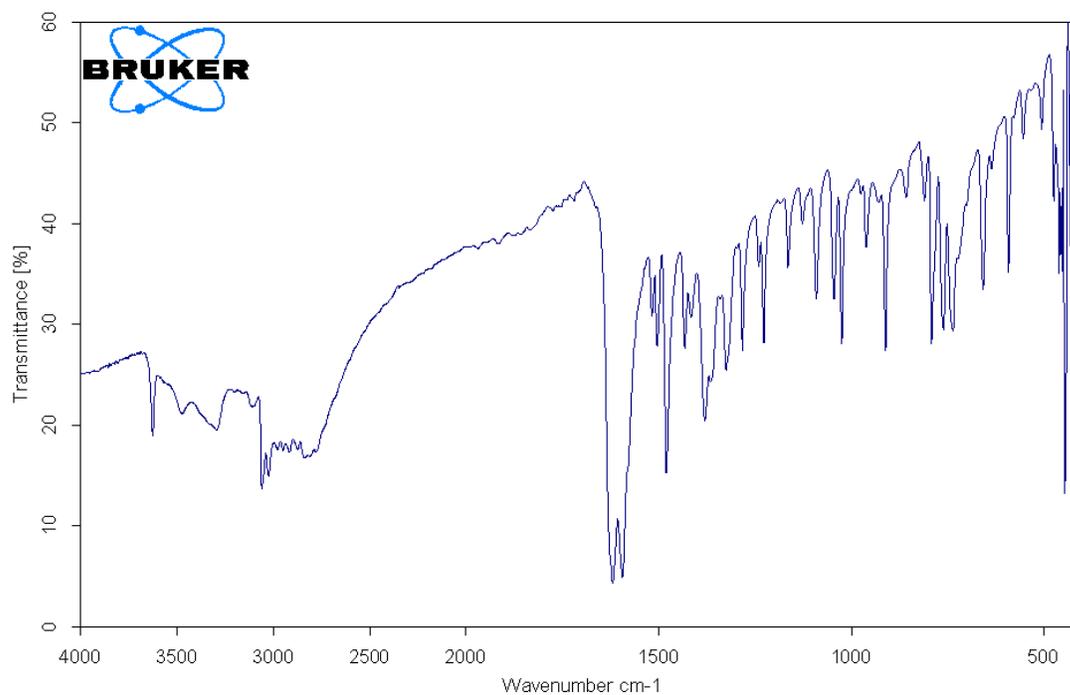
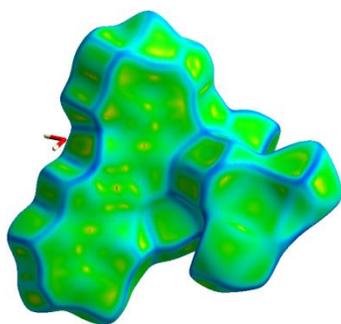
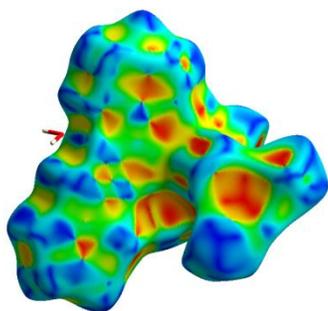
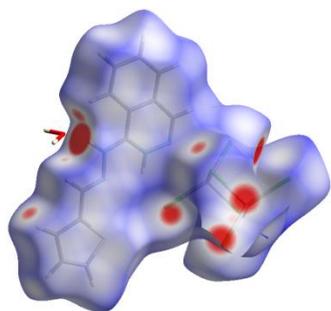
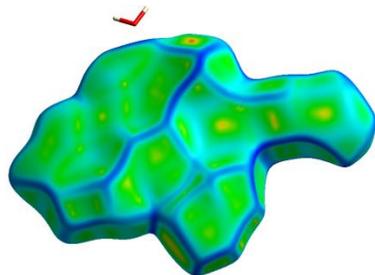
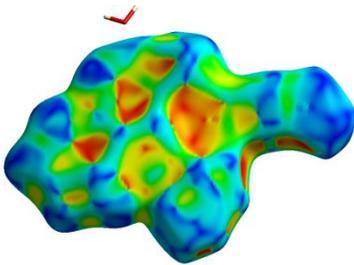
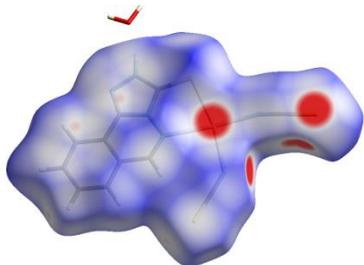
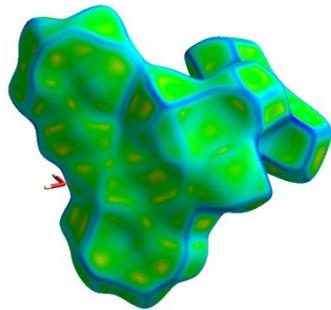
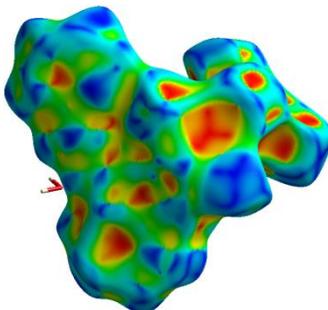
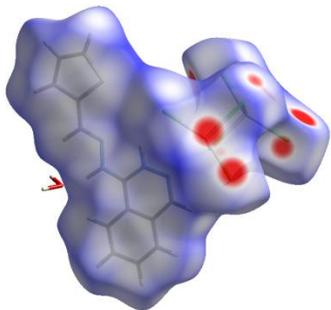


Figure S7. FTIR spectra of $[\text{Cd}_3(\text{Hydralazine})_2(\text{H}_2\text{O})_2\text{Cl}_6] \cdot 3$.

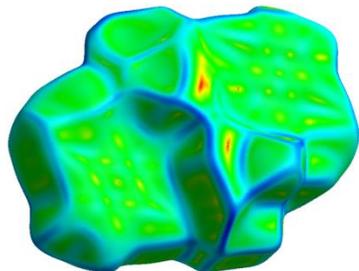
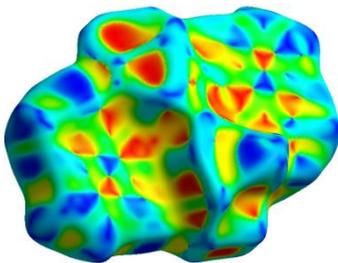
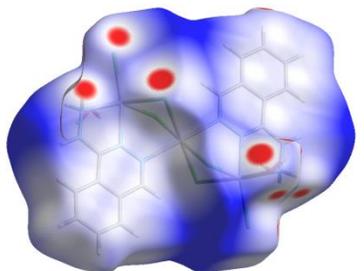
1



2



3



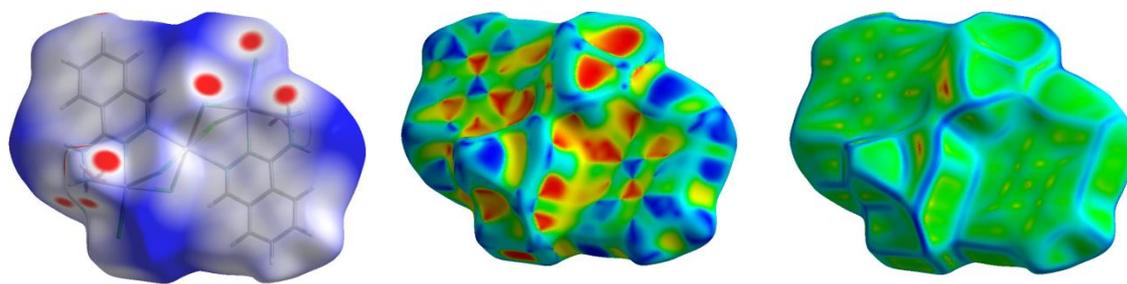


Figure S8. Hirshfeld d_{norm} (-0.2-2.0), shape index (SI) and curvedness surfaces of the studied complexes.