

Electronic Supplementary Information

Coordination polymers fabricated from $\text{Cd}(\text{NO}_3)_2$ and N,N',O -pincer type isonicotinoylhydrazone based polytopyc ligands – an insight from experimental and theoretical investigations

Ghodrat Mahmoudi,^{*a} Farhad Akbari Afkhami,^b Ali Akbar Khandar,^c Jonathan M. White,^d Waldemar Maniukiewicz,^{*e} Maria G. Babashkina,^f Mariusz P. Mitoraj,^{*g} Filip Sagan^g and Damir A. Safin^{*fhi}

^a Department of Chemistry, Faculty of Science, University of Maragheh, P.O. Box 55181-83111, Maragheh, Iran. E-mail: ghodratmahmoudi@gmail.com

^b Department of Chemistry, The University of Alabama, Box 870336, 250 Hackberry Lane, Tuscaloosa, Alabama 35487, USA

^c Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, 51666-16471, Tabriz, Iran

^d BIO-21 Molecular Science and Biotechnology, University of Melbourne, Parkville, Victoria 3052, Australia

^e Institute of General and Ecological Chemistry, Lodz University of Technology, Żeromskiego 116, 90-924 Łódź, Poland. E-mail: waldemar.maniukiewicz@p.lodz.pl

^f Advanced Materials for Industry and Biomedicine laboratory, Kurgan State University, Sovetskaya Str. 63/4, 640020 Kurgan, Russian Federation. E-mail: damir.a.safin@gmail.com

^g Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University, R. Gronostajowa 2, 30-387 Cracow, Poland. E-mail: mitoraj@chemia.uj.edu.pl

^h Innovation Center for Chemical and Pharmaceutical Technologies, Ural Federal University named after the First President of Russia B.N. Yeltsin, Mira Str. 19, Ekaterinburg, 620002, Russian Federation

ⁱ University of Tyumen, Volodarskogo Str. 6, 625003 Tyumen, Russian Federation

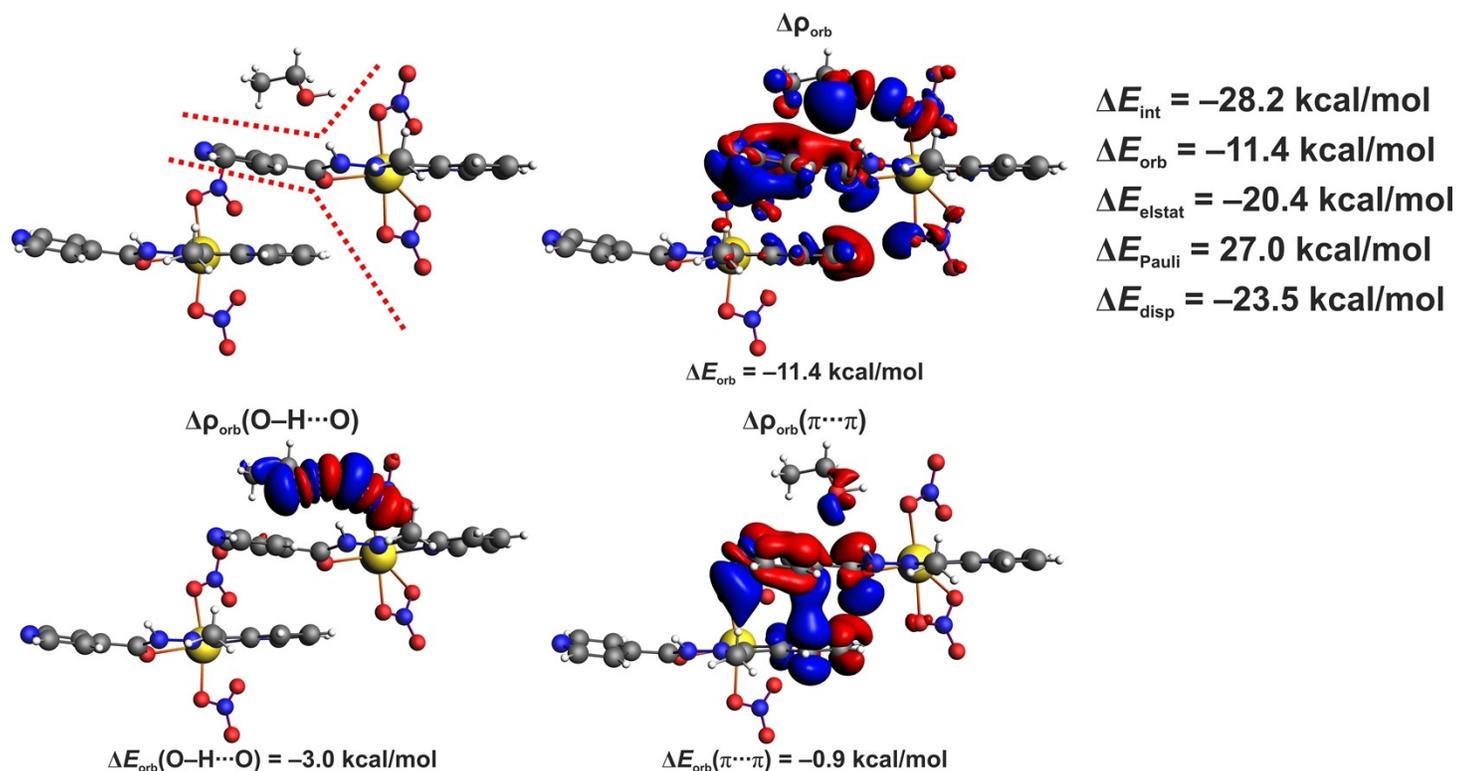


Fig. S1 ETS-NOCV energy decomposition results for the cluster model of **2**. (top) The considered model including fragmentation pattern, ETS based results, overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} . (bottom) The constituting NOCVs based deformation density contributions $\Delta\rho_{\text{orb}}(i)$ with the corresponding energies $\Delta E_{\text{orb}}(i)$.

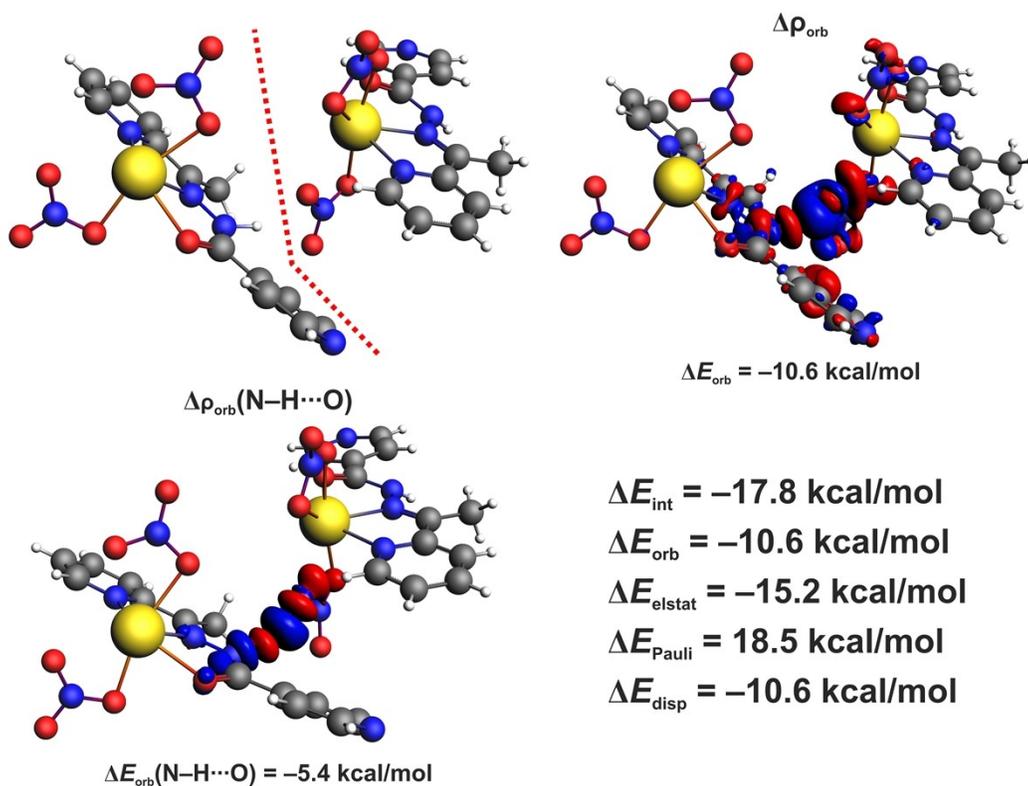


Fig. S2 ETS-NOCV energy decomposition results for the cluster model of **2**. (top) The considered model including fragmentation pattern, ETS based results, overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} . (bottom) The constituting NOCVs based deformation density contributions $\Delta\rho_{\text{orb}}(i)$ with the corresponding energies $\Delta E_{\text{orb}}(i)$.

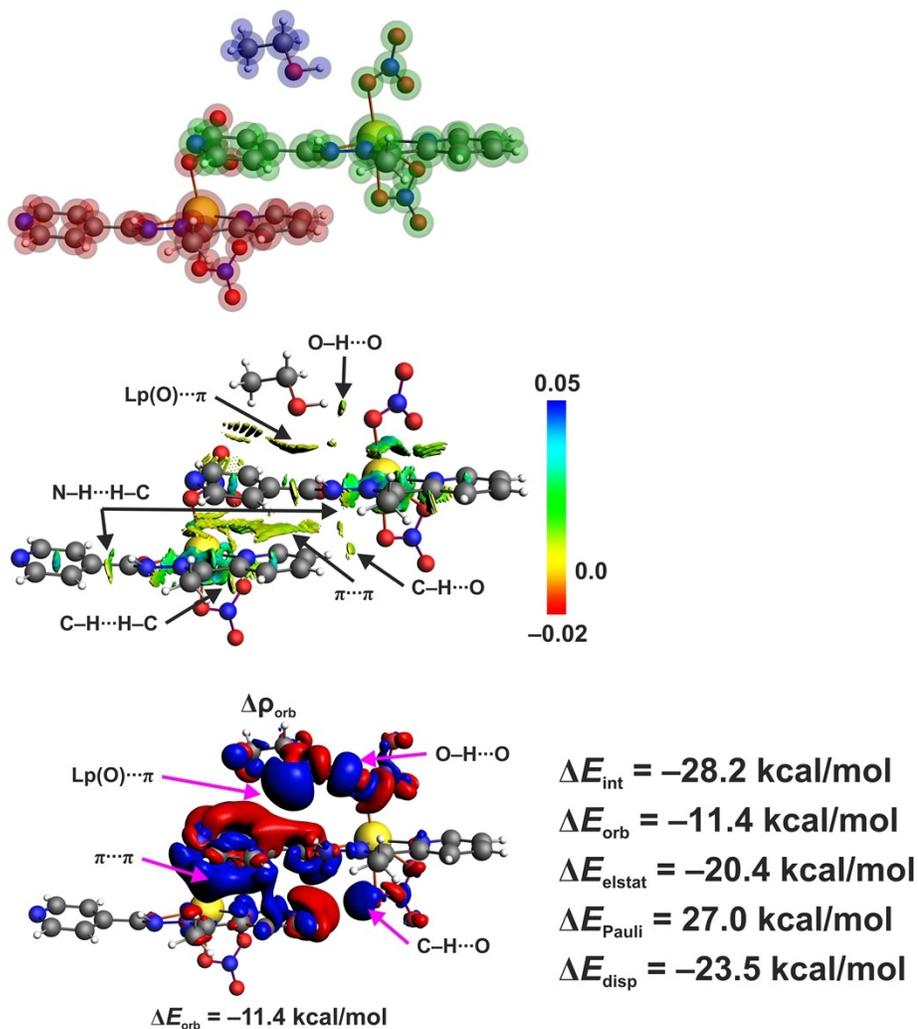


Fig. S3 ETS-NOCV energy decomposition results for the cluster model of **2**. (top) The considered model, (middle) NCI contour plot and (bottom) overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} .

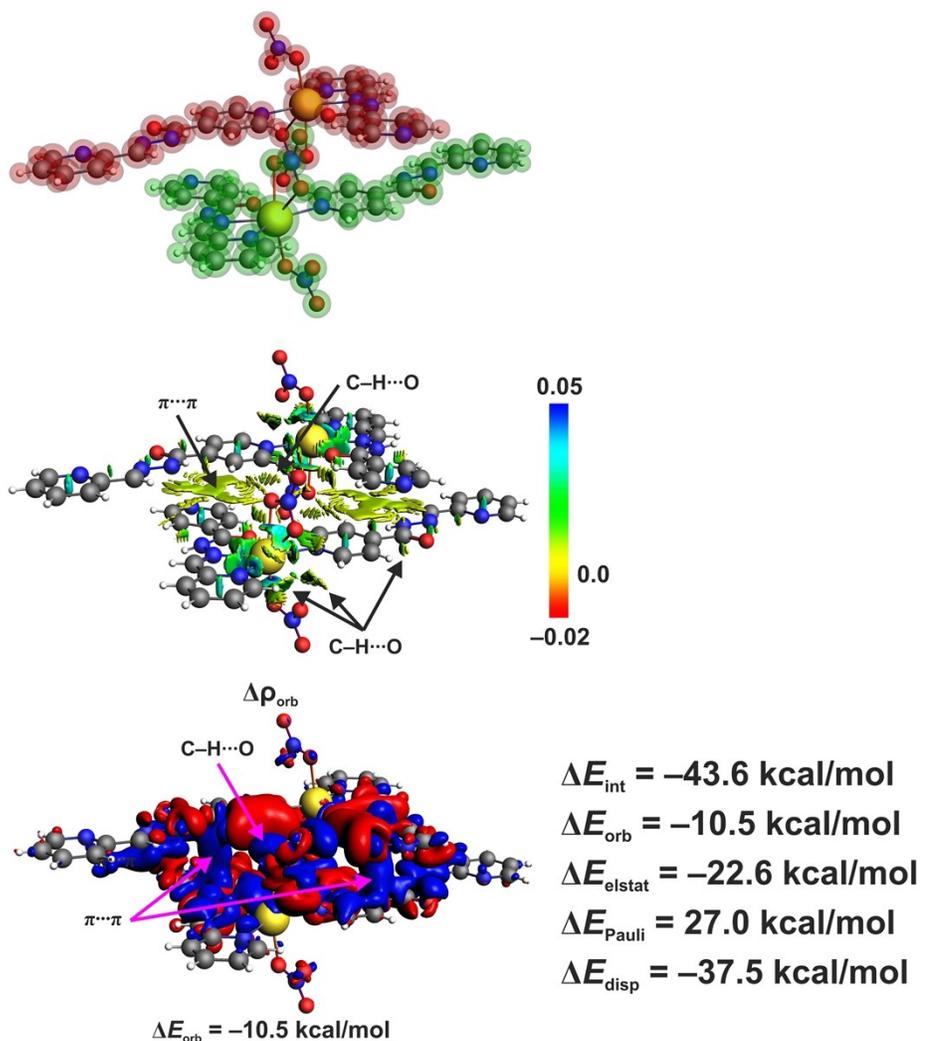


Fig. S4 ETS-NOCV energy decomposition results for the cluster model of **1**. (top) The considered model, (middle) NCI contour plot and (bottom) overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} .

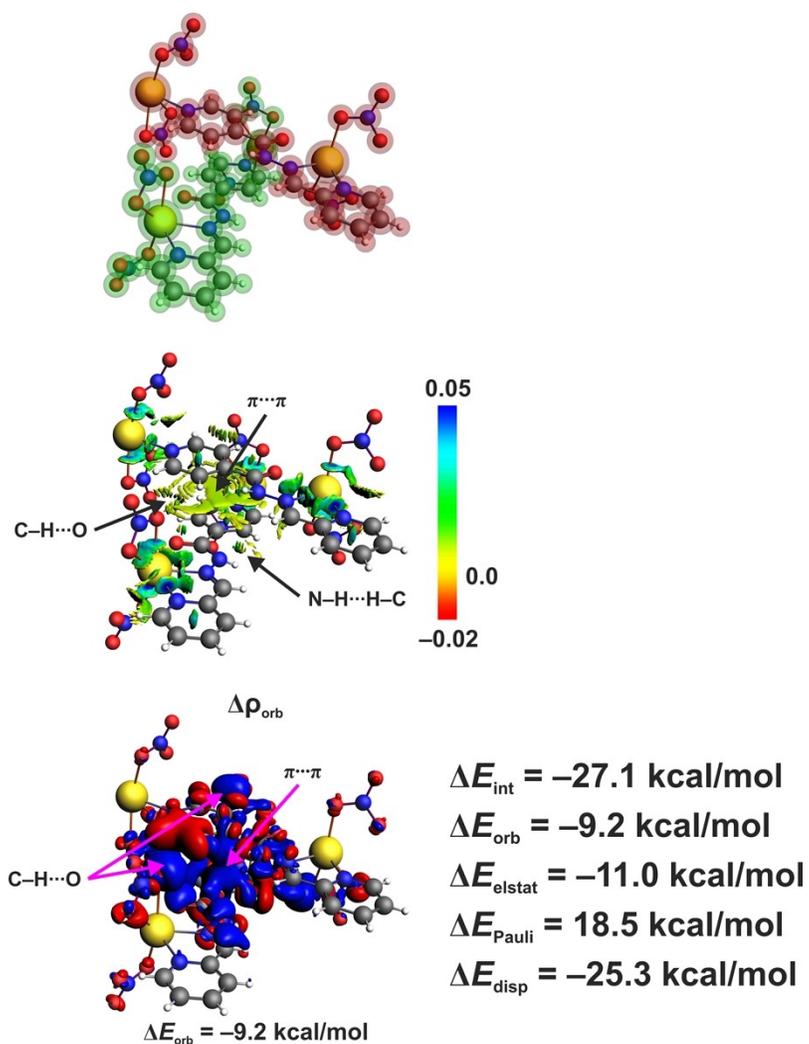
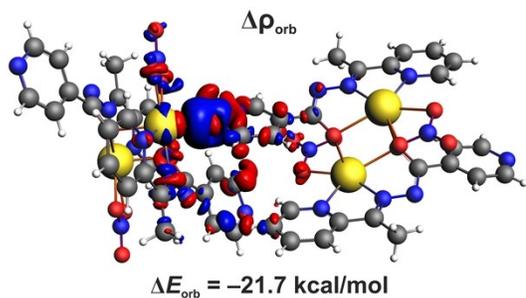
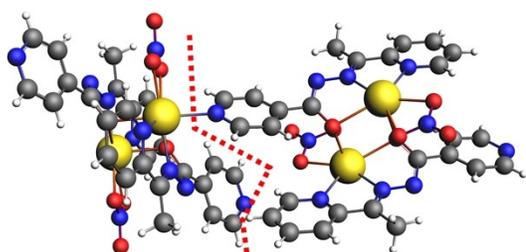


Fig. S5 ETS-NOCV energy decomposition results for the cluster model of **1**. (top) The considered model, (middle) NCI contour plot and (bottom) overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} .



$$\begin{aligned} \Delta E_{\text{int}} &= -32.7 \text{ kcal/mol} \\ \Delta E_{\text{orb}} &= -21.7 \text{ kcal/mol} \\ \Delta E_{\text{elstat}} &= -62.2 \text{ kcal/mol} \\ \Delta E_{\text{Pauli}} &= 74.3 \text{ kcal/mol} \\ \Delta E_{\text{disp}} &= -23.0 \text{ kcal/mol} \end{aligned}$$

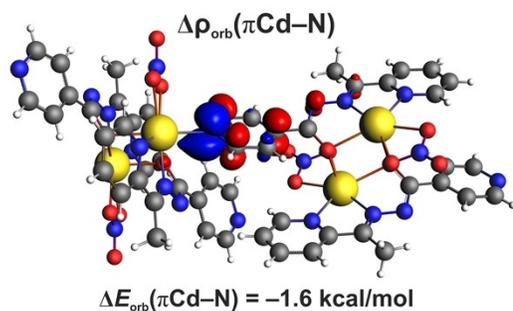
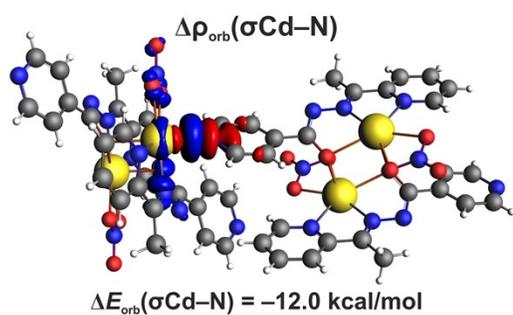


Fig. S6 ETS-NOCV energy decomposition results, describing the Cd–N bond in the cluster model of **3**. (top) ETS based results, overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} . (bottom) The constituting NOCVs based deformation density contributions $\Delta\rho_{\text{orb}}(i)$ with the corresponding energies $\Delta E_{\text{orb}}(i)$.

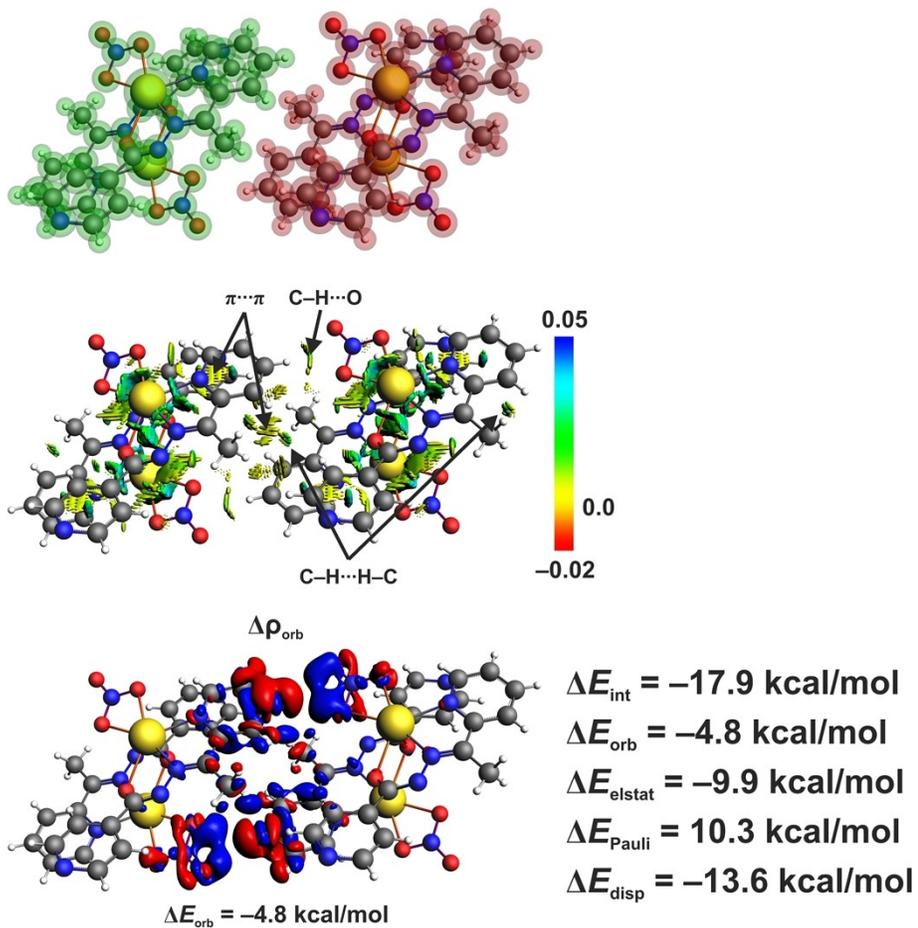


Fig. S7 ETS-NOCV energy decomposition results for the cluster model of **3**. (top) The considered model, (middle) NCI contour plot and (bottom) overall deformation density $\Delta\rho_{\text{orb}}$ with the corresponding energy ΔE_{orb} .