

Supporting Information

Designing and exploration of the biological potentials of novel centrosymmetric heteroleptic Copper(II) carboxylates

Viola ¹, Niaz Muhammad ^{*1}, Awal Noor ^{*2}, Muhammad Sirajuddin ³, Maciej Kubicki ⁴, Shahnaz Rahim ¹, Abdus Samad ⁵, Shaukat Shujah ⁶, Abdul Wadood ⁵ and Saqib Ali ⁷

¹ Department of Chemistry, Abdul Wali Khan University Mardan, Mardan 23200, Pakistan.

² Department of Basic Sciences, Preparatory Year Deanship, King Faisal University, Al-Hassa 31982, Saudi Arabia.

³ Department of Chemistry, University of Science and Technology Bannu, Bannu 28100, Pakistan.

⁴ Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland.

⁵ Department of Biochemistry, Abdul Wali Khan University Mardan, Mardan 23200, Pakistan.

⁶ Department of Chemistry, Kohat University of Science & Technology, Kohat, 26000 Pakistan.

⁷ Department of Chemistry, Quaid-I-Azam University Islamabad, Islamabad 45320, Pakistan.

* Correspondence: drniaz@awkum.edu.pk (N.M.); anoor@kfu.edu.sa (A.N.)

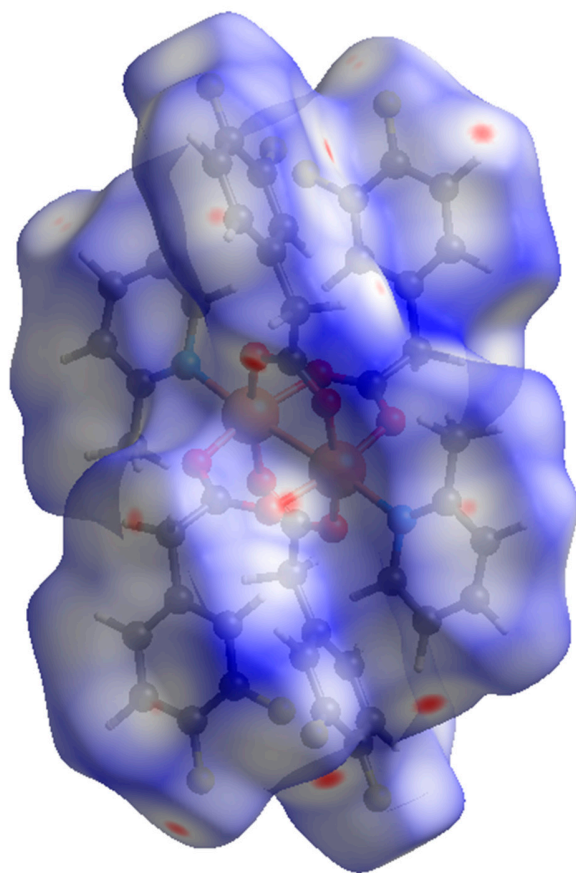


Figure S1. View of the three-dimensional Hirshfeld surface of **1** plotted over d_{norm} in the range -0.1216 to 1.3131 .

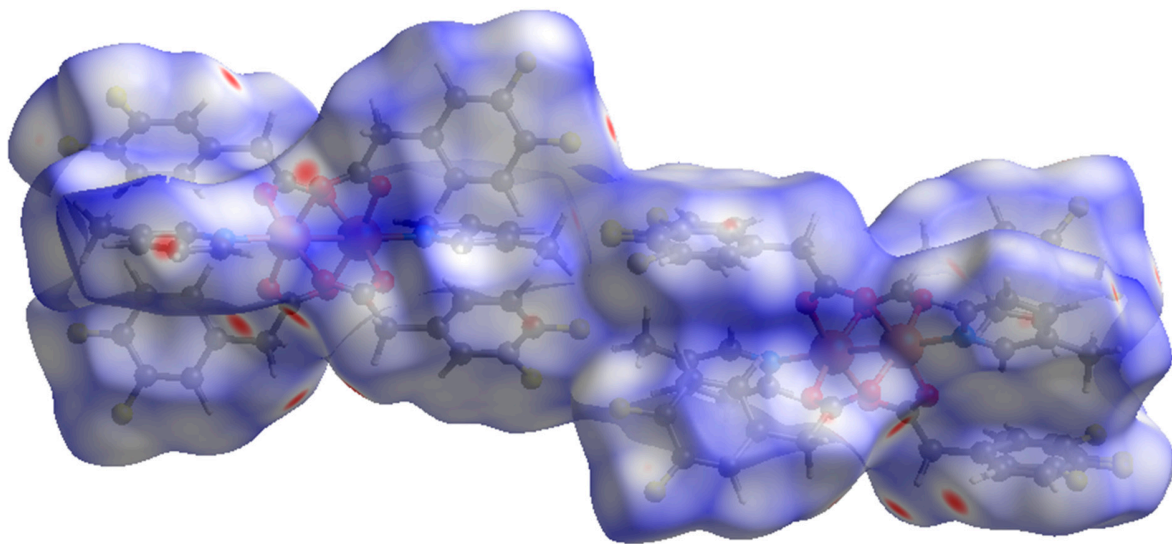


Figure S2. View of the three-dimensional Hirshfeld surface of **2** plotted over d_{norm} in the range -0.1965 to 1.4003 .

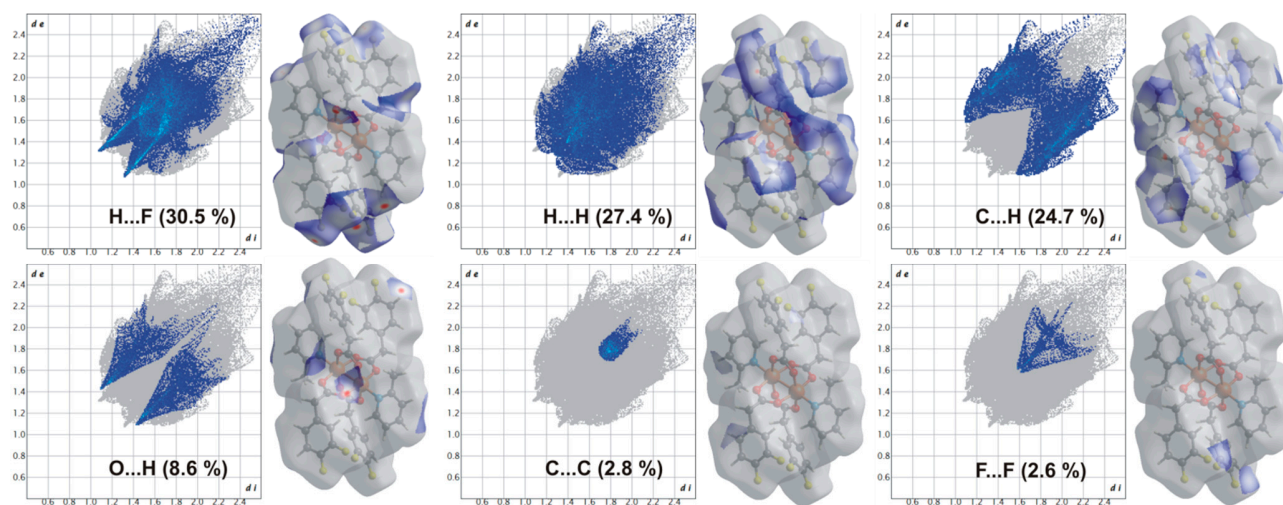


Figure S3. Two-dimensional fingerprint plots for all intermolecular contacts in 1. The percentage of contribution is specified for each contact.

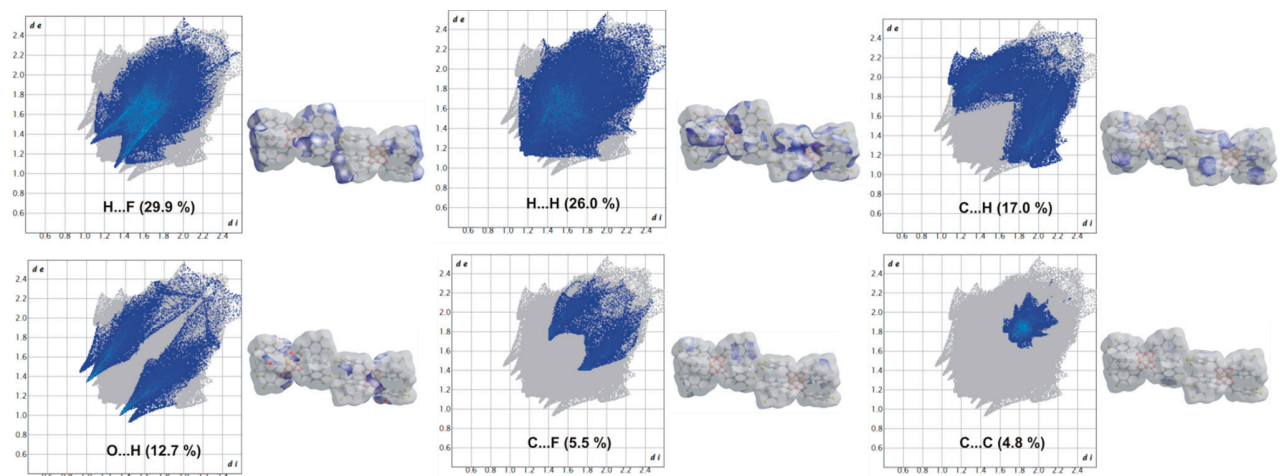


Figure S4. Two-dimensional fingerprint plots for all intermolecular contacts in 2. The percentage of contribution is specified for each contact.

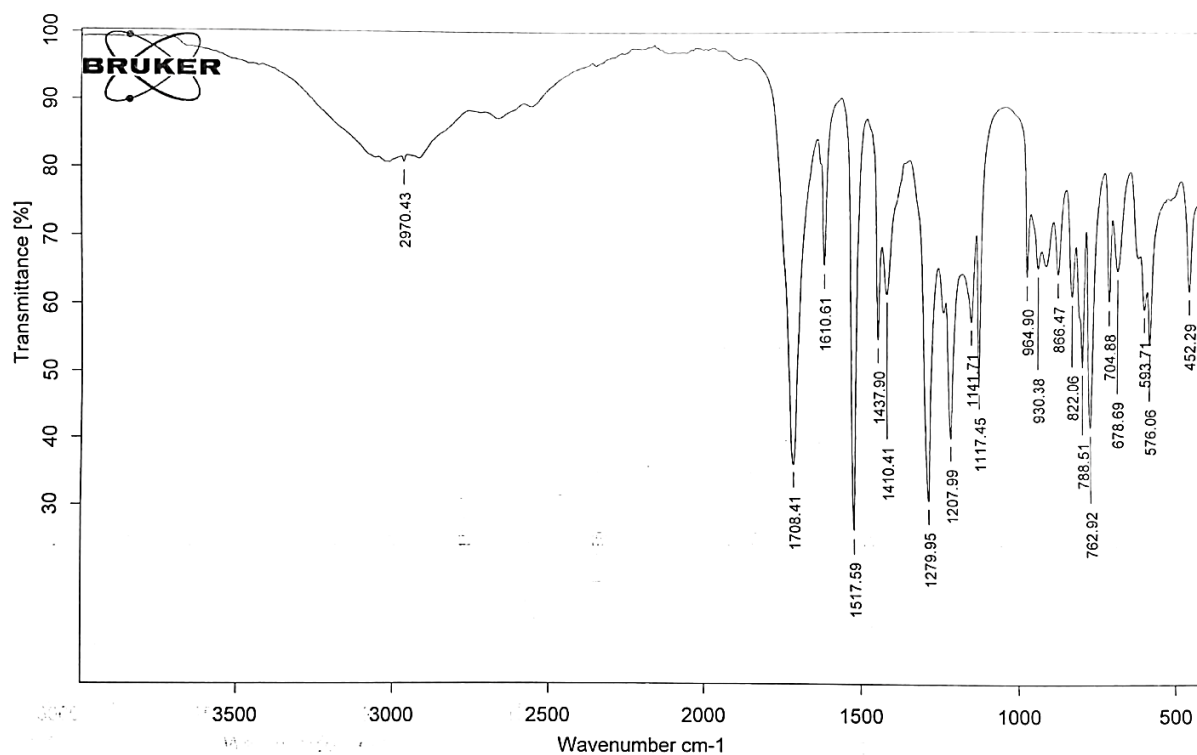


Figure S5: FTIR spectrum of ligand acid.

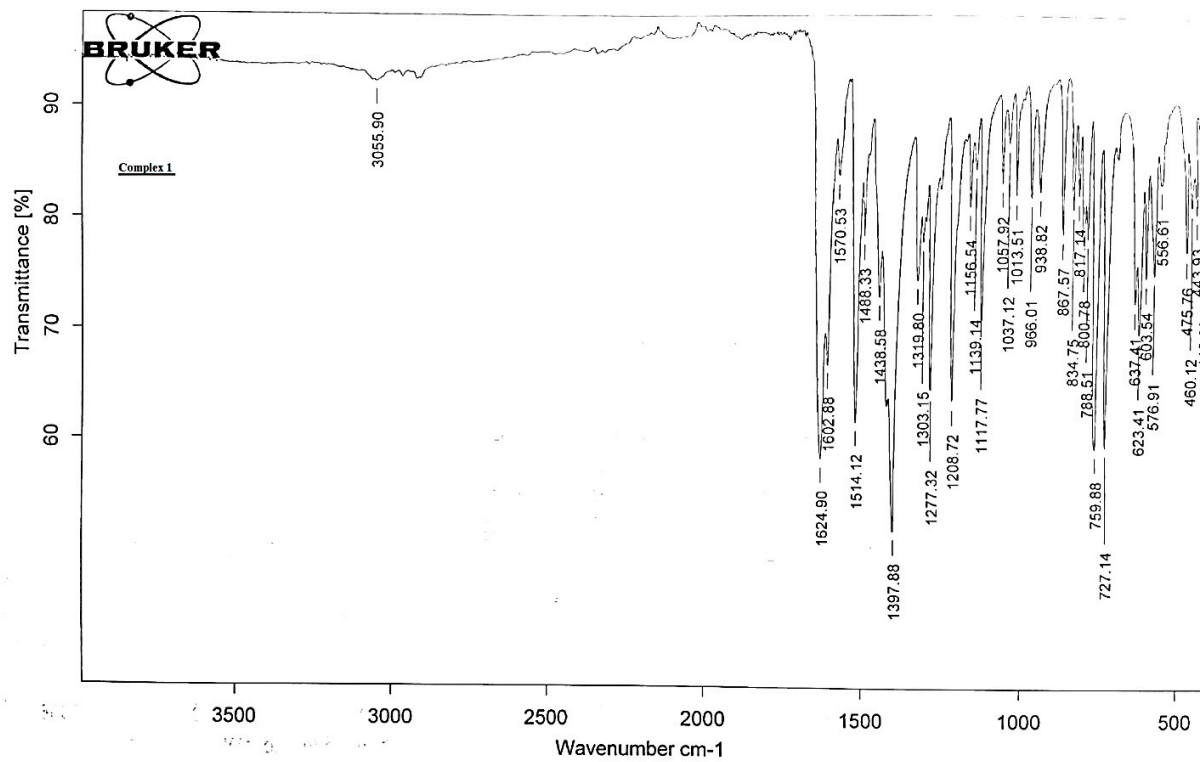


Figure S6: FTIR spectrum of complex 1.

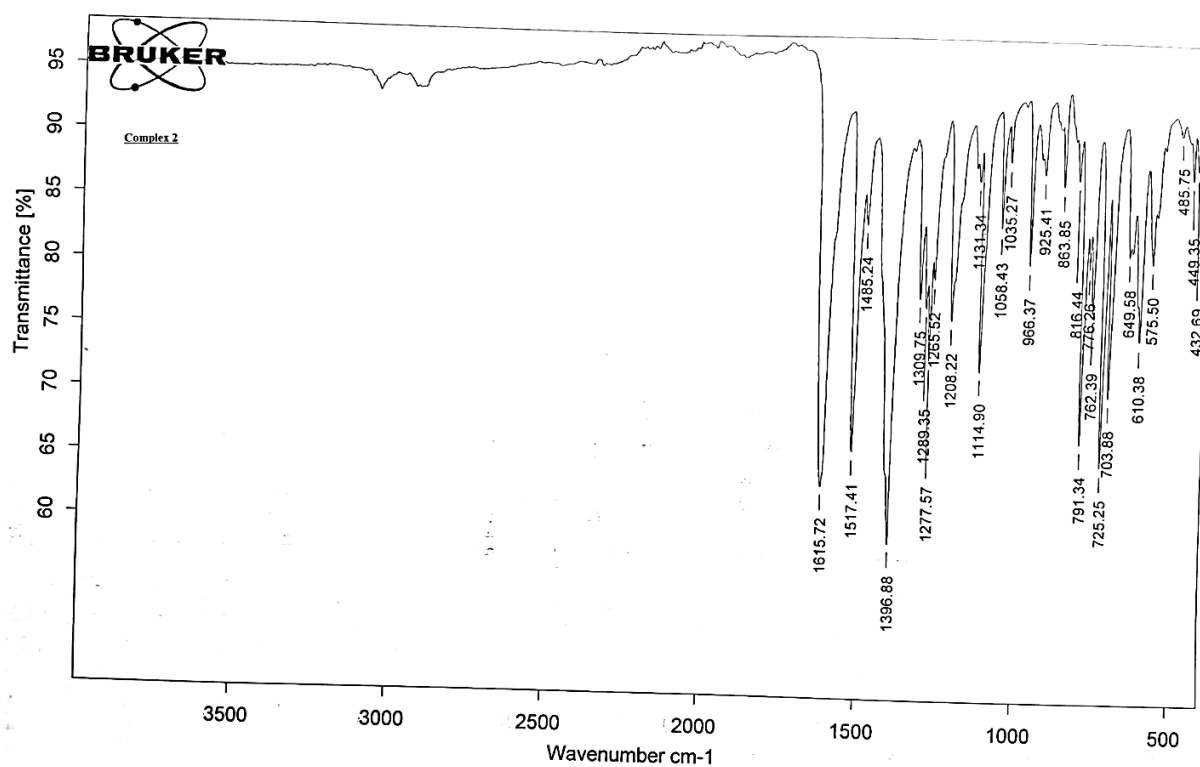


Figure S7: FTIR spectrum of complex 2.

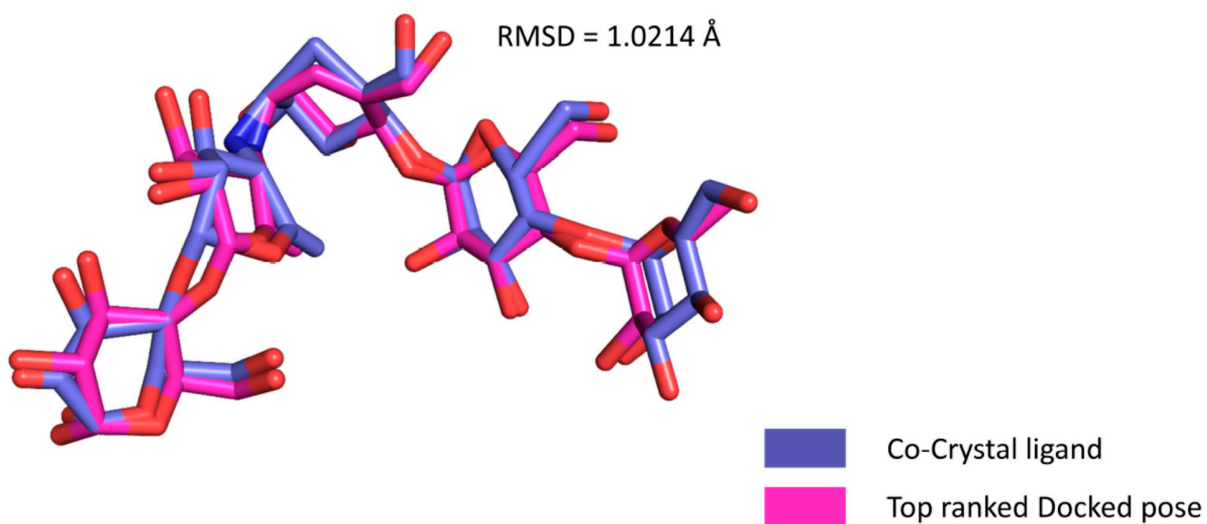


Figure S8: Co-crystal Ligand and Top ranked docked pose.