

Structure directing role of CH \cdots X (X = C, N, S, Cl) interactions in three ionic cobalt(III) complexes: X-ray investigation and DFT study using QTAIM Vr predictor to eliminate the effect of pure coulombic forces

Susovan Bera,^a Sudip Bhunia,^a Rosa M. Gomila,^b Michael G. B. Drew,^c Antonio Frontera,^{b,*} and Shouvik Chattopadhyay^{a,*}

^a*Department of Chemistry, Inorganic Section, Jadavpur University, Kolkata - 700032, India. Tel: +91-33-24572941, E-mail: shouvik.chem@gmail.com*

^b*Department of Chemistry, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Balears), SPAIN. E-mail: toni.frontera@uib.es*

^c*School of Chemistry, The University of Reading, P.O. Box 224, Whiteknights, Reading RG6 6AD, United Kingdom*

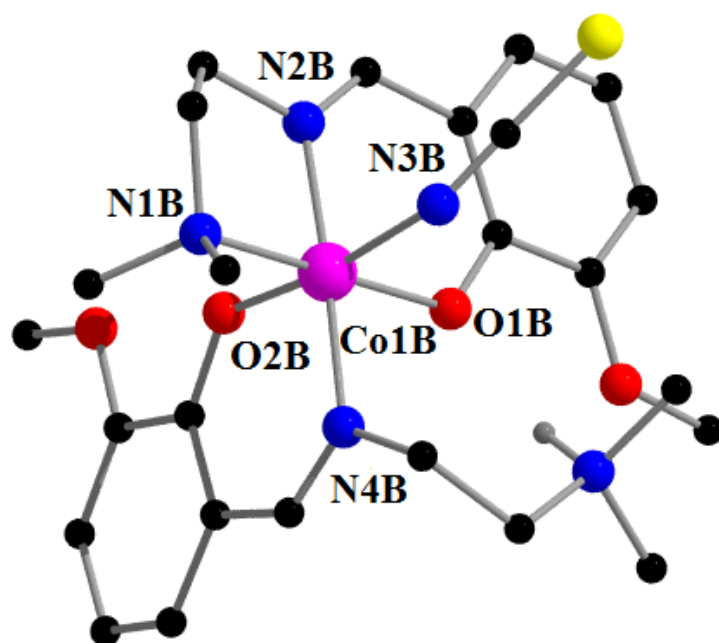


Fig. S1: Perspective view of the cationic part (Unit B) of complex **3** with selective atom numbering scheme. Only one hydrogen atom (attached with the amine nitrogen atom) is shown.

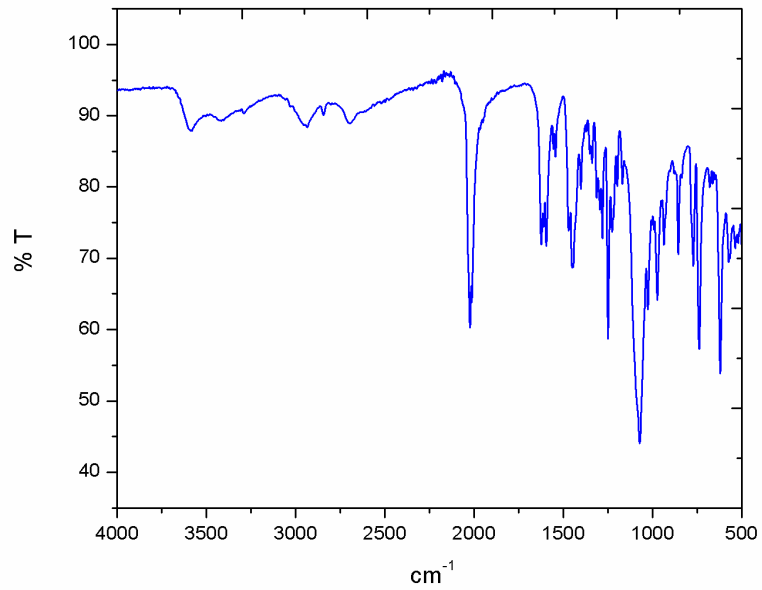


Fig. S2:IR spectrum of complex 1.

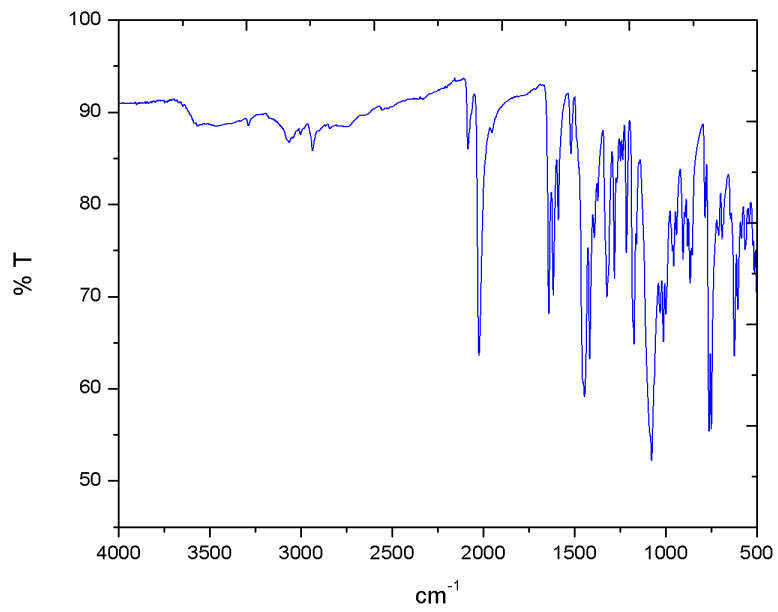


Fig. S3:IR spectrum of complex 2.

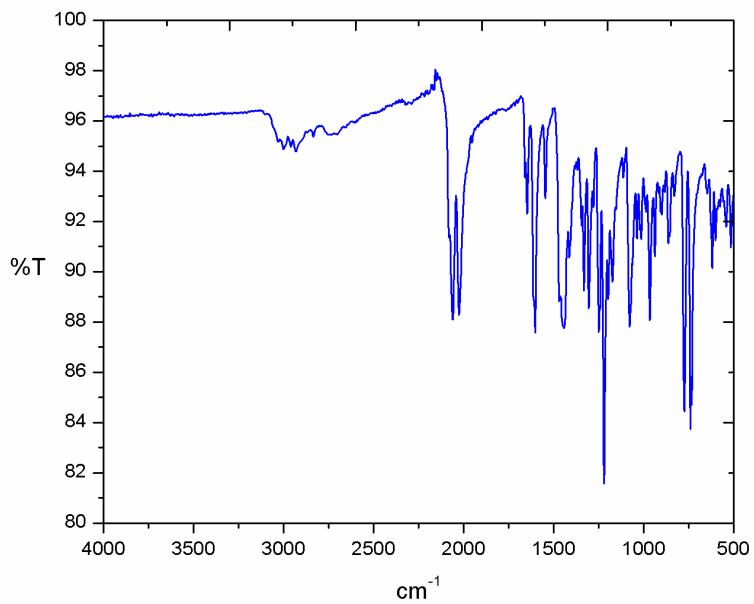


Fig. S4: IR spectrum of complex 3.

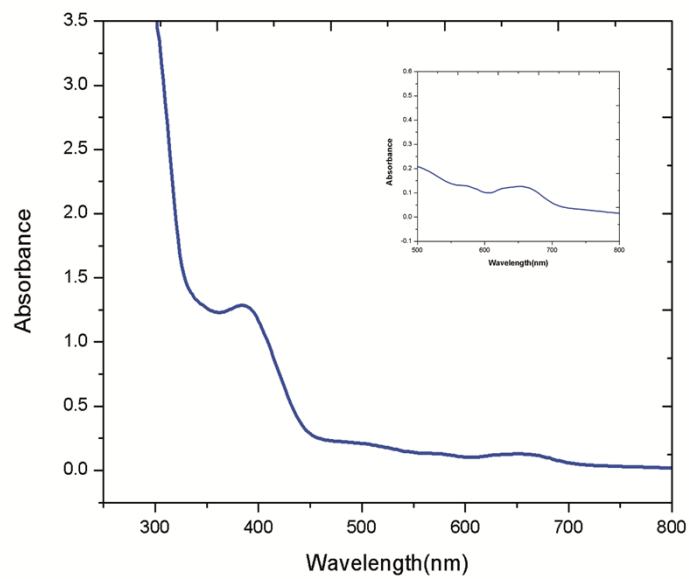


Fig. S5: UV-Vis spectrum of complex 3.

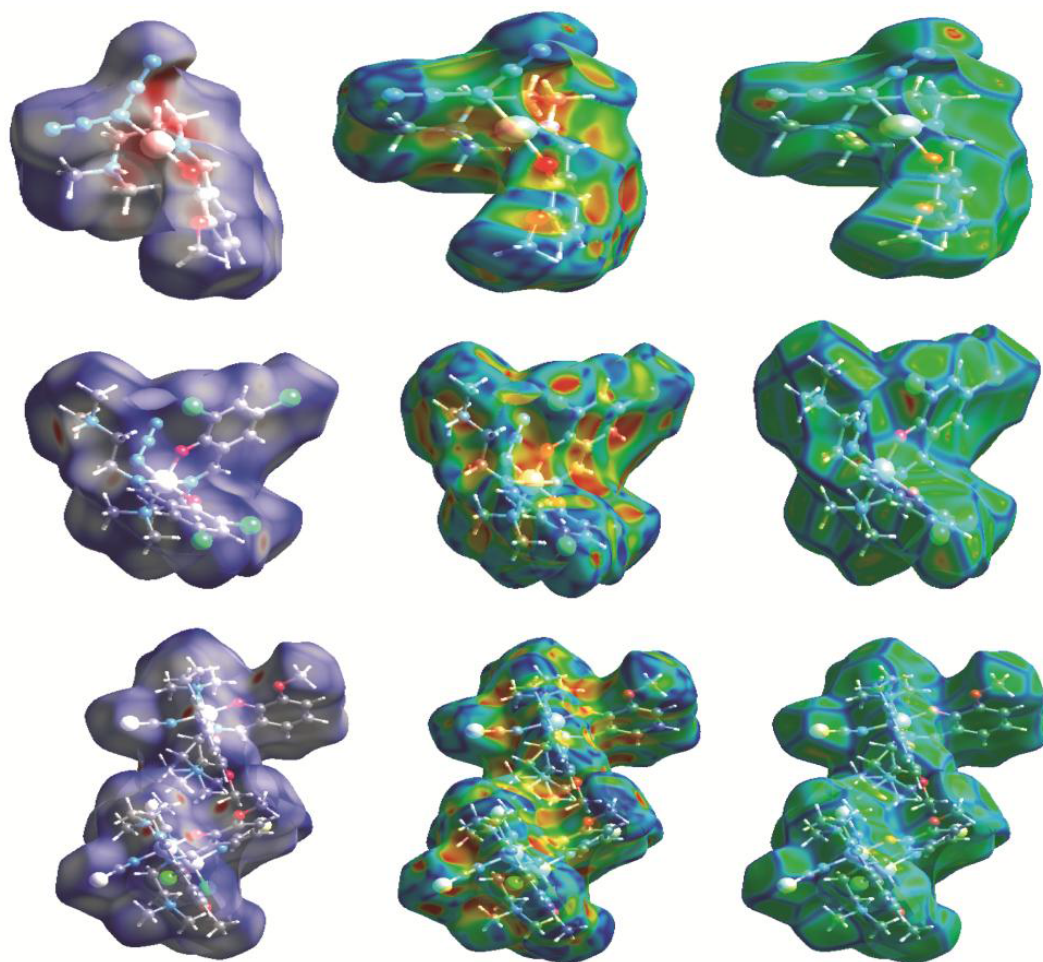


Fig. S6: Hirshfeld surfaces of complexes **1**, **2** and **3** mapped over d_{norm} (left), shape index (middle) and curvedness (right).

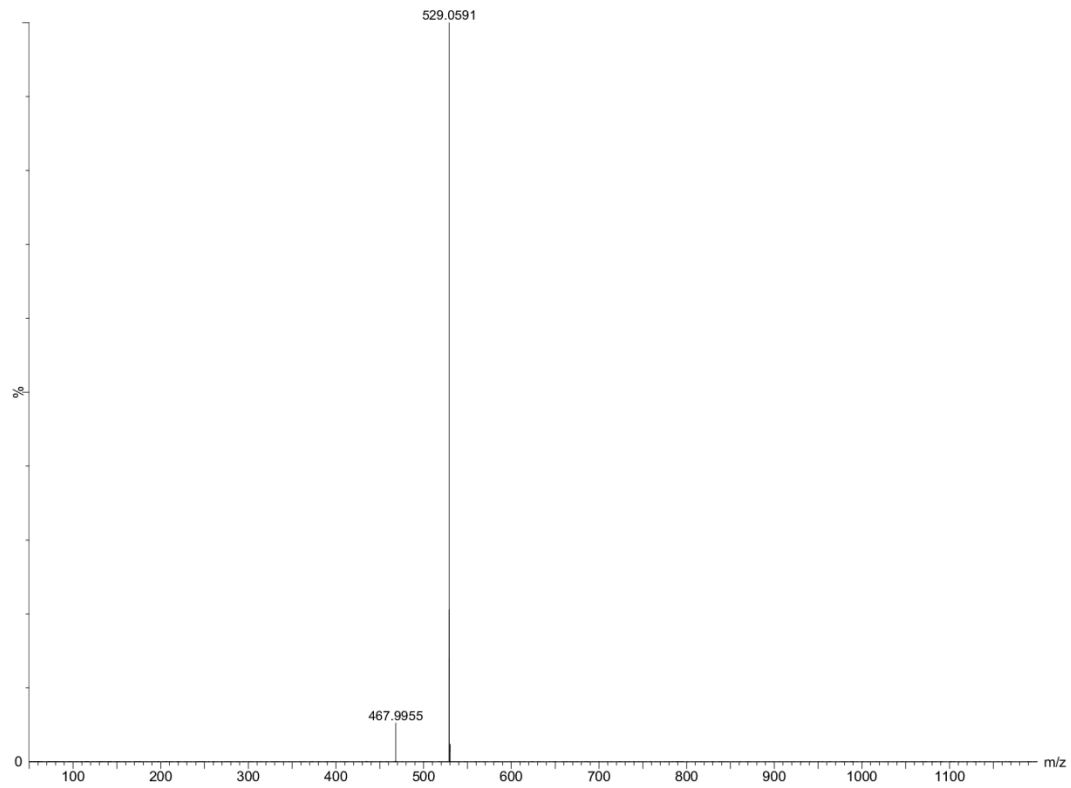


Fig. S7: ESI-MS spectrum of complex **1** in acetonitrile medium.

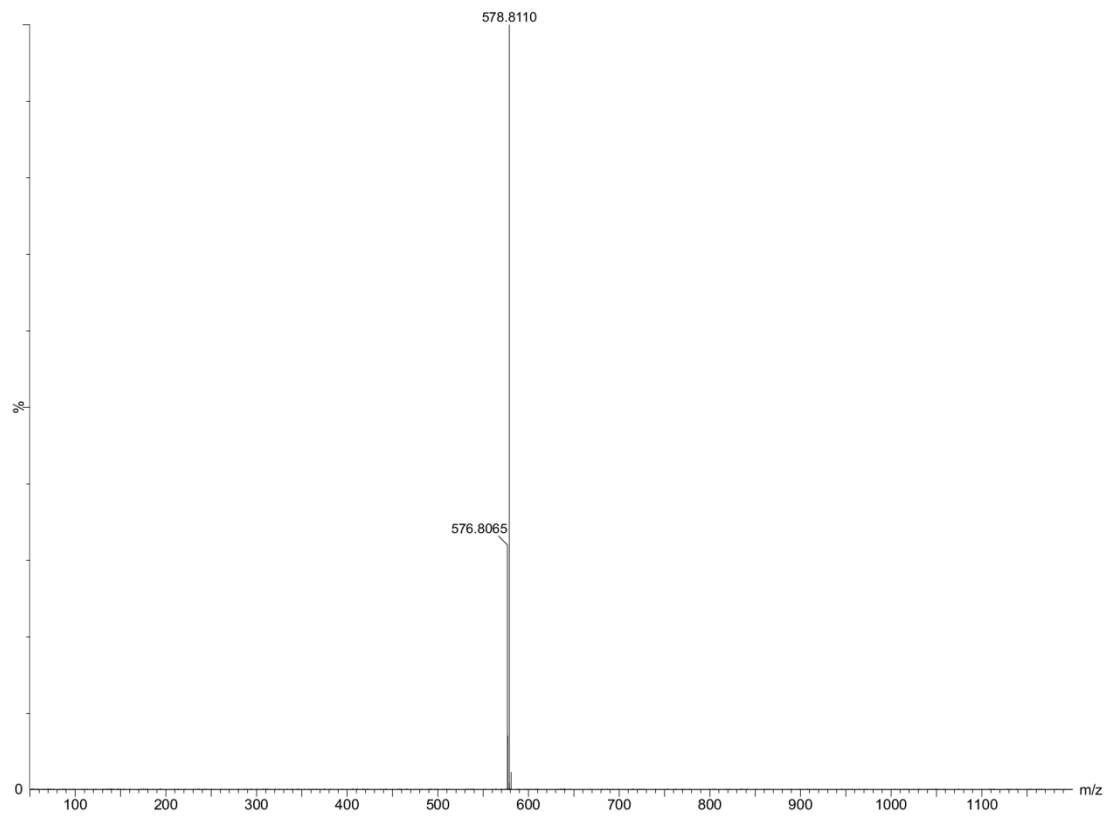


Fig. S8: ESI-MS spectrum of complex **2** in acetonitrile medium.

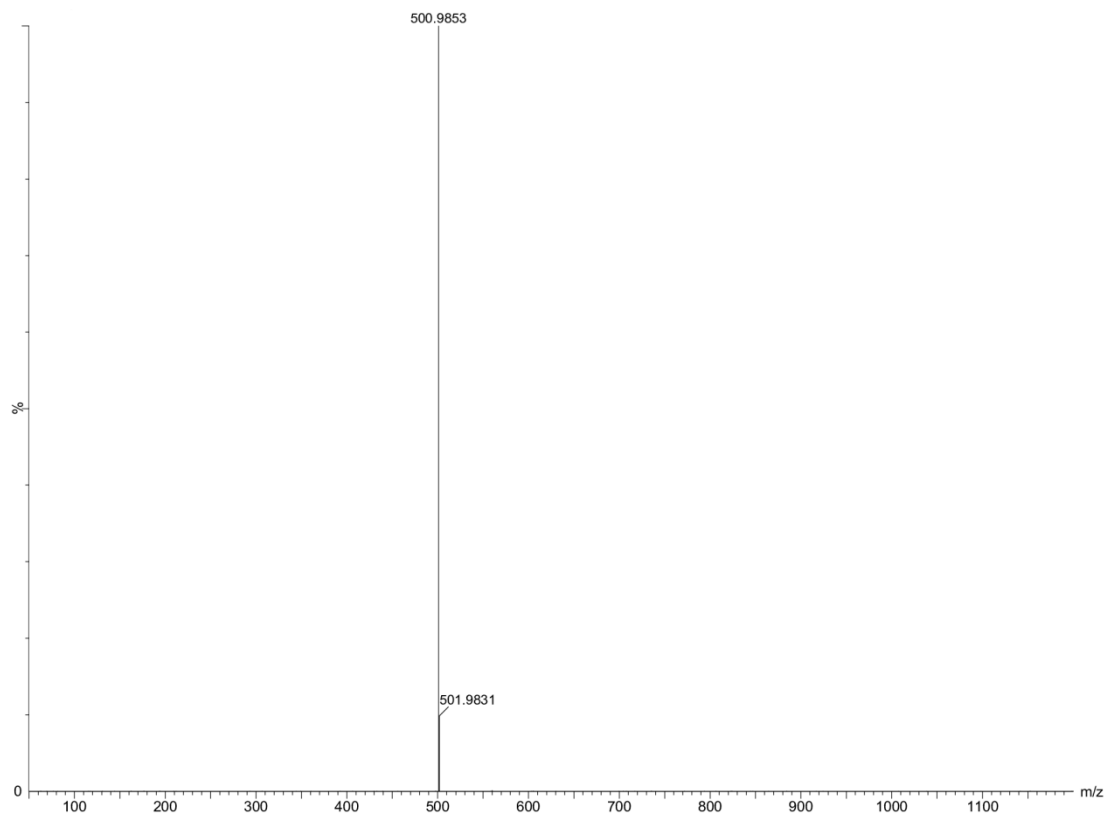


Fig. S9: ESI-MS spectrum of complex **3** in acetonitrile medium.

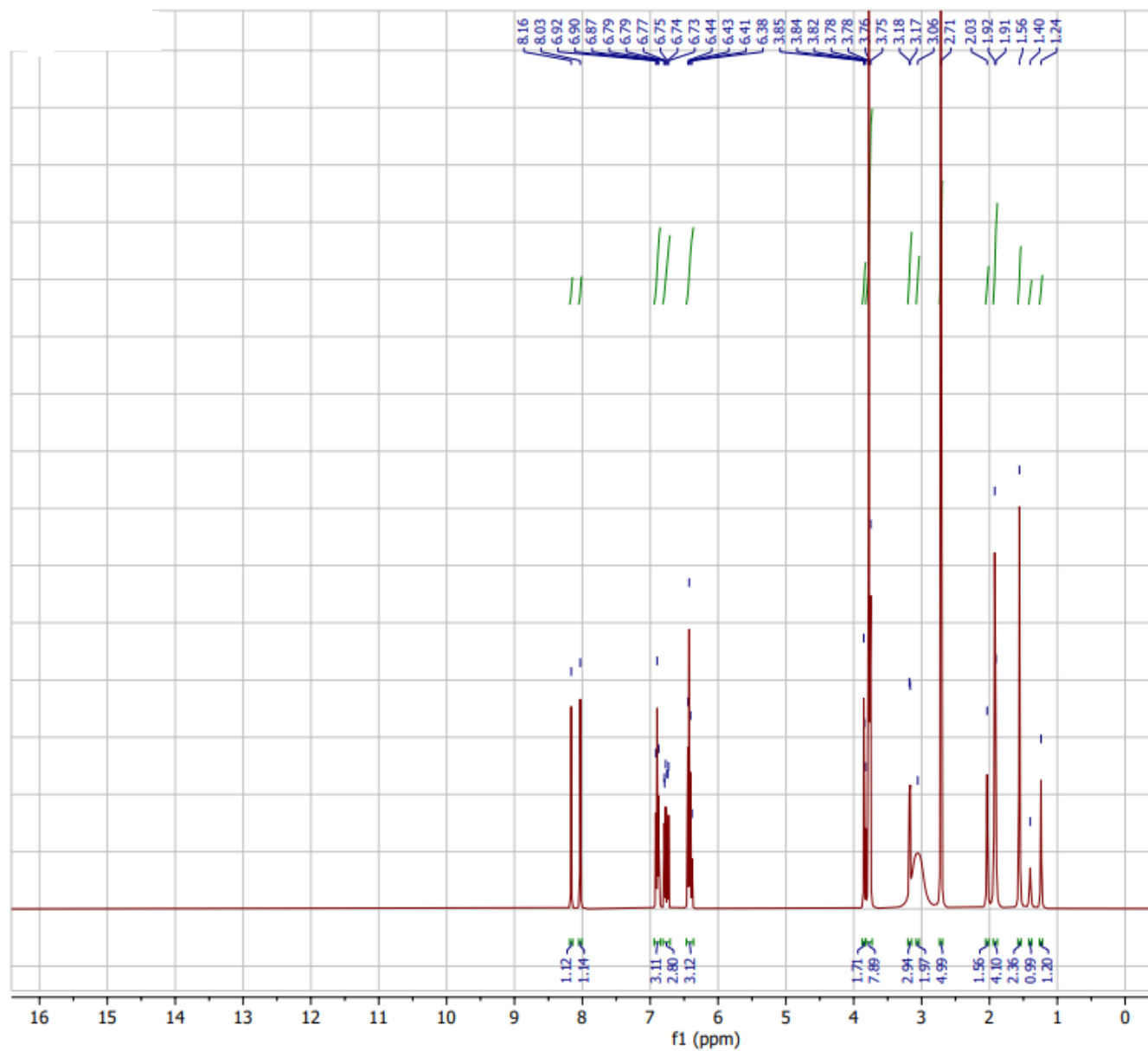


Fig. S10: ^1H NMR spectrum of complex 1.

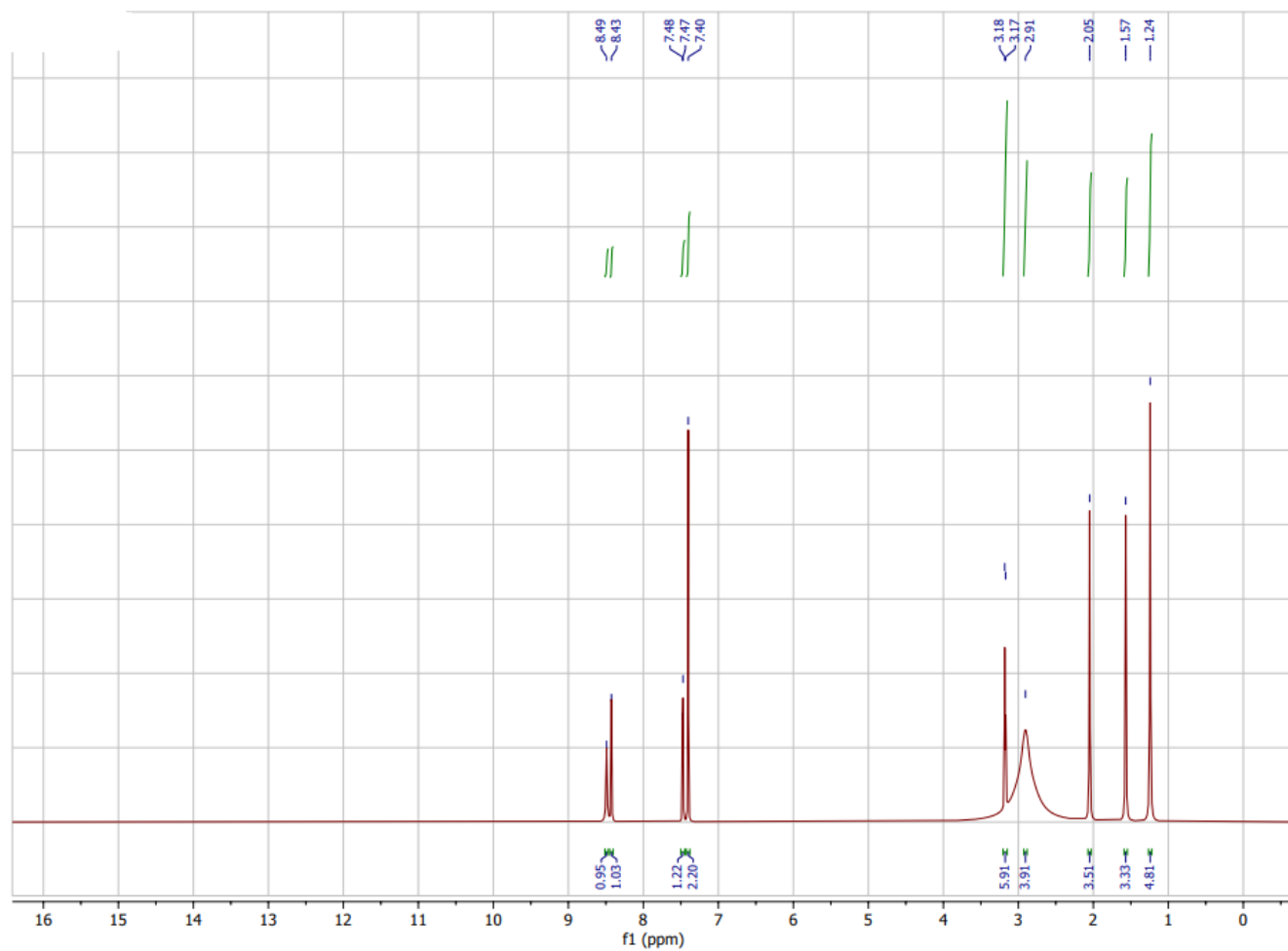


Fig. S11: ¹H NMR spectrum of complex 2.