Synthesis, Structural Characterization, and Theoretical Analysis of Novel Zinc(II) Schiff Base Complexes with Halogen and Hydrogen Bonding Interactions

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Hirshfeld surface analysis

Crystal Explorer 21.5 [S1] software has been used to calculate Hirshfeld surfaces [S2-S4] and the related two-dimensional fingerprint [S5, S6] plots. The bond lengths to hydrogen atoms have been set to standard values. The distance from the point to the nearest nucleus external to the surface (d_e) and the distance to the nearest nucleus internal to the surface (d_i) are defined for each point on the Hirshfeld surface to calculate the normalized contact distance (d_{norm}) using the appropriate formula.[S7]

The d_{norm} value may be less than zero or more than zero depending on the relative values of intermolecular contacts and van der Waals separations. The Hirshfeld surface with a red-white-blue color scheme is displayed with the d_{norm} parameter. Shorter contacts are indicated by the bright red spots. White areas represent contacts around the van der Waals

separation and blue regions, on the other hand, signify absence of any close contacts. It is needless to say that the Hirshfeld surface is unique for a given CIF.[S8]

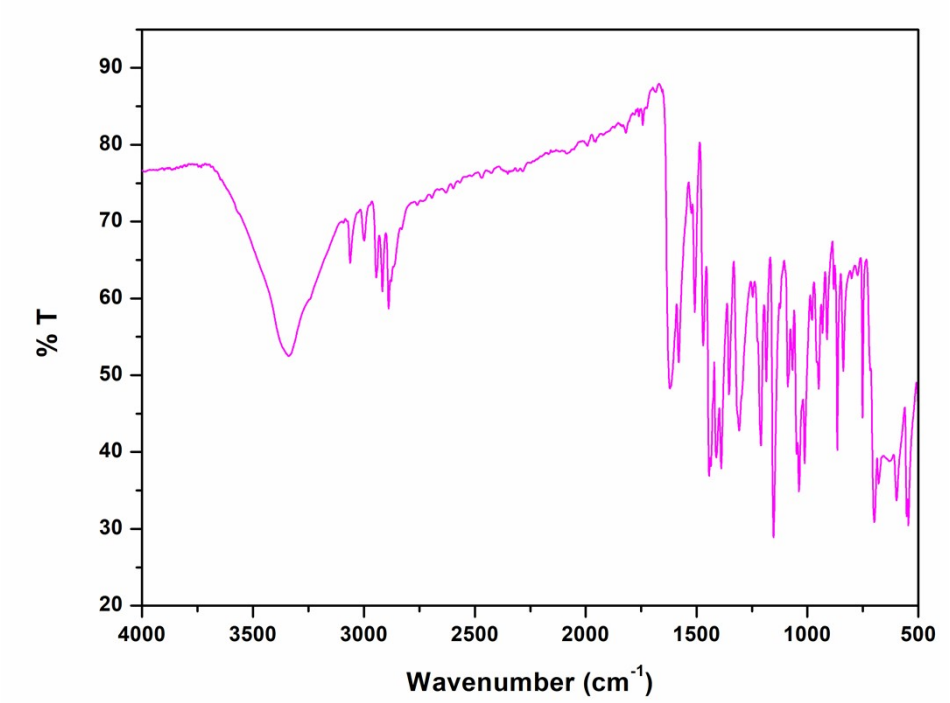

Fig. S1. IR spectrum of complex **1**.

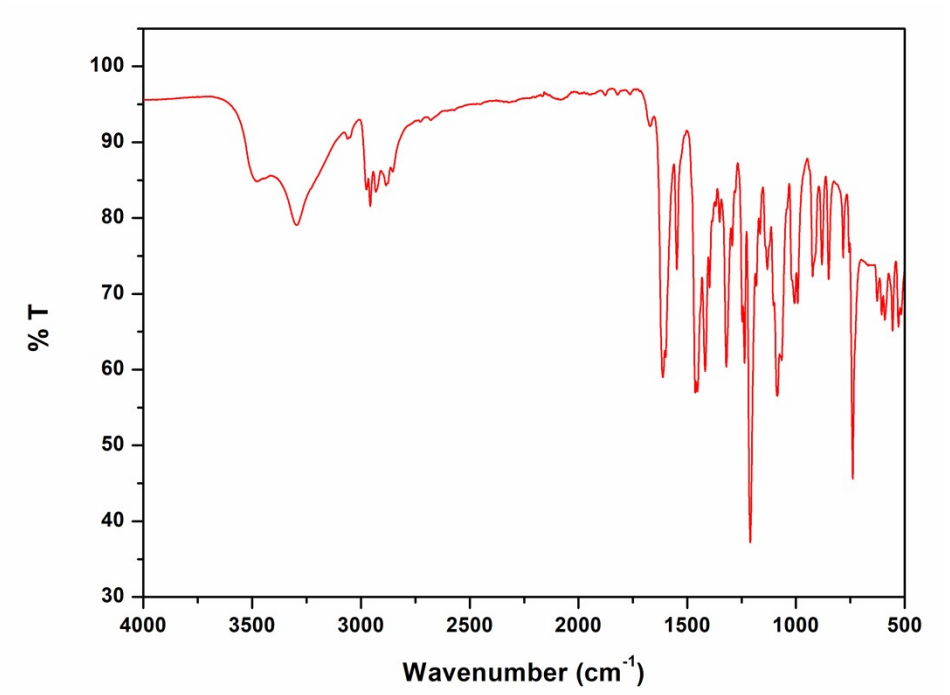

Fig. S2. IR spectrum of complex **2**.

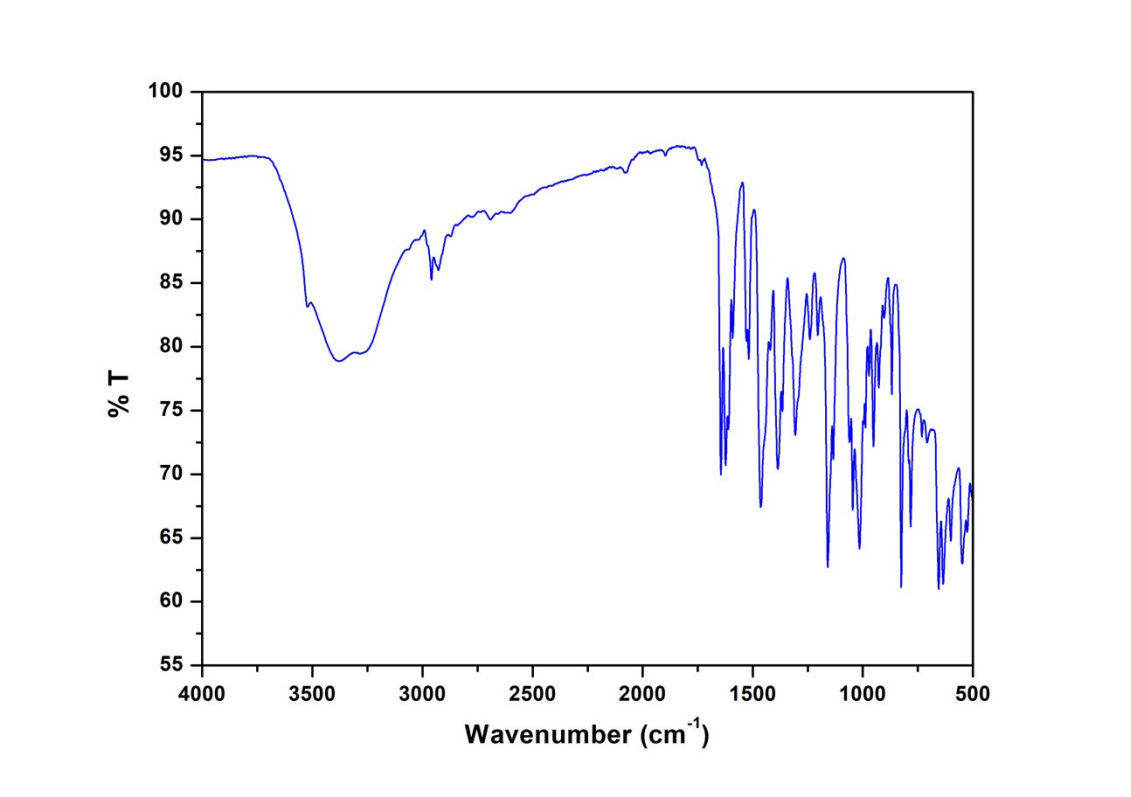

Fig. S3. IR spectrum of complex **3**.

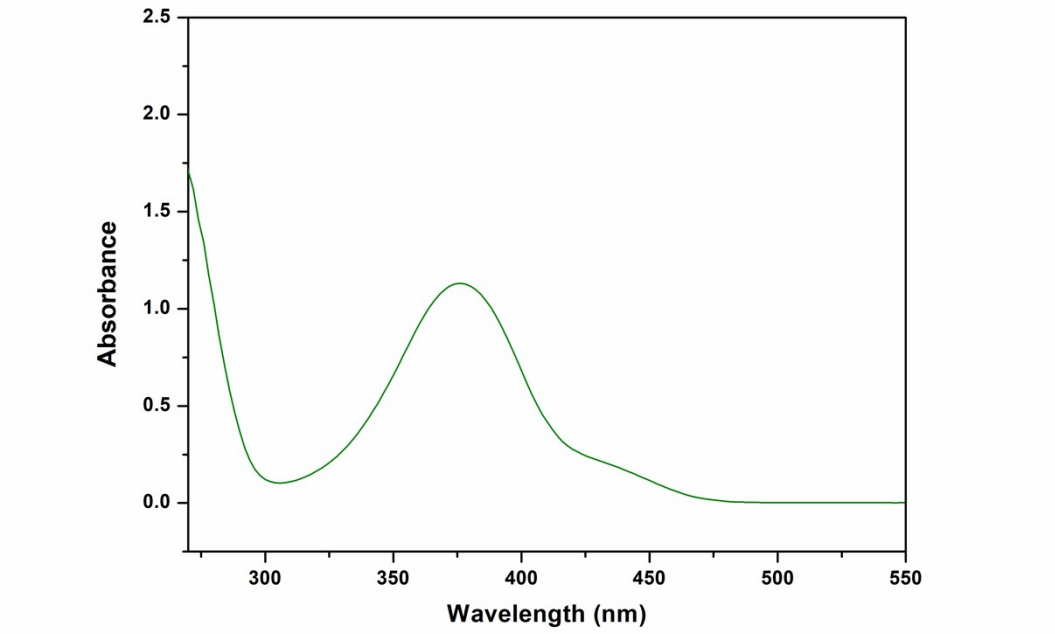

Fig. S4. The UV spectrum of complex **1** in methanol.

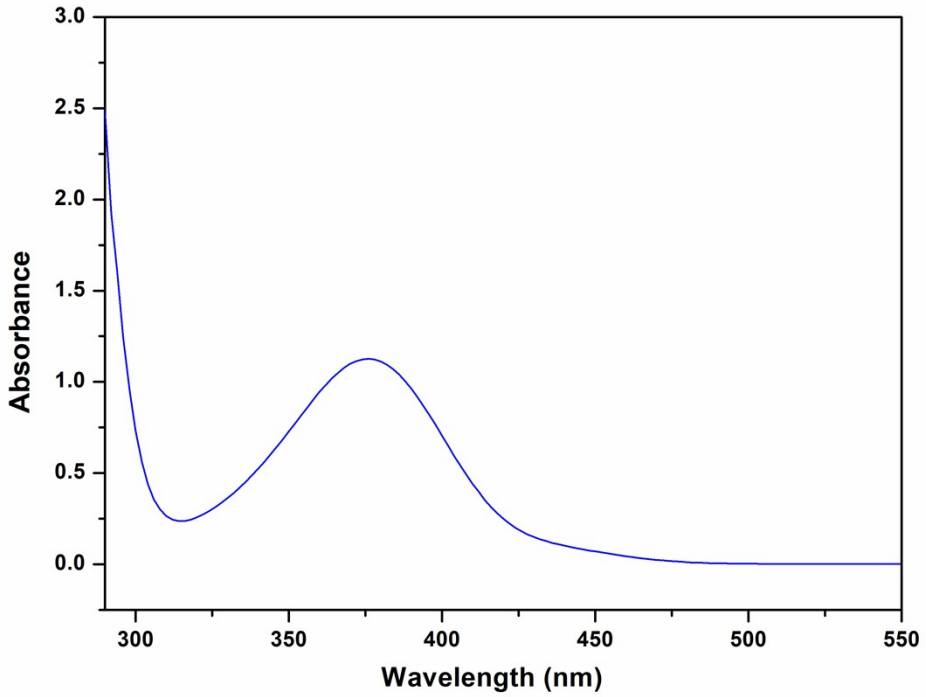

Figure S5. The UV spectrum of complex **2** in methanol.

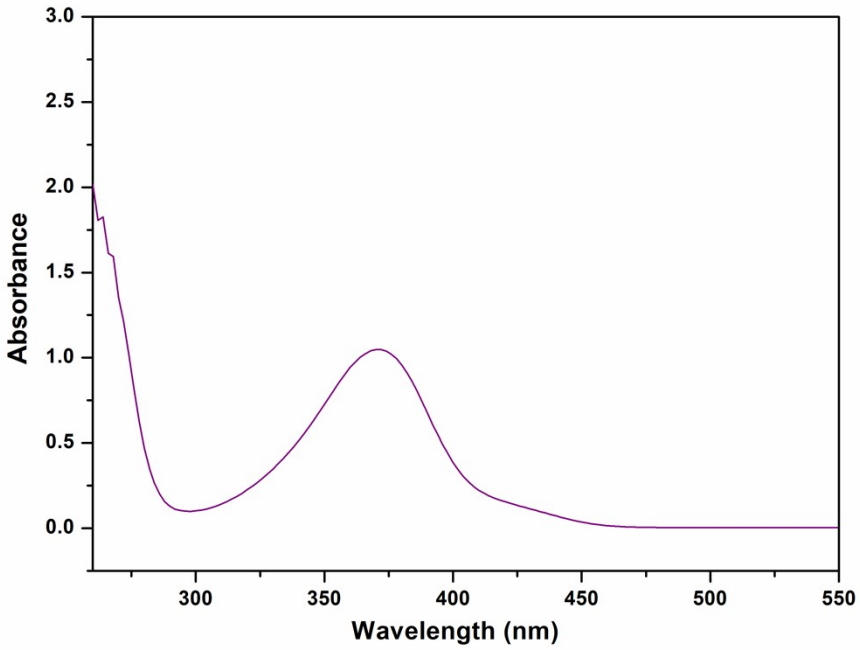

Fig. S6. The UV spectrum of complex **3** in methanol.

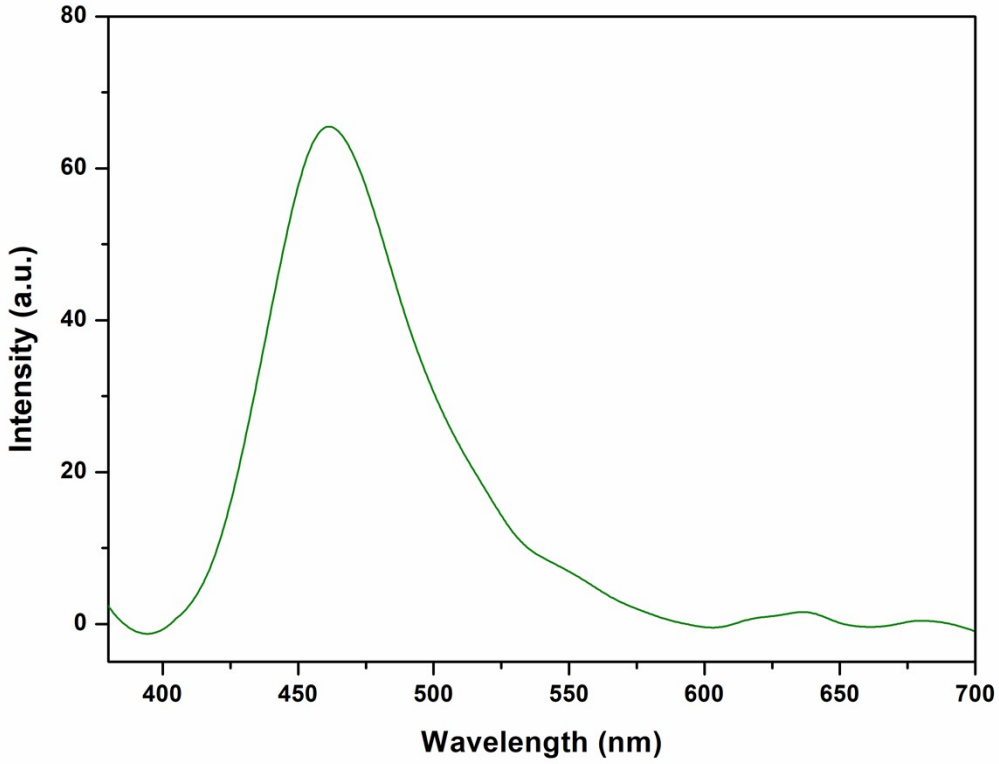

Fig. S7. The fluorescence spectrum of complex **3**.

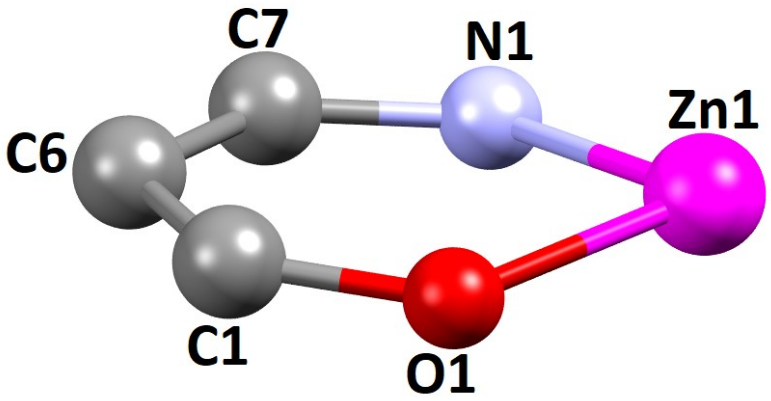

Fig. S8. The perspective view of envelope conformation of saturated six-member ring [Zn(1)-O(1)-C(1)-C(6)-C(7)-N(1)] in complex **1**.

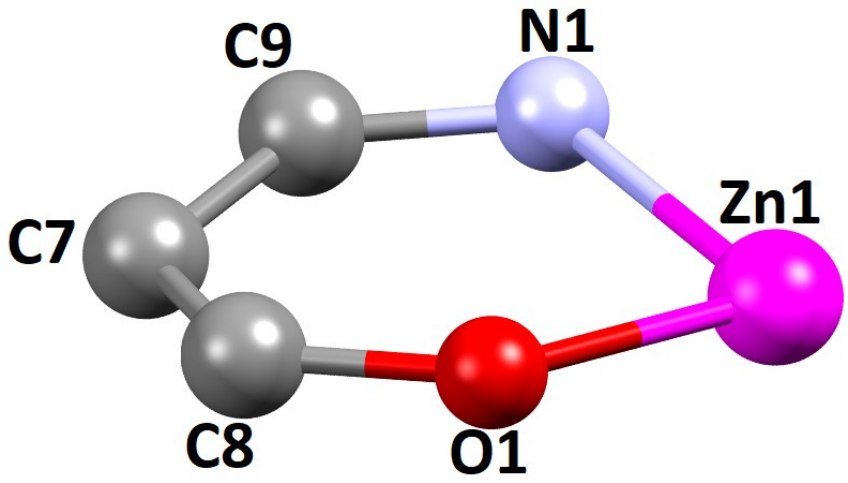

Fig. S9. The perspective view of envelope conformation of saturated six-member ring [Zn(1)-O(1)-C(8)-C(7)-C(9)-N(1)] in complex **2**.

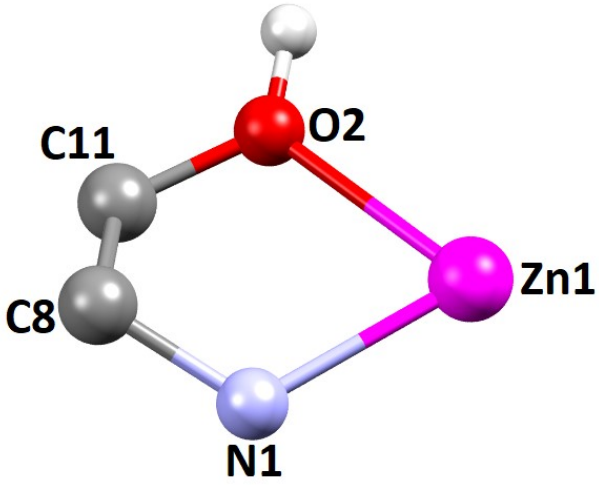

Fig. S10. The perspective view of envelope conformation of saturated five-member ring [Zn(1)-O(2)-C(11)-C(8)-N(1)] in complex **3**.

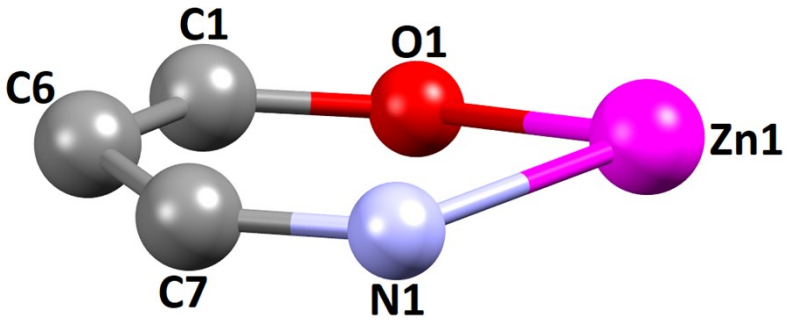

Fig. S11. The perspective view of screw-boat conformation of saturated six-member ring [Zn(1)-O(1)-C(8)-C(7)-C(9)-N(1)] in complex **3**.

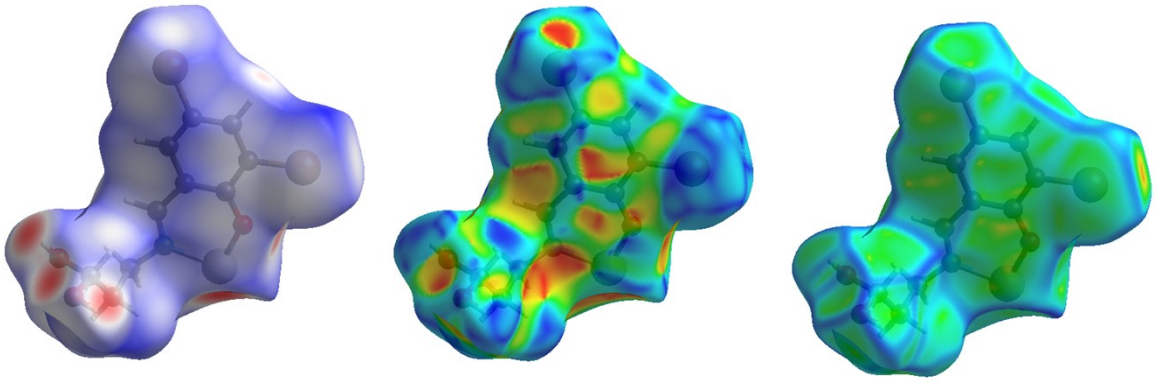

Fig. S12. Hirshfeld surfaces of complex **1**, mapped over d_{norm} (left), shape index (middle) and curvedness (right).

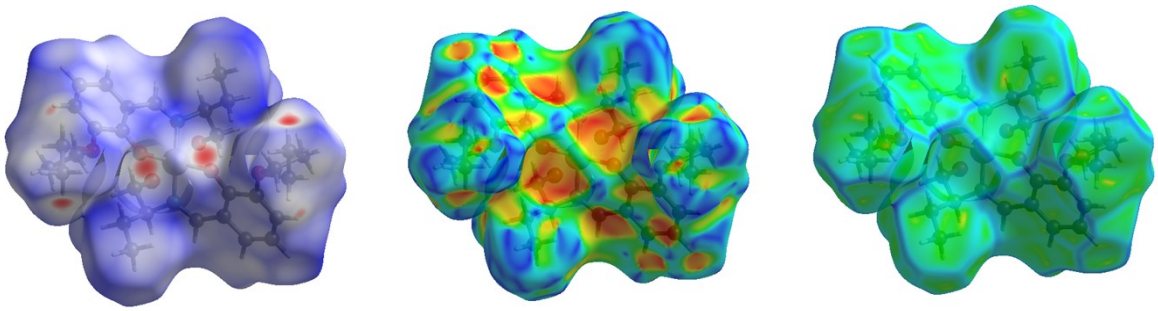

Fig. S13. Hirshfeld surfaces of complex **2**, mapped over d_{norm} (left), shape index (middle) and curvedness (right).

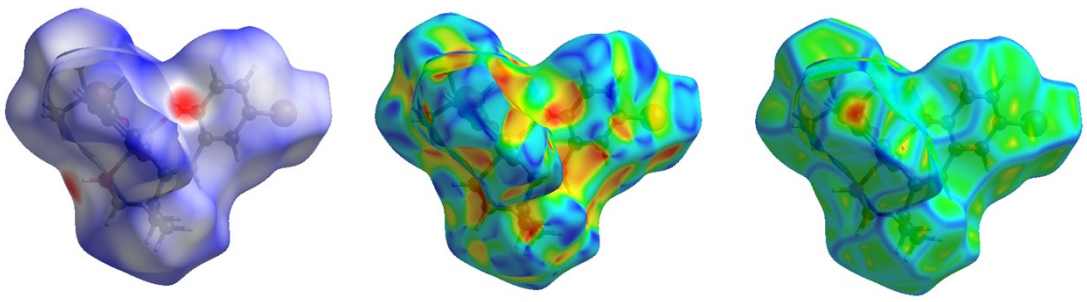

Fig. S14. Hirshfeld surfaces of complex **3**, mapped over d_{norm} (left), shape index (middle) and curvedness (right).

References

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