Synthesis, Structural Characterization, and DFT Investigation of a Mixed-Valence Co(III)/Co(II) Complex Stabilized by Supramolecular Interactions

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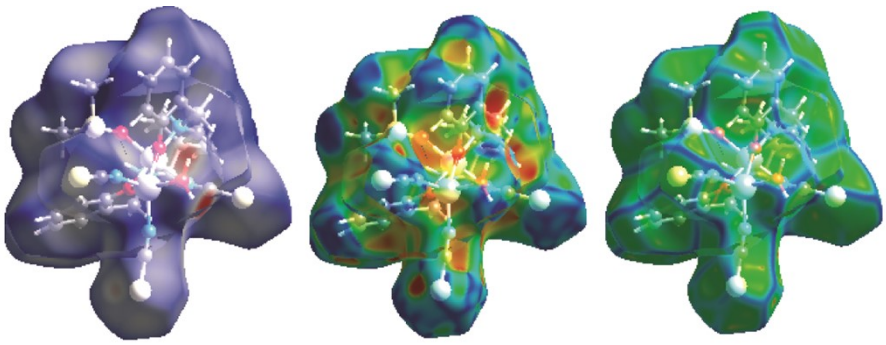

Fig. S1: Hirshfeld surface of the complex mapped over d_{norm} (left), shape index (middle) and curvedness (right).

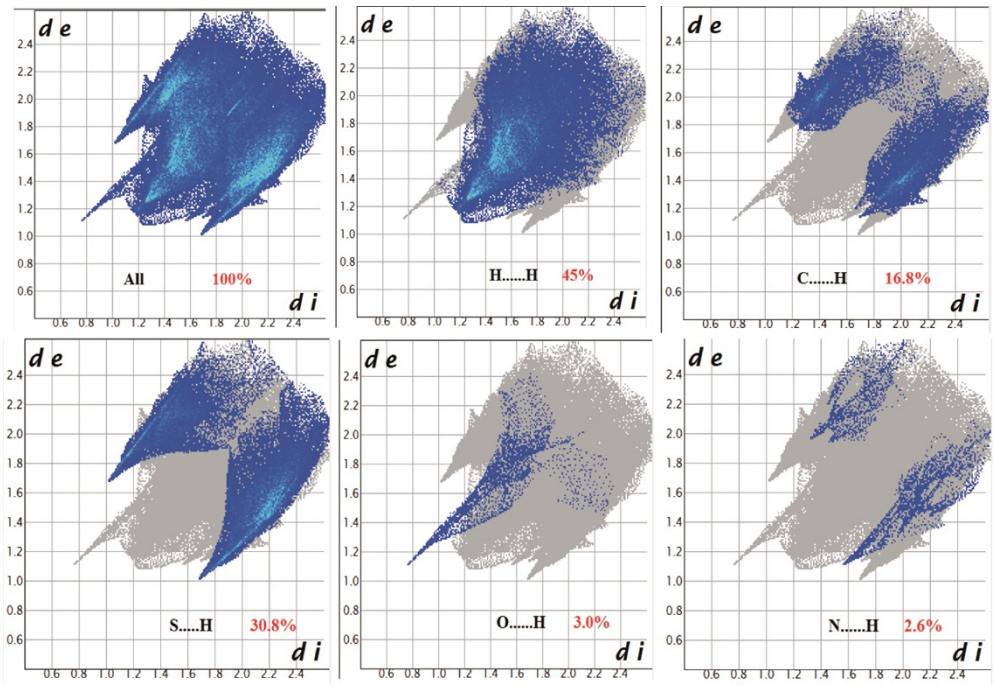

Fig. S2: Fingerprint plot of the complex: Full and resolved into H···H/H···H, C···H/H···C, S···H/H···S, O···H/H···O, and N···H/H···N contacts contributed to the total Hirshfeld Surface area.

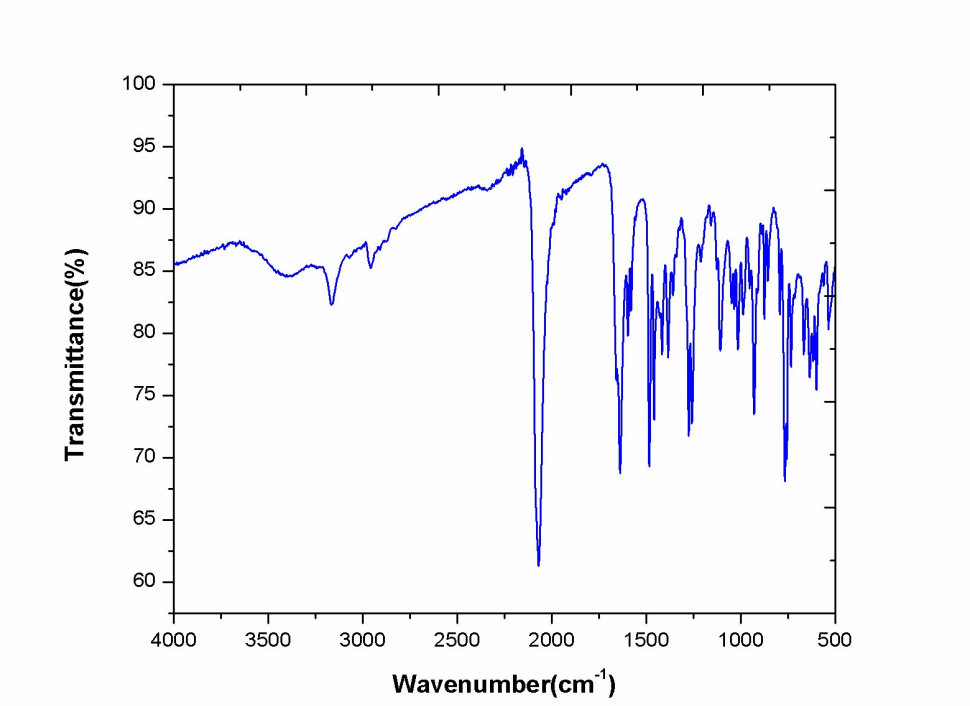

Fig. S3: IR spectrum of the complex**.**

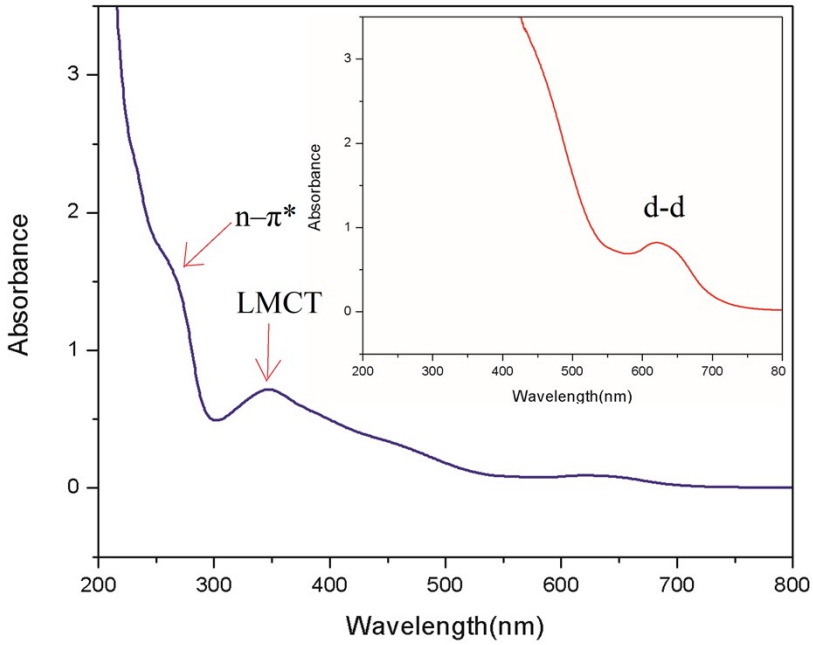

Fig. S4: UV spectrum of the complex**.** Inset shows the spectrum in the range of 400-800 nm.

Table S1: Selected bond angles (°) of the complex**.**

O(1)-Co(1)-O(2)	78.64(17)
O(1)-Co(1)-O(3)	94.31(17)
O(1)-Co(1)-N(1)	93.39(19)
O(1)-Co(1)-N(2)	171.8(2)
O(1)-Co(1)-N(3)	88.7(2)
O(2)-Co(1)-O(3)	93.92(19)
O(2)-Co(1)-N(1)	172.00(18)

O(2)-Co(1)-N(2)	93.17(19)
O(2)-Co(1)-N(3)	89.9(2)
O(3)-Co(1)-N(1)	85.97(19)
O(3)-Co(1)-N(2)	86.00(19)
O(3)-Co(1)-N(3)	175.56(19)
N(1)-Co(1)-N(2)	94.8(2)
N(1)-Co(1)-N(3)	90.6(2)
N(2)-Co(1)-N(3)	91.5(2)
O(1)-Co(2)-O(2)	72.69(16)
O(1)-Co(2)-O(4)	88.39(17)
O(1)-Co(2)-N(4)	153.2(2)
O(1)-Co(2)-N(5)	105.0(2)
O(2)-Co(2)-O(4)	152.58(18)
O(2)-Co(2)-N(4)	94.9(2)
O(2)-Co(2)-N(5)	109.5(2)
O(4)-Co(2)-N(4)	93.5(2)
O(4)-Co(2)-N(5)	94.3(2)
O(4)-Co(2)-N(5)	101.6(3)