Supplementary file

Field induced single molecule magnetic behavior of a mononuclear cobalt (II) Schiff base complex derived from 5-bromo vanillin

Fikre Elemo[1, 2], Sören Schlittenhardt[3], Taju Sani[1, 2], Cyril Rajnák[5], Wolfgang Linert[6], Roman Boča[5], Madhu Thomas*[1, 2] and Mario Ruben*[3,4,7]

[1]Department of Industrial Chemistry, College of Applied Science, Addis Ababa Science and Technology University, P.o.Box, 16417,Addis Ababa, Ethiopia
[2]Nanotechnology Centre of Excellence, Addis Ababa Science and Technology University, Addis Ababa, Ethiopia, P.o.Box, 16417
[3]Karlsruhe Institute of Technology, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany
[4]Karlsruhe Institute of Technology, Institute for Quantum Materials and Technologies, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany
[5]Department of Chemistry, Faculty of Natural Sciences, University of SS Cyril and Methodius, 91701 Trnava, Slovakia
[6]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna,
Austria,
[7]Centre Européen de Science Qantique (CESQ); Institut de Science et d'Ingénierie Supramoléculaires (ISIS, UMR 7006), CNRS-Université de Strasbourg, 8 allée Gaspard Monge BP 70028 67083 Strasbourg Cedex, France
* Correspondence: Madhu Thomas, e-mail; madhu.thomas@aastu.edu.et and Mario Ruben, email; mario.ruben@kit.edu

Table S1. Crystal data and structure refinement for $Co(C_{19}H_{17}BrN_3O_3)_2$

The compound	$Co(C_{19}H_{17}BrN_3O_3)_2.4CH_3OH$
Empirical formula	$C_{42}H_{50}Br_2CoN_6O_{10}$
Formula weight	1017.63
Temperature/K	160.00
Crystal system	monoclinic
Space group	Cc
a/Å	19.3278(4)
b/Å	20.4812(4)
c/Å	22.8624(6)
α/°	90
β/°	102.070(2)
γ/°	90
Volume/$Å^3$	8850.2(43)
Z	8
$\rho_{calc}g/cm^3$	1.528
μ/mm^{-1}	3.903
F(000)	4168
Crystal size/mm^3	0.1 × 0.08 × 0.08
Radiation	GaK\α (λ = 1.34143)
2Θ range for data collection/°	5.54 to 125.1
Index ranges	-21 ≤ h ≤ 25, -26 ≤ k ≤ 27, -30 ≤ l ≤ 19
Reflections collected	47072
Independent reflections	14114 [R_{int} = 0.0261, R_{sigma} = 0.0212]
Data/restraints/parameters	14114/2/1127
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0315, wR_2 = 0.0790
Final R indexes [all data]	R_1 = 0.0348, wR_2 = 0.0804
Largest diff. peak/hole / e $Å^{-3}$	0.56/-0.43
Flack parameter	0.099(3)
CCDC number	2170911

Table S2. Selected bond Lengths for $Co(C_{19}H_{17}BrN_3O_3)_2$

Atom	Atom	Length/Å
Co1	O6	2.210(2)
Co1	O2	2.041(2)
Co1	O5	2.066(3)
Co1	O3	2.189(2)
Co1	N1	2.087(2)
Co1	N4	2.086(2)
Co2	O12	2.191(2)
Co2	O11	1.995(2)
Co2	O9	2.242(2)
Co2	O8	2.015(2)
Co2	N7	2.079(2)
Co2	N10	2.092(2)

Table S3. Selected bond Angles for $Co(C_{19}H_{17}BrN_3O_3)_2$

Atom	Atom	Atom	Angle/°
O2	Co1	O6	88.71(9)
O5	Co1	O6	167.37(8)
O5	Co1	O2	99.07(9)
O3	Co1	O6	83.99(9)
O3	Co1	O2	166.17(9)
O3	Co1	O5	90.27(9)
N1	Co1	O6	99.40(10)
N1	Co1	O2	87.89(9)
N1	Co1	O5	90.87(10)
N1	Co1	O3	81.76(9)
N4	Co1	O6	81.41(10)
N4	Co1	O2	97.32(9)
N4	Co1	O5	87.70(11)
N4	Co1	O3	93.19(9)
N4	Co1	N1	174.75(10)
O11	Co2	O12	167.24(8)
O9	Co2	O12	82.46(8)
O9	Co2	O11	89.05(9)
O8	Co2	O12	89.63(9)
O8	Co2	O11	100.30(10)
O8	Co2	O9	167.21(9)
N7	Co2	O12	93.89(10)
N7	Co2	O11	94.17(10)
N7	Co2	O9	80.99(9)
N7	Co2	O8	89.57(9)
N10	Co2	O12	82.05(10)
N10	Co2	O11	88.89(10)
N10	Co2	O9	92.71(9)
N10	Co2	O8	96.15(9)
N10	Co2	N7	172.94(11)
C66	O12	Co2	104.9(2)
C28	O6	Co1	105.0(2)
C59	O11	Co2	127.6(2)
C47	O9	Co2	104.88(19)
C2	O2	Co1	125.70(18)

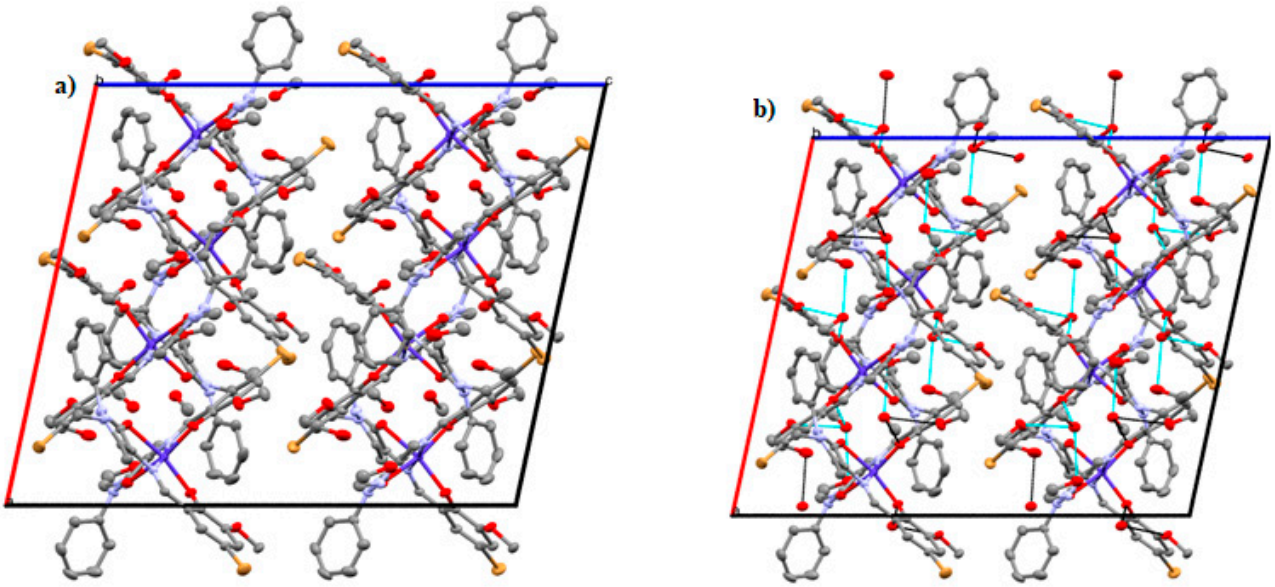

Figure S1. Crystal packing along b axis a) without H-bonding b) with H-bonding

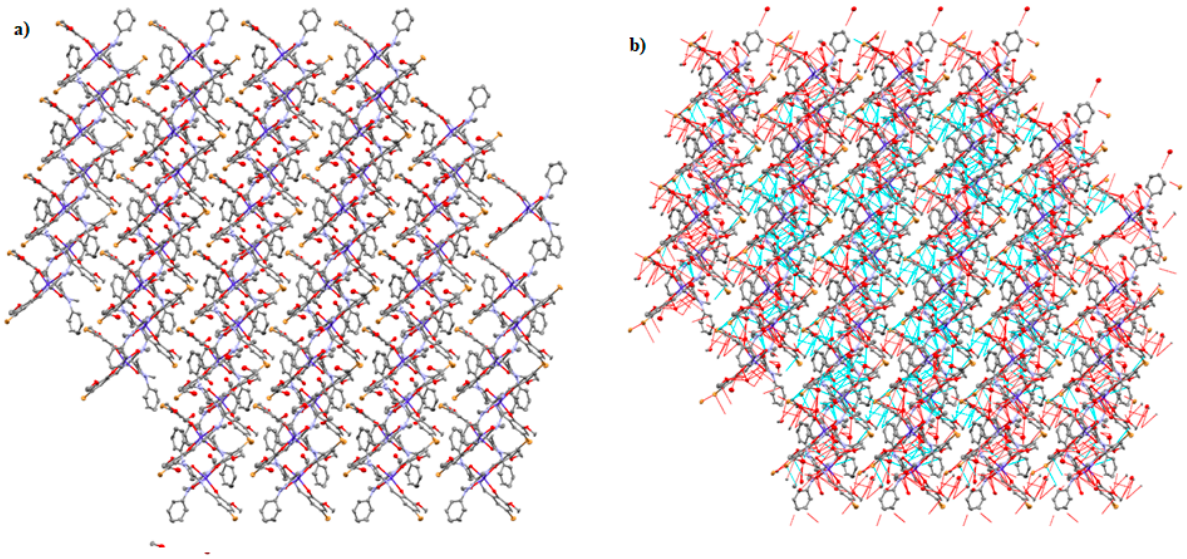

Figure S2. Crystal packing along b axis a) without H-bonding b) with H-bonding

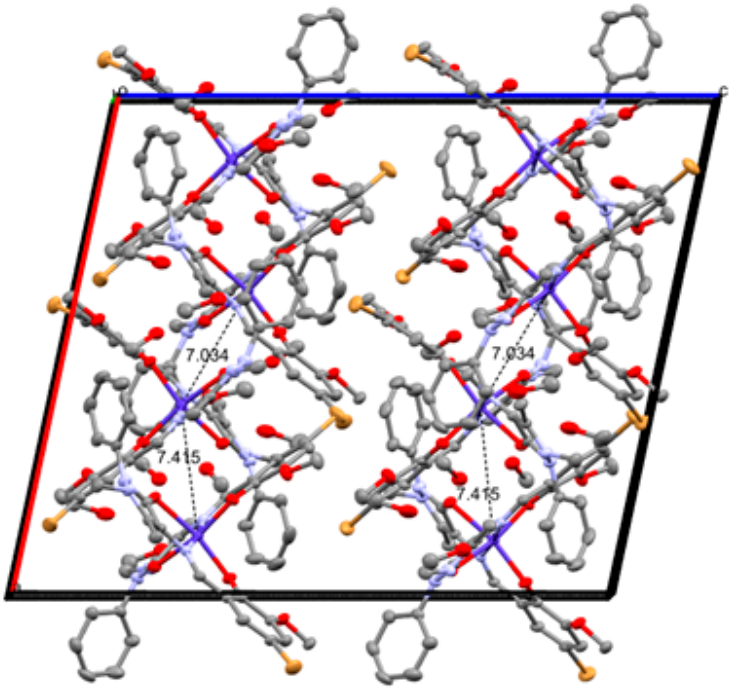

Figure S3. Intralayer M…M distances in the molecule