"A trigonal prismatic Cu_6-pyrazolato complex containing a μ_6-F ligand"

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Electronic Supplementary Information

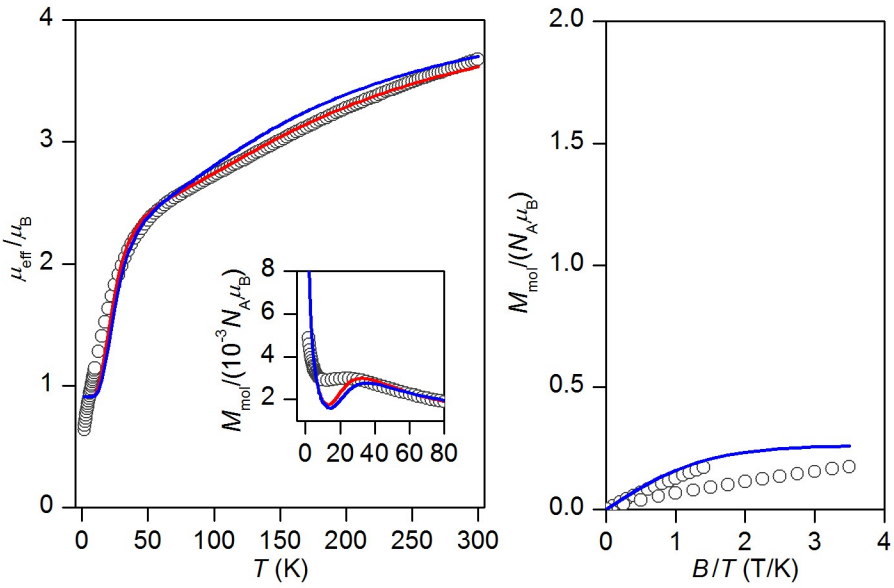

Figure S1. The magnetic data for **2,** the temperature dependence of the effective magnetic moment and molar magnetization measured at $B = 0.1$ T; the reduced isothermal magnetizations measured at $T = 2$ and 5 K. Open circles – experimental data, red solid lines – calculated data using equation 1, with $J_1 = -151$ cm^{-1}, $J_2 = -47$ cm^{-1}, $|d_z| = 0.0$ cm^{-1} and $x_{PI} = 4.2\%$; blue solid line – calculated data using equation 1, with $J_1 = -130$ cm^{-1}, $J_2 = -51$ cm^{-1}, $|d_z| = 0.0$ cm^{-1} and $x_{PI} = 4.2\%$;

Table S1 Energies of spin states calculated using B3LYP/TZP with/without the fluoride ion inside the cage

$[\{Cu_3(\mu_3\text{-}OH)(\mu\text{-}pz)_3\}_2(\mu\text{-}3,5\text{-}Ph_2pz)_3(\mu_6\text{-}F)]$

Spin State	Energy (eV)	M_S
(ααα) (ααα)	-600.790735	**3**
(ααα) (βββ)	-600.810576	**0**
(ααβ) (ααβ)	-600.854794	**1**

$[\{Cu_3(\mu_3\text{-}OH)(\mu\text{-}pz)_3\}_2(\mu\text{-}3,5\text{-}Ph_2pz)_3]^+$

Spin State	Energy (eV)	M_S
(ααα) (ααα)	-588.948680	**3**
(ααα) (βββ)	-588.968982	**0**
(ααβ) (ααβ)	-589.056991	**1**

Table S2

Cartesian coordinates for the optimized geometry of $[\{Cu_3(\mu_3\text{-}OH)(\mu\text{-}pz)_3\}_2(\mu\text{-}3,5\text{-}Ph_2pz)_3]^+$ ($\boldsymbol{M_S}$ = 3, B3LYP/TZP).

Energy	**-21.64347217 au**		
Cu	1.972077	0.000000	1.690446
Cu	-0.986038	1.707869	1.690446
Cu	-0.986038	-1.707869	1.690446
Cu	1.972077	0.000000	-1.690446
Cu	-0.986038	1.707869	-1.690446
Cu	-0.986038	-1.707869	-1.690446
N	1.913519	-1.949638	1.876473
N	-2.645196	0.682337	-1.876473
N	0.731676	2.631975	1.876473
N	-2.645196	-0.682337	-1.876473
N	0.731676	2.631975	-1.876473
N	-2.645196	-0.682337	1.876473
N	1.913519	1.949638	1.876473
N	1.913519	-1.949638	-1.876473
N	-2.645196	0.682337	1.876473
N	0.731676	-2.631975	1.876473
N	1.913519	1.949638	-1.876473
N	0.731676	-2.631975	-1.876473
N	-1.851723	-3.207278	-0.675812
N	3.703446	0.000000	0.675812
N	-1.851723	-3.207278	0.675812
N	-1.851723	3.207278	0.675812
N	3.703446	0.000000	-0.675812
N	-1.851723	3.207278	-0.675812
C	-3.919207	-1.097266	-1.941489
C	2.909863	-2.845500	1.941489
C	2.909863	2.845500	1.941489
C	1.009343	3.942765	-1.941489
C	1.009343	-3.942765	-1.941489
C	2.384069	-4.129329	1.999672
C	2.384069	4.129329	1.999672
C	2.909863	2.845500	-1.941489
C	1.009343	-3.942765	1.941489
C	1.009343	3.942765	1.941489
C	2.384069	4.129329	-1.999672
C	-3.919207	-1.097266	1.941489
C	2.384069	-4.129329	-1.999672
C	-3.919207	1.097266	1.941489

C	-3.919207	1.097266	-1.941489
C	-4.768138	0.000000	1.999672
C	2.909863	-2.845500	-1.941489
C	-4.768138	0.000000	-1.999672
C	-2.489039	4.311143	-1.097222
C	-2.489039	4.311143	1.097222
C	-2.916554	5.051620	0.000000
C	-2.489039	-4.311143	1.097222
C	-2.489039	-4.311143	-1.097222
C	-2.916554	-5.051620	0.000000
O	0.000000	0.000000	2.238811
O	0.000000	0.000000	-2.238811
C	4.978079	0.000000	1.097222
C	4.978079	0.000000	-1.097222
C	5.833108	0.000000	0.000000
H	-3.454164	-5.982788	0.000000
H	2.920489	-5.058435	-2.067620
H	3.936611	-2.524252	-1.926731
H	0.217761	-4.671331	-1.926731
H	2.920489	-5.058435	2.067620
H	6.908329	0.000000	0.000000
H	3.936611	2.524252	-1.926731
H	2.920489	5.058435	-2.067620
H	0.217761	4.671331	-1.926731
H	-4.154372	2.147079	-1.926731
H	-5.840978	0.000000	-2.067620
H	-4.154372	-2.147079	-1.926731
H	-5.840978	0.000000	2.067620
H	3.936611	2.524252	1.926731
H	2.920489	5.058435	2.067620
H	0.217761	4.671331	1.926731
H	0.000000	0.000000	-3.208466
H	0.000000	0.000000	3.208466
H	-3.454164	5.982788	0.000000
H	-4.154372	2.147079	1.926731
H	-4.154372	-2.147079	1.926731
H	5.212042	0.000000	-2.148564
H	5.212042	0.000000	2.148564
H	3.936611	-2.524252	1.926731
H	0.217761	-4.671331	1.926731
H	-2.606021	4.513761	2.148564
H	-2.606021	4.513761	-2.148564
H	-2.606021	-4.513761	2.148564

H	-2.606021	-4.513761	-2.148564

Table S3 Cartesian coordinates for the optimized geometry of [{$Cu_3(\mu_3\text{-}OH)(\mu\text{-}pz)_3\}_2(\mu\text{-}3,5\text{-}Ph_2pz)_3(\mu_6\text{-}F)$] ($\boldsymbol{M_S}$ = 3, B3LYP/TZP)

Energy	**-22.07865368 au**		
Cu	1.867640	0.000000	1.707754
Cu	-0.933820	1.617424	1.707754
Cu	-0.933820	-1.617424	1.707754
Cu	1.867640	0.000000	-1.707754
Cu	-0.933820	1.617424	-1.707754
Cu	-0.933820	-1.617424	-1.707754
N	1.911258	-1.955806	1.941690
N	-2.649406	0.677295	-1.941690
N	0.738148	2.633101	1.941690
N	-2.649406	-0.677295	-1.941690
N	0.738148	2.633101	-1.941690
N	-2.649406	-0.677295	1.941690
N	1.911258	1.955806	1.941690
N	1.911258	-1.955806	-1.941690
N	-2.649406	0.677295	1.941690
N	0.738148	-2.633101	1.941690
N	1.911258	1.955806	-1.941690
N	0.738148	-2.633101	-1.941690
N	-1.803070	-3.123008	-0.673390
N	3.606139	0.000000	0.673390
N	-1.803070	-3.123008	0.673390
N	-1.803070	3.123008	0.673390
N	3.606139	0.000000	-0.673390
N	-1.803070	3.123008	-0.673390
C	-3.920943	-1.098019	-1.992815
C	2.911384	-2.846627	1.992815
C	2.911384	2.846627	1.992815
C	1.009560	3.944646	-1.992815
C	1.009560	-3.944646	-1.992815
C	2.386499	-4.133537	2.042029
C	2.386499	4.133537	2.042029
C	2.911384	2.846627	-1.992815
C	1.009560	-3.944646	1.992815
C	1.009560	3.944646	1.992815

C	2.386499	4.133537	-2.042029
C	-3.920943	-1.098019	1.992815
C	2.386499	-4.133537	-2.042029
C	-3.920943	1.098019	1.992815
C	-3.920943	1.098019	-1.992815
C	-4.772998	0.000000	2.042029
C	2.911384	-2.846627	-1.992815
C	-4.772998	0.000000	-2.042029
C	-2.439686	4.225660	-1.096419
C	-2.439686	4.225660	1.096419
C	-2.868872	4.969031	0.000000
C	-2.439686	-4.225660	1.096419
C	-2.439686	-4.225660	-1.096419
C	-2.868872	-4.969031	0.000000
O	0.000000	0.000000	2.567982
O	0.000000	0.000000	-2.567982
F	0.000000	0.000000	0.000000
C	4.879372	0.000000	1.096419
C	4.879372	0.000000	-1.096419
C	5.737743	0.000000	0.000000
H	-3.406557	-5.900329	0.000000
H	2.923624	-5.063865	-2.089010
H	3.936795	-2.521507	-1.967083
H	0.215292	-4.670118	-1.967083
H	2.923624	-5.063865	2.089010
H	6.813114	0.000000	0.000000
H	3.936795	2.521507	-1.967083
H	2.923624	5.063865	-2.089010
H	0.215292	4.670118	-1.967083
H	-4.152087	2.148610	-1.967083
H	-5.847248	0.000000	-2.089010
H	-4.152087	-2.148610	-1.967083
H	-5.847248	0.000000	2.089010
H	3.936795	2.521507	1.967083
H	2.923624	5.063865	2.089010
H	0.215292	4.670118	1.967083
H	0.000000	0.000000	-3.533993
H	0.000000	0.000000	3.533993
H	-3.406557	5.900329	0.000000
H	-4.152087	2.148610	1.967083
H	-4.152087	-2.148610	1.967083
H	5.109035	0.000000	-2.148732
H	5.109035	0.000000	2.148732

H	3.936795	-2.521507	1.967083
H	0.215292	-4.670118	1.967083
H	-2.554518	4.424554	2.148732
H	-2.554518	4.424554	-2.148732
H	-2.554518	-4.424554	2.148732
H	-2.554518	-4.424554	-2.148732