Supporting Information

Modulation of Magnetic Anisotropy and Exchange Interaction in Phenoxide Bridged Dinuclear Co(II) Complexes

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Table S1: Processing parameters and crystallographic data for complexes 1–4

Complex	**1**	**2**	**3**	**4**
CCDC No.	1970738	1970739	1970740	1970741
Empirical formula	$C_{32}H_{31}Co_2N_7O_2S_2$	$C_{28}H_{28}Cl_2Co_2N_4O_2$	$C_{28}H_{28}Br_2Co_2N_4O_2$	$C_{28}H_{27}Co_2I_2N_4O_2$
Formula weight	727.62	641.30	730.22	823.19
Temperature/K	140	140	140	140
Crystal system	monoclinic	triclinic	triclinic	monoclinic
Space group	$P2_1/n$	P-1	P-1	C2/c
a/Å	9.2730(2)	9.3471(9)	9.4036(11)	34.9535(15)
b/Å	18.9557(4)	10.4181(11)	10.4446(13)	19.1821(6)
c/Å	19.2243(4)	15.7332(15)	15.7606(19)	9.7347(3)
α/°	90	91.224(4)	91.825(4)	90
β/°	103.0350(10)	91.138(3)	91.751(4)	104.011(4)
γ/°	90	112.712(3)	113.722(4)	90
Volume/Å^3	3292.10(12)	1412.3(2)	1414.9(3)	6332.8(4)
Z	4	2	2	8
ρ_{calc}g/cm^3	1.468	1.508	1.714	1.727
μ/mm^{-1}	1.175	1.396	4.029	3.027
F(000)	1496.0	656.0	728.0	3192.0
Crystal size/mm^3	0.2 × 0.13 × 0.07	0.71 × 0.59 × 0.47	0.68 × 0.54 × 0.41	0.1 × 0.08 × 0.07
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.816 to 59.222	4.726 to 49.658	4.736 to 50.178	4.246 to 50.19
Index ranges	-12 ≤ h ≤ 12, -24 ≤ k ≤ 26, -26 ≤ l ≤ 26	-11 ≤ h ≤ 10, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18	-39 ≤ h ≤ 41, -22 ≤ k ≤ 21, -11 ≤ l ≤ 11
Reflections collected	37590	46991	25805	27283
Independent reflections	9212 [R_{int} = 0.0467, R_{sigma} = 0.0431]	4846 [R_{int} = 0.1471, R_{sigma} = 0.0708]	5001 [R_{int} = 0.1350, R_{sigma} = 0.1063]	5637 [R_{int} = 0.0590, R_{sigma} = 0.0609]
Data/restraints/parameters	9212/0/407	4846/0/343	5001/48/343	5637/0/350
Goodness-of-fit on F^2	1.048	1.055	1.030	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0360, wR_2 = 0.0757	R_1 = 0.0467, wR_2 = 0.0710	R_1 = 0.0600, wR_2 = 0.0976	R_1 = 0.0408, wR_2 = 0.0820
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.0842	R_1 = 0.0904, wR_2 = 0.0823	R_1 = 0.1097, wR_2 = 0.1116	R_1 = 0.0654, wR_2 = 0.0916
Largest diff. peak/hole / e Å^{-3}	0.51/-0.43	0.35/-0.33	0.80/-0.76	0.65/-0.81

[a]$R_1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. [b]$wR_2 = [\Sigma w(Fo^2 - Fc^2)/(Fo^2)^2]^{1/2}$

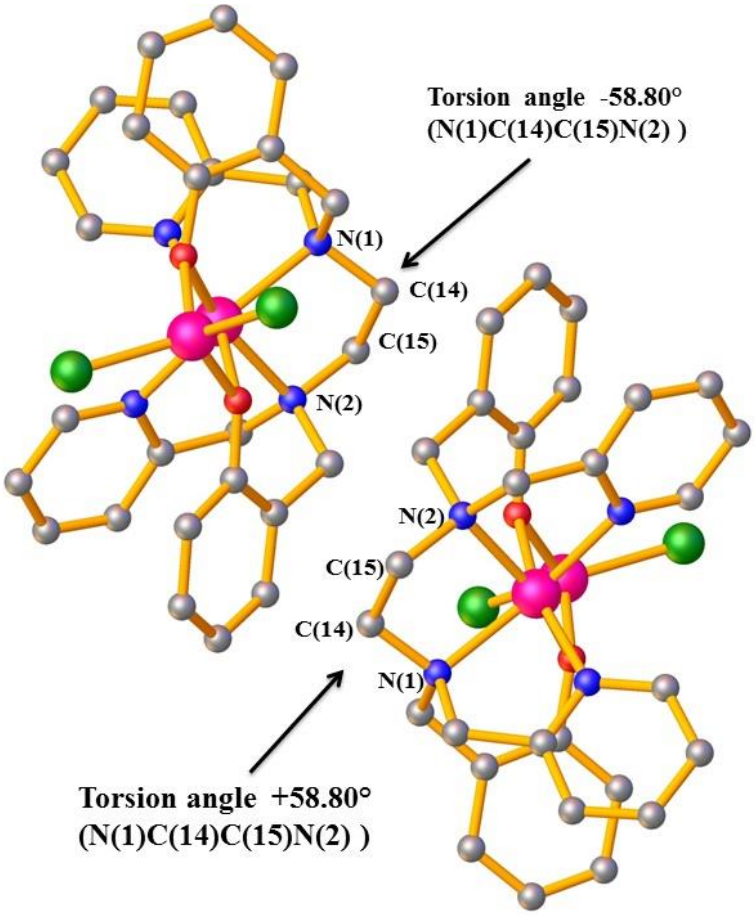

Figure S1. Enantiomeric pair of the complex **2** with the torsion angles of -58.80° and +58.80°.

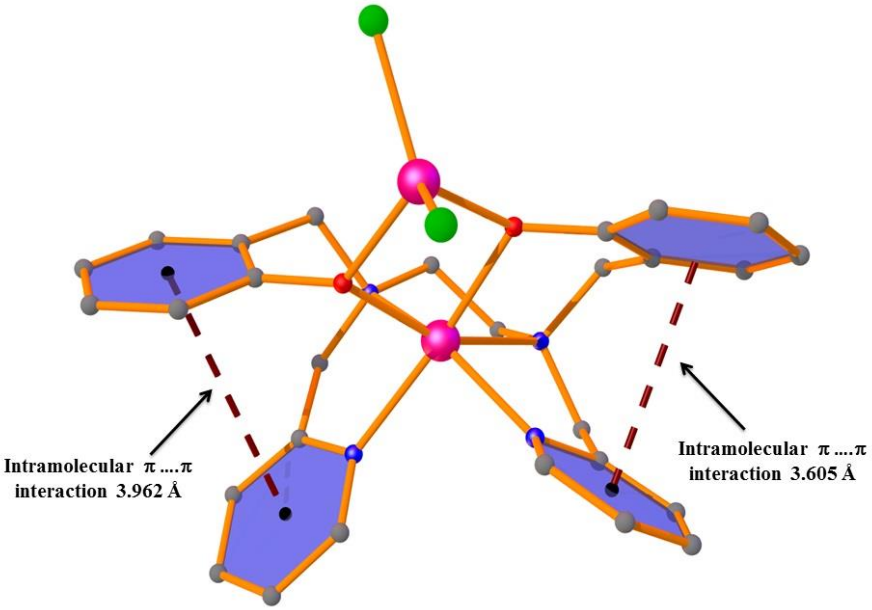

Figure S2. Intramolecular π····π interaction in complex **2**.

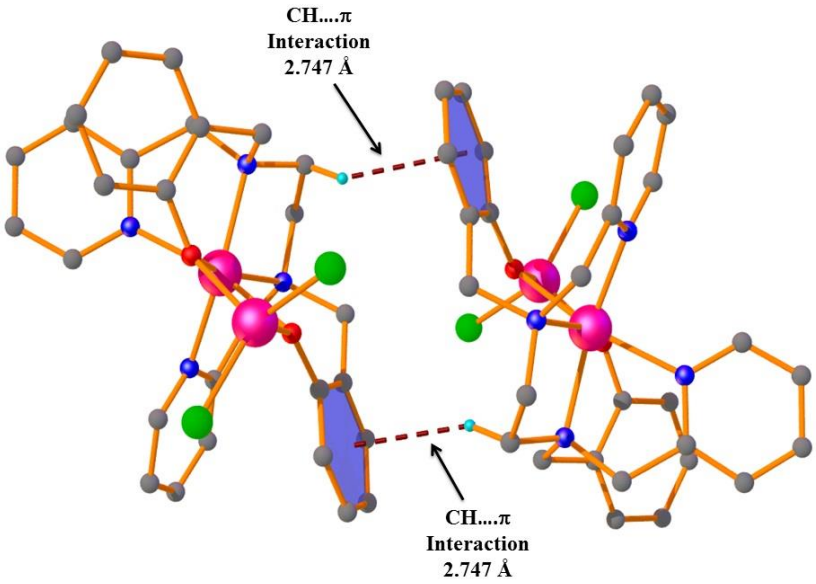

Figure S3. CH····π interaction (H-CH_2 of from ethylene diamine) in complex **2** forming a dimeric structure.

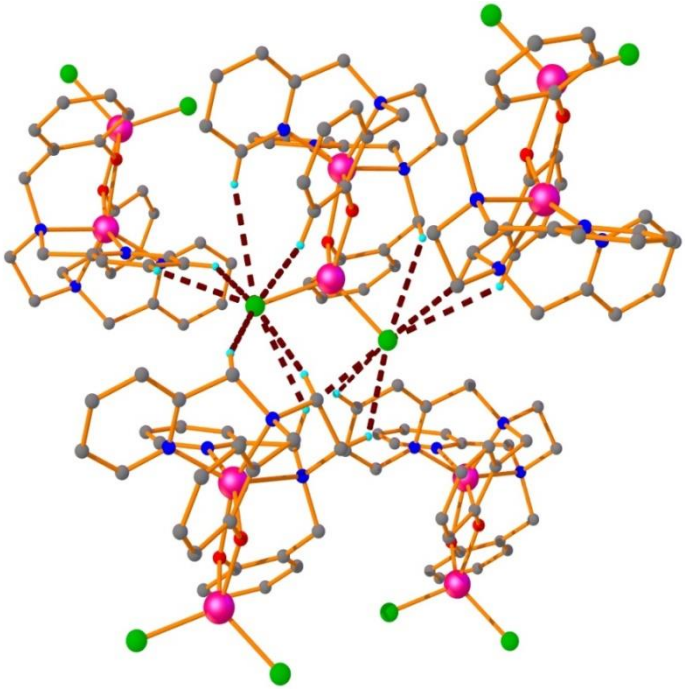

Figure S4. One unit of complex 2 is in in H····Cl (H-bonding) interaction with the four neighbouring dinuclear units of complex **2**.

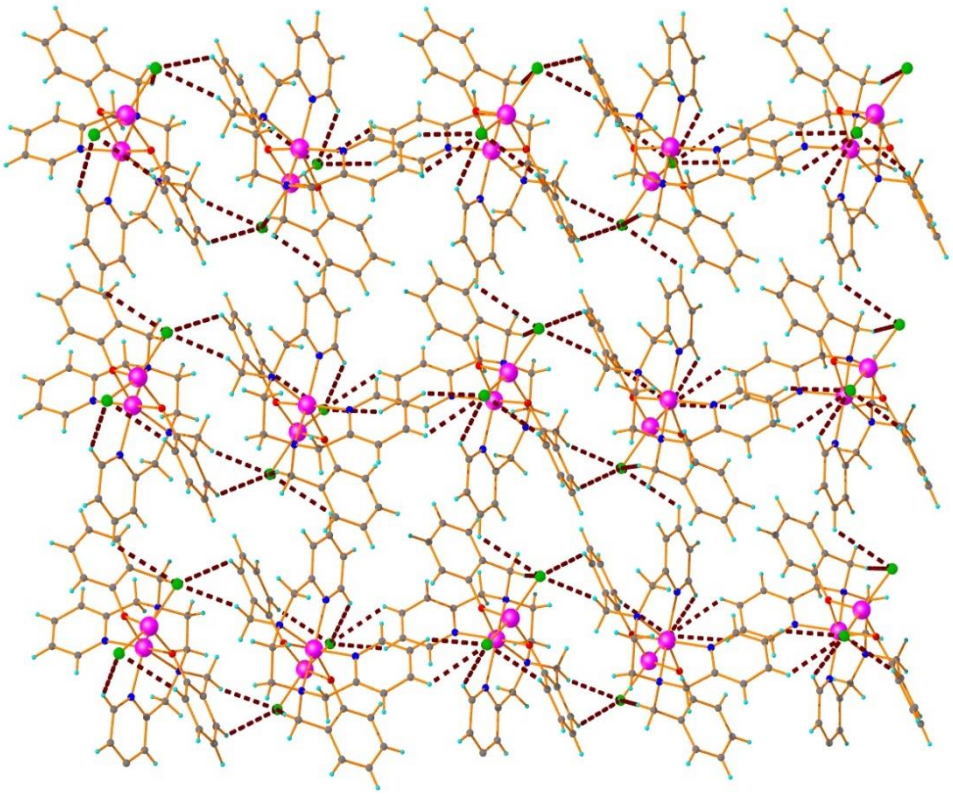

Figure S5. H····Cl interaction in 3D packed structure of complex **2**.

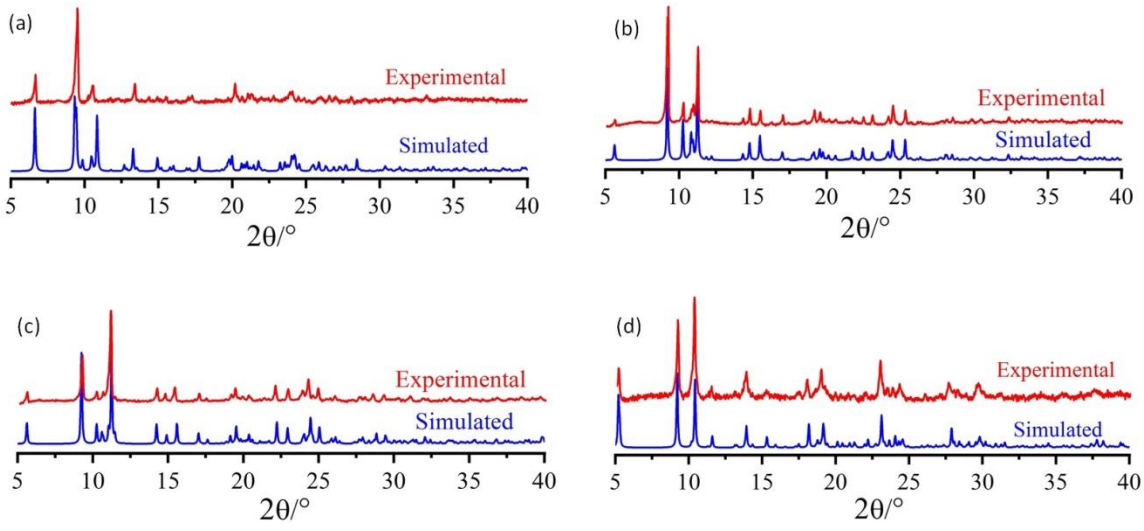

Figure S6. Simulated and experimental pattern of PXRD for complexes **1**-**4** from (a) to (d) respectively.

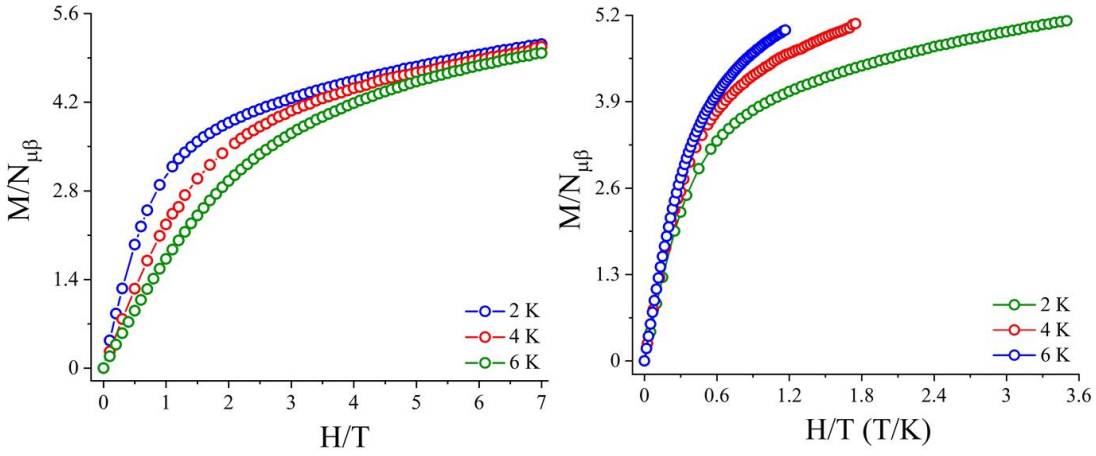

Figure S7a. *M*/NμB vs. H plot for complex **2** (left) at the indicated temperatures, and reduced magnetization plot (right).

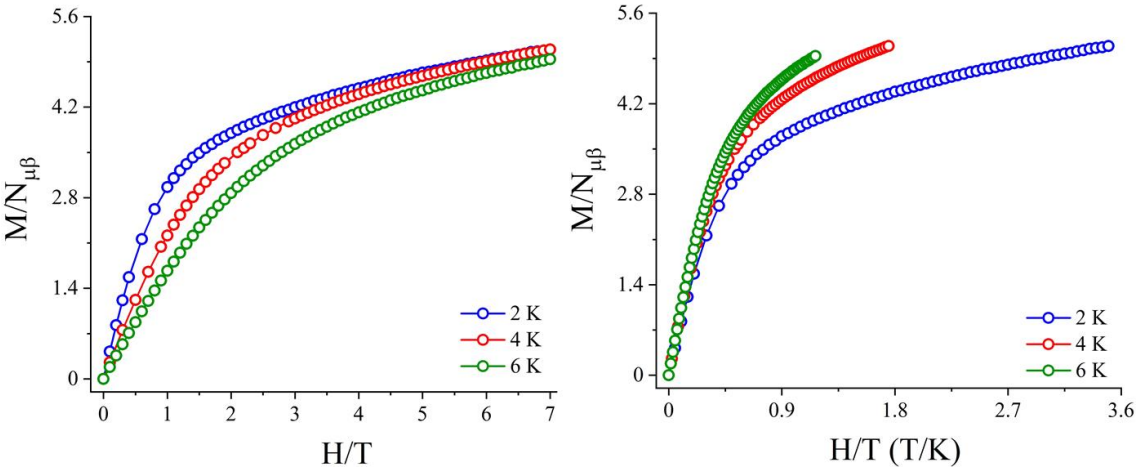

Figure S7b. *M*/NμB vs. H plot for complex **3** (left) at the indicated temperatures, and reduced magnetization plot (right).

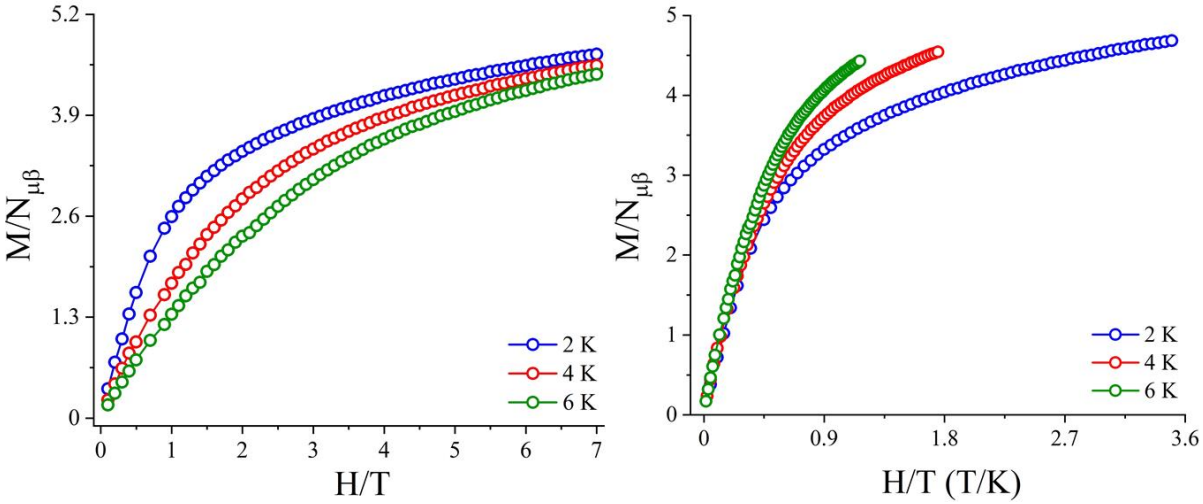

Figure S7c. *M*/NμB vs. H plot for complex **4** (left) at the indicated temperatures, and reduced magnetization plot (right).

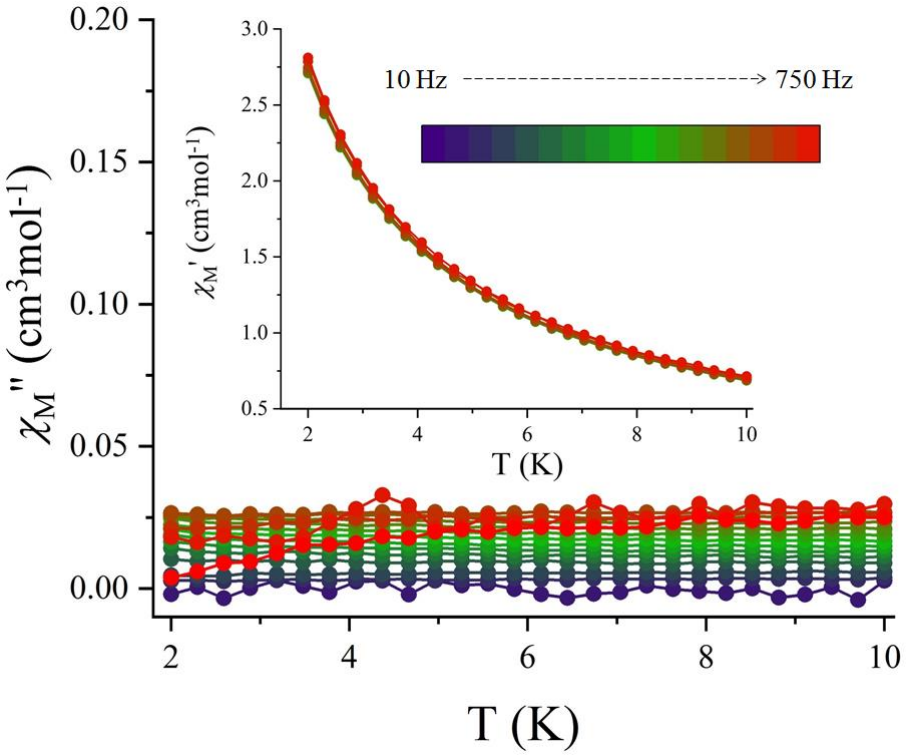

Figure S8a. Temperature dependent out of phase (χ'') magnetic susceptibility plot of complex **1** under zero DC field (**inset:** In phase (χ') magnetic susceptibility plot of complex **1**).

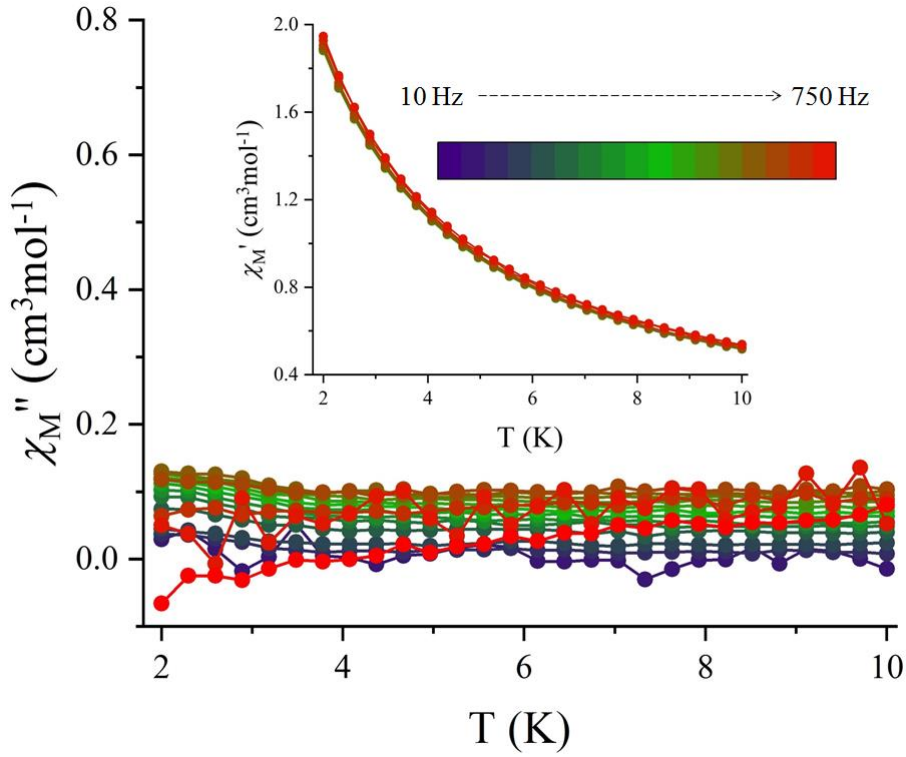

Figure S8b. Temperature dependent out of phase (χ'') magnetic susceptibility plot of complex **4** under zero DC field (**inset:** In phase (χ') magnetic susceptibility plot of complex **4**).

Table S2a: Bond lengths relating to the coordination sphere at the metal centres of all dinuclear complexes from **1** to **4**

1		**2**		**3**		**4**	
Co1 O1	2.1491(13)	Co1O1	2.142(2)	Co1 O1	2.137(4)	Co1 O1	2.140(3)
Co1 O2	2.0649(14)	Co1O2	2.066(2)	Co1 O2	2.079(4)	Co1 O2	2.029(3)
Co1 N3	2.1244(18)	Co1N3	2.125(3)	Co1 N3	2.114(6)	Co1 N3	2.146(4)
Co1 N1	2.1852(15)	Co1N1	2.185(3)	Co1 N1	2.180(6)	Co1 N1	2.181(4)
Co1 N2	2.1792(17)	Co1N2	2.178(3)	Co1 N2	2.171(6)	Co1 N2	2.186(4)
Co1 N4	2.1429(16)	Co1N4	2.146(3)	Co1 N4	2.132(6)	Co1 N4	2.151(4)
Co2 O1	1.9504(13)	Co2O1	1.964(2)	Co2 O1	1.967(4)	Co2 O1	1.959(3)
Co2 O2	1.9446(14)	Co2O2	1.983(2)	Co2 O2	1.979(5)	Co2 O2	1.939(3)
Co2 N5	1.9555(19)	Co2Cl1	2.2562(11)	Co2Br1	2.3998(12)	Co2I1	2.6055(8)
Co2 N6	1.9479(19)	Co2Cl2	2.2322(12)	Co2 Br2	2.3776(11)	Co2I2	2.5502(8)

Table S2b: Bond Angles relating to the coordination sphere at the metal centres of all dinuclear complexes from **1** to **4**

Complex **1**		Complex **2**		Complex **3**		Complex **4**	
Co2O1Co1	98.21(5)	Co2 O1Co1	100.40(11)	Co2 O1 Co1	100.2(3)	Co2 O1 Co1	98.57(14)
Co2 O2 Co1	101.31(6)	Co2 O2 Co1	98.42(10)	Co2 O2 Co1	98.1(3)	Co2 O2 Co1	103.12(16)
N6 Co2 N5	113.76(8)	Cl1 Co2 Cl2	113.92(5)	Br2 Co2 Br1	114.4(6)	I2 Co2 I1	115.39(3)

Shape Analysis

Table S3:
Octahedral Co(II) centre

HP-6	1	D6h	Hexagon
PPY-6	2	C5v	Pentagonal pyramid
OC-6	3	Oh	Octahedron
TPR-6	4	D3h	Trigonal prism
JPPY-6	5	C5v	Johnson pentagonal pyramid J2

Structure [ML_6]	**HP-6**	**PPY-6**	**OC-6**	**TPR-6**	**JPPY-6**
Complex **1**	31.609	18.134	5.264	**4.347**	22.085
Complex **2**	31.290	18.572	4.689	**4.752**	22.448
Complex **3**	31.154	19.093	4.335	**5.137**	23.071
Complex **4**	31.131	18.334	5.896	**3.745**	22.186

Highlighted red colour shows the possible geometries of the metal centres with minimum distortions.

Table S4:
Tetrahedral Co(II) centre

SP-4	1	D4h	Square
T-4	2	Td	Tetrahedron
SS-4	3	C2v	Seesaw
vTBPY-4	4	C3v	Vacant trigonal bipyramid

Structure [ML_4]	**SP-4**	**T-4**	**SS-4**	**vTBPY-4**
Complex **1**	28.673	**1.869**	9.033	2.957
Complex **2**	28.451	**2.655**	9.394	3.227
Complex **3**	27.817	**3.268**	9.692	3.497
Complex **4**	28.663	**4.652**	10.405	3.675

Highlighted red colour shows the possible geometries of the metal centres with minimum distortions.

Table S5: Intramolecular π····π Stacking distances

Complex	**1**	**2**	**3**	**4**
π····π (Å)	3.796	3.605	3.674	3.886
π····π (Å)	3.782	3.962	3.935	3.949

Table S6: Distance between the two cobalt centres in all four complexes

Complex	**1**	**2**	**3**	**4**
Distance (Co1····Co2) (Å)	3.101	3.111	3.102	3.108

CASSCF calculations on DFT optimized geometries:

Geometry optimizations using DFT method were also carried out (uB3LYP functional with TZV basis set for Co and SVP for others) for complex **1** in gas phase, to check how the ZFS parameters change upon optimization. It was found that the octahedral site anisotropy (D_{oh}) is unaltered upon geometry optimization while the tetrahedral site, the sign of D_{Td} became negative (-22 cm^{-1}) in the optimized structure compared to positive (+13.9 cm^{-1}) in X-Ray structure. The optimization geometry for the octahedral site was obtained by replacing the T_d site with Zn(II) ion and similarly, for the geometry optimization for the T_d site was performed by replacing the O_h site with Zn(II) ion. The optimized coordinates and subsequent ZFS are tabulated results below. The drastic change in the *D* value of the tetrahedral site is attributed to the change in NCS-Co-NCS angle, which changes from 113.75° in the X-Ray structure to 128.29° in the optimized geometry.

Table S7: Comparison of the ZFS parameters computed on X-ray geometry and on optimised geometry.

Octahedral site optimized coordinate $D_{Oh\text{-}opt}$ = -57.0 cm^{-1}, E/D = 0.065				Tetrahedral site optimized coordinate $D_{Td\text{-}opt}$ = -22.0 cm^{-1}, E/D = 0.238			
Co	-0.00208	-0.80245	-0.49179	Co	-0.04907	2.062797	0.760545
Zn	0.069344	2.071012	0.788152	Zn	0.053775	-0.80176	-0.46921
S	2.343469	5.39629	-1.62868	S	1.833369	5.664503	-1.59152
S	-1.97228	0.878826	4.809976	S	-2.04987	0.908111	4.822164
O	-1.04455	1.006853	-0.55576	O	-1.09144	0.977255	-0.5638
O	1.180045	0.352851	0.65243	O	1.177469	0.458119	0.649624
N	-1.76706	-1.62288	0.39179	N	-1.67889	-1.68559	0.469192
N	-1.20481	-1.39861	-2.32222	N	-1.12769	-1.49015	-2.29895
N	1.670759	-0.99565	-1.99537	N	1.765999	-0.9253	-2.00147
N	1.161054	-2.53106	0.262822	N	1.34301	-2.52026	0.278428
N	-0.78222	2.013193	2.53658	N	-0.87149	1.968944	2.504415
N	0.985972	3.5135	-0.06422	N	0.713854	3.572945	-0.10053
C	-1.28462	1.545645	3.504455	C	-1.36986	1.53889	3.49297
C	2.443084	-2.23224	-1.77335	C	2.608241	-2.10669	-1.75568
H	3.505424	-2.09048	-2.03561	H	3.661047	-1.90551	-2.01787
H	2.061944	-3.01536	-2.44973	H	2.276916	-2.92199	-2.42037
C	2.323829	-2.76642	-0.36567	C	2.527182	-2.63522	-0.33928
C	2.517251	0.332829	0.703382	C	2.513002	0.5076	0.690465
C	3.26469	0.245106	-0.49808	C	3.263293	0.434049	-0.51115
C	-2.65367	-2.16092	-0.46376	C	-2.52958	-2.26683	-0.39363
C	-2.33436	1.164984	-0.85143	C	-2.38576	1.052355	-0.86666
C	1.026717	-1.00383	-3.32235	C	1.093312	-0.99707	-3.30841
H	1.723728	-1.35022	-4.11026	H	1.787469	-1.32408	-4.10716
H	0.765078	0.032488	-3.57748	H	0.772467	0.018858	-3.57844
C	-0.22506	-1.88058	-3.31523	C	-0.1151	-1.93997	-3.27032
H	-0.66221	-1.91268	-4.33236	H	-0.54328	-2.02365	-4.2883
H	0.047229	-2.91634	-3.06118	H	0.213355	-2.95166	-2.98639
C	1.561413	4.315376	-0.72559	C	1.188746	4.464369	-0.72937

C	-2.14907	-1.3293	1.644512	C	-2.08872	-1.38746	1.711811
H	-1.41204	-0.84837	2.292385	H	-1.37985	-0.87194	2.364304
C	-2.12304	-2.45321	-1.85248	C	-1.9807	-2.57116	-1.77784
H	-1.55457	-3.39748	-1.80529	H	-1.35934	-3.4794	-1.70072
H	-2.96075	-2.61528	-2.55593	H	-2.81364	-2.80713	-2.46589
C	1.927732	-3.82815	2.134752	C	2.212752	-3.71612	2.168286
H	1.724594	-4.2223	3.13196	H	2.041591	-4.12334	3.166257
C	2.526178	0.222871	-1.81055	C	2.5309	0.350962	-1.82558
H	1.855212	1.094636	-1.87525	H	1.799566	1.172428	-1.89305
H	3.247367	0.288702	-2.64658	H	3.247846	0.465552	-2.66042
C	-3.19384	1.963545	-0.06649	C	-3.2881	1.818883	-0.09811
H	-2.7862	2.471285	0.810222	H	-2.9019	2.368342	0.762887
C	-2.87685	0.501123	-1.98243	C	-2.8892	0.335213	-1.98369
C	3.201293	0.401184	1.93198	C	3.19471	0.636082	1.916072
H	2.611805	0.482706	2.848072	H	2.600557	0.707021	2.82999
C	-1.94757	-0.23626	-2.90257	C	-1.92363	-0.37174	-2.89225
H	-2.50869	-0.59222	-3.78823	H	-2.46529	-0.76474	-3.77456
H	-1.18501	0.470484	-3.26207	H	-1.19401	0.365213	-3.25933
C	-4.54253	2.093659	-0.39417	C	-4.6411	1.870073	-0.42799
H	-5.18417	2.720501	0.231133	H	-5.31623	2.474989	0.183452
C	3.140481	-4.07075	1.484994	C	3.45143	-3.83431	1.532195
H	3.922493	-4.66362	1.965429	H	4.285462	-4.3387	2.026073
C	-4.23619	0.645678	-2.29256	C	-4.25454	0.400646	-2.2959
H	-4.63424	0.140648	-3.17903	H	-4.62457	-0.14326	-3.17149
C	-3.95857	-2.46322	-0.06694	C	-3.82845	-2.61145	-0.01027
H	-4.6613	-2.89281	-0.78375	H	-4.50484	-3.07496	-0.73127
C	3.341309	-3.53111	0.216725	C	3.611575	-3.28594	0.26152
H	4.280749	-3.68401	-0.31826	H	4.568914	-3.34405	-0.26022
C	0.972244	-3.04969	1.486206	C	1.190159	-3.04423	1.503238
H	0.018723	-2.82619	1.967868	H	0.210653	-2.91431	1.969113
C	-5.07857	1.433255	-1.50666	C	-5.13895	1.157886	-1.52652
H	-6.13488	1.540582	-1.76303	H	-6.19902	1.20316	-1.78587
C	-4.35249	-2.17486	1.241331	C	-4.25191	-2.3215	1.288184
H	-5.37357	-2.38688	1.56777	H	-5.26935	-2.56698	1.602288
C	-3.43518	-1.58767	2.114609	C	-3.37033	-1.6897	2.167234
H	-3.69037	-1.30063	3.136109	H	-3.65119	-1.40016	3.181266
C	4.665003	0.227497	-0.43865	C	4.66277	0.492596	-0.4526
H	5.237176	0.181047	-1.37085	H	5.235895	0.458454	-1.38485
C	4.59533	0.37956	1.967862	C	4.587649	0.690343	1.950294
H	5.109545	0.441254	2.93095	H	5.09853	0.799639	2.910928
C	5.337471	0.290996	0.783905	C	5.332385	0.616023	0.76687
H	6.42939	0.286819	0.812614	H	6.423018	0.670947	0.793177

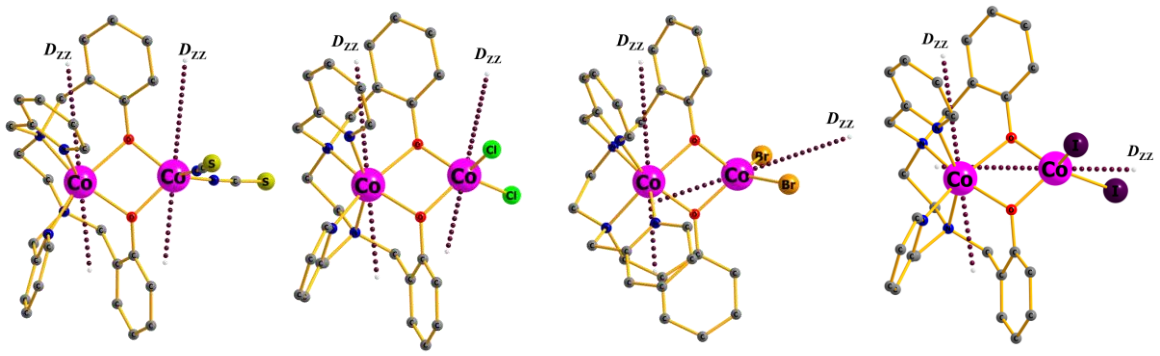

Figure S9. D_{zz} orientations on the local magnetic Co(II) centres plotted on the four complexes.

Table S8: CASSCF/NEVPT2 computed local ZFS parameters of the four complexes:

Complexes	Method	D_{Oh} (cm^{-1})	E/D	D_{Td} (cm^{-1})	E/D
1	NEVPT2	-43.7	0.11	12.8	0.23
	CASSCF	-60.4	0.11	13.9	0.23
2	NEVPT2	-41.5	0.12	14.2	0.30
	CASSCF	-58.2	0.12	15.1	0.32
3	NEVPT2	-45.2	0.13	-15.7	0.16
	CASSCF	-62.9	0.13	-17.6	0.10
4	NEVPT2	-37.5	0.09	-20.2	0.06
	CASSCF	-53.8	0.09	-22.7	0.06

Table S9: Multi-configurational wavefunction description and their contribution towards *D* and *E*/*D* parameter for six-coordinate site for complex **1**.

CASSCF Spin-free Energy of Complex 1 for Co(Oh) center (cm^{-1})	Multi-configurational CASSCF wavefunction $(d_{z^2})(d_{x^2-y^2})(d_{xy})(d_{yz})(d_{xz})$	Contribution towards D_{oh} (cm^{-1})	Contribution towards E_{oh} (cm^{-1})
0.0	2 2 1 1 1 (74%) 2 1 2 1 1 (19%)	0.0	0.00
905.4	2 1 2 1 1 (73%) 2 2 1 1 1 (15%)	-81.0	-0.06
3058.7	1 1 2 2 1 (26%) 1 2 1 1 2 (26%)	8.3	-8.56
7007.5	1 1 2 2 1 (30%) 2 1 1 1 2 (24%)	5.6	3.88
7300.7	1 2 1 2 1 (49%) 2 1 1 2 1 (20%)	5.4	-0.74

Table S10: Comparison of the 1st excited state contribution towards the *D* parameter of the six coordinate Co(II) centre in all four complexes.

Complexes	D_{Oh} in cm^{-1}	Contribution to D_{oh} from 1st excited state (cm^{-1})	CASSCF Energy of 1st excited state (cm^{-1})
1	-60.4	-81.0	905.4
2	-58.2	-79.0	925.0
3	-62.9	-83.5	823.4
4	-53.8	-73.3	1079.7

Table S11: Comparison of the first four excited state contributions towards the *D* parameter of the four coordinate Co(II) centre in all four complexes.

Complexes	D_{Td} (cm^{-1})	Contribution to D_{Td} from first four excited states (cm^{-1})	CASSCF Energy of first four excited states (cm^{-1})
1	13.9	18.9 5.2 -9.5 0.3	2894 4041 4780 5814
2	15.1	25.4 2.1 -15.6 7.5	2110 2652 3192 4390
3	-17.6	-55.0 12.6 10.5 11.6	1890 2330 2729 4295
4	-22.7	-60.2 11.7 8.9 13.1	1602 2064 2419 4299

Table S12: Multi-configurational wavefunction description and their contribution towards *D* and *E*/*D* parameter for four-coordinate site for complex **1**.

CASSCF Spin-free Energy of Complex 1 for Co(Td) center (cm^{-1})	**Multi-configurational CASSCF wavefunction (d_{yz})(d_{z^2})($d_{x^2-y^2}$)(d_{xy})(d_{xz})**	**Contribution towards D_{Td} (cm^{-1})**	**Contribution towards E_{Td} (cm^{-1})**
0.0	2 1 2 1 1 (38%) 2 2 1 1 1 (25%) 2 1 1 2 1 (16%)	0.0	0.00
2893.9	1 2 2 1 1 (55%) 1 2 1 2 1 (28%)	18.9	18.68
4041.7	2 1 1 1 2 (45%) 1 1 1 2 2 (15%)	5.1	-10.39
4780.4	2 1 1 2 1 (31%) 1 2 1 2 1 (17%)	-9.5	-4.62

Table S13: Multi-configurational wavefunction description and their contribution towards *D* and *E*/*D* parameter for six-coordinate site for complex **3**.

CASSCF Spin-free Energy of Complex 3 for Co(Td) center (cm^{-1})	**Multi-configurational CASSCF wavefunction ($d_{x^2-y^2}$)(d_{z^2})(d_{xy})(d_{xz})(d_{yz})**	**Contribution towards D_{Td} (cm^{-1})**	**Contribution towards E_{Td} (cm^{-1})**
0.0	2 2 1 1 1 (49%) 1 2 2 1 1 (28%)	0.0	0.00
1889.8	1 2 2 1 1 (46%) 2 2 1 1 1 (30%)	-55.0	0.16
2329.7	2 1 1 1 2 (62%) 1 2 1 1 2 (19%)	12.6	-0.96
2729.2	1 1 2 1 2 (40%) 1 1 2 2 1 (17%)	10.5	6.76

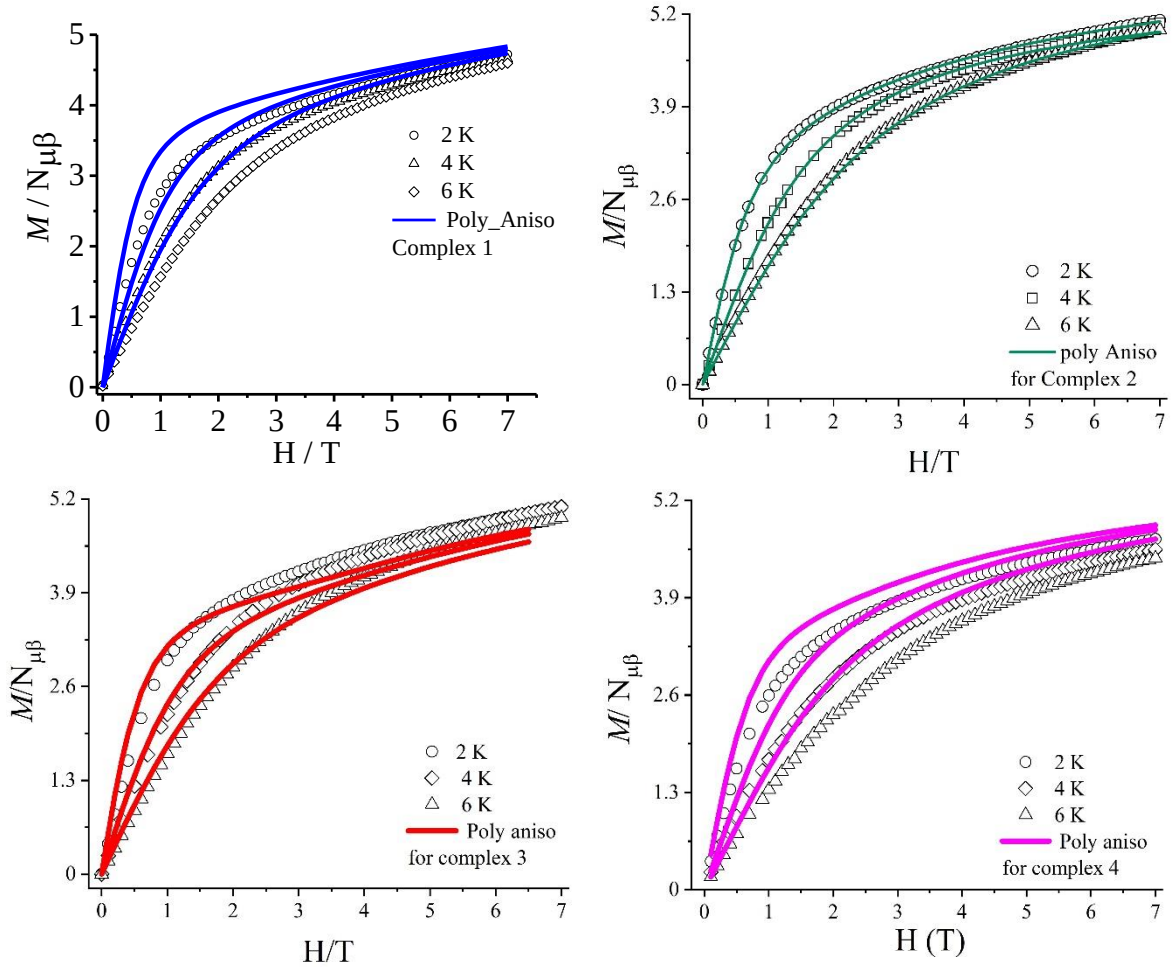

Figure S10. Comparison of experimental χT vs T and M vs H curve with the POLY_ANISO fitted values.

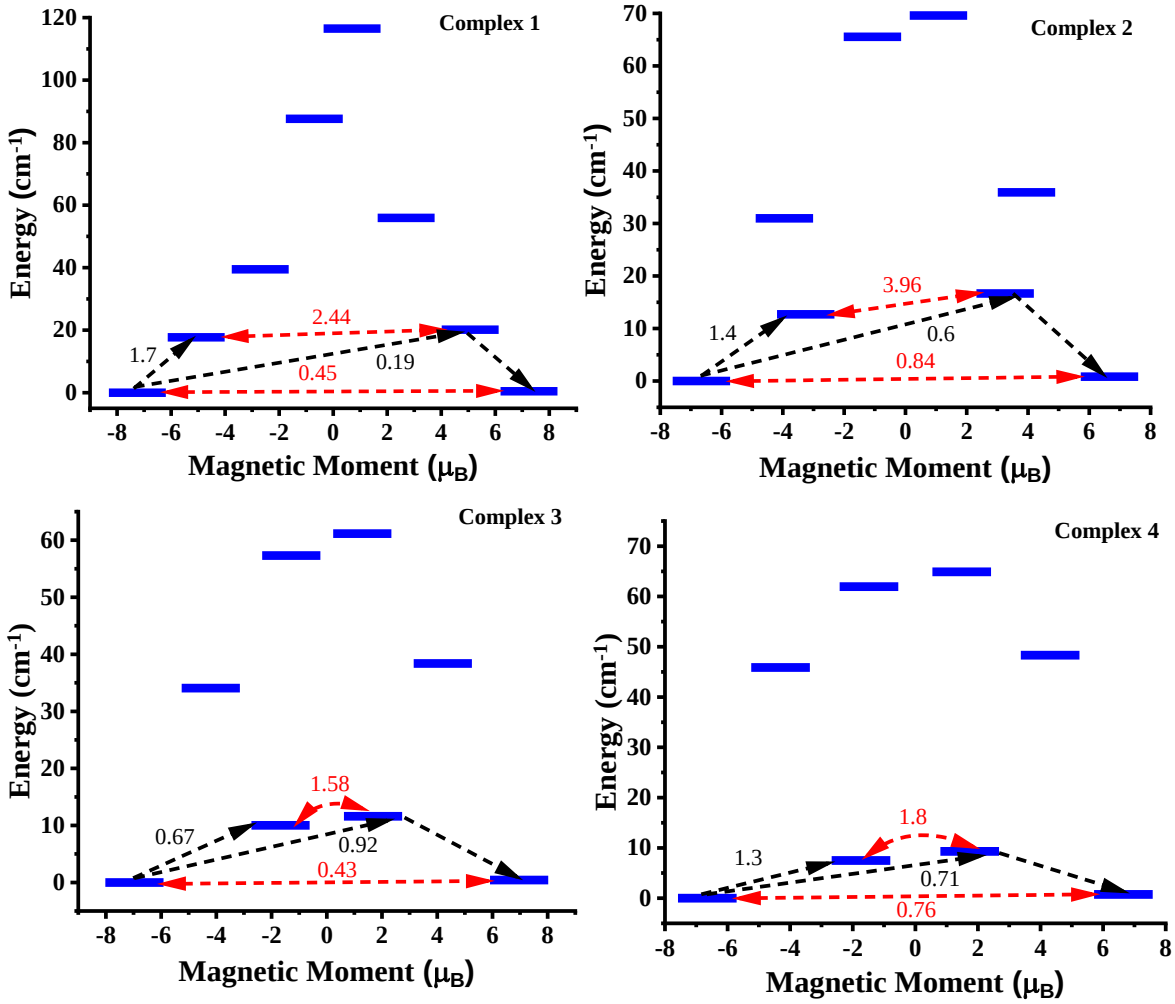

Figure S11: POLY_ANISO computed energy barrier of the exchange coupled states of four complexes. The dotted red arrows with numbers in red are tunnel splitting of the respective non-Kramers pairs and dotted black arrows with numbers in black indicate the transition probability and mixing coefficient with the opposite non-Kramers pair.

List of bond length for Complexes 1-4

Table S14a:
Bond Lengths for Complex 1

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O1	2.1491(13)	C24	C25	1.387(3)
Co1	O2	2.0649(14)	C22	C17	1.393(3)
Co1	N3	2.1244(18)	C22	C21	1.394(3)
Co1	N1	2.1852(15)	C17	C16	1.503(3)
Co1	N2	2.1792(17)	C17	C18	1.394(3)
Co1	N4	2.1429(16)	C9	C8	1.504(3)
Co2	O1	1.9504(13)	C9	C10	1.380(3)
Co2	O2	1.9446(14)	C1	C2	1.395(3)
Co2	N5	1.9555(19)	C1	C6	1.402(3)
Co2	N6	1.9479(19)	C15	C14	1.514(3)
S2	C30	1.616(2)	C13	C12	1.382(3)
S1	C29	1.615(2)	C27	C26	1.379(4)
O1	C1	1.350(2)	C27	C28	1.380(3)
O2	C22	1.358(2)	C2	C3	1.385(3)
N3	C9	1.345(3)	C6	C7	1.505(3)
N3	C13	1.343(3)	C6	C5	1.390(3)
N1	C14	1.484(3)	C21	C20	1.387(4)
N1	C8	1.478(3)	C3	C4	1.379(3)
N1	C7	1.496(2)	C26	C25	1.380(3)
N2	C23	1.483(2)	C5	C4	1.391(3)
N2	C15	1.478(2)	C10	C11	1.374(4)
N2	C16	1.497(3)	C11	C12	1.376(4)
N4	C24	1.335(3)	C18	C19	1.386(4)
N4	C28	1.345(3)	C20	C19	1.369(4)
N5	C29	1.156(3)	C31	C32	1.408(5)
N6	C30	1.160(3)	C31	N7	1.097(4)
C23	C24	1.497(3)			

Table S14b:
Bond Lengths for Complex 2

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O2	2.066(2)	C23	C24	1.504(5)
Co1	O1	2.142(2)	C24	C25	1.377(5)
Co1	N1	2.185(3)	C1	C6	1.387(5)
Co1	N2	2.178(3)	C1	C2	1.400(5)
Co1	N4	2.146(3)	C9	C8	1.502(5)
Co1	N3	2.125(3)	C9	C10	1.382(5)
Co2	Cl1	2.2562(11)	C28	C27	1.363(5)
Co2	Cl2	2.2322(12)	C7	C6	1.498(5)
Co2	O2	1.983(2)	C14	C15	1.519(5)
Co2	O1	1.964(2)	C13	C12	1.384(5)
O2	C22	1.354(4)	C6	C5	1.390(5)
O1	C1	1.349(4)	C17	C16	1.492(5)
N1	C7	1.492(4)	C17	C18	1.394(5)
N1	C8	1.482(5)	C18	C19	1.372(6)
N1	C14	1.485(4)	C2	C3	1.375(6)

N2	C23	1.487(4)	C21	C20	1.380(6)
N2	C15	1.482(4)	C27	C26	1.371(6)
N2	C16	1.494(5)	C25	C26	1.368(6)
N4	C24	1.329(4)	C5	C4	1.372(6)
N4	C28	1.342(4)	C3	C4	1.375(7)
N3	C9	1.339(5)	C10	C11	1.371(6)
N3	C13	1.333(5)	C12	C11	1.360(6)
C22	C17	1.401(5)	C19	C20	1.369(6)
C22	C21	1.386(5)			

Table S14c:
Bond Lengths for Complex 3

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	Co2	2.3998(12)	C8	C9	1.534(9)
Br2	Co2	2.3776(11)	C7	C6	1.502(10)
Co1	O1	2.137(4)	C9	C10	1.350(9)
Co1	O2	2.079(4)	C23	C24	1.496(9)
Co1	N1	2.180(6)	C28	C27	1.378(10)
Co1	N3	2.114(6)	C10	C11	1.389(10)
Co1	N4	2.132(6)	C22	C17	1.427(10)
Co1	N2	2.171(6)	C22	C21	1.388(10)
Co2	O1	1.967(4)	C14	C15	1.515(9)
Co2	O2	1.979(5)	C27	C26	1.378(10)
O1	C1	1.345(8)	C2	C3	1.375(10)
O2	C22	1.341(8)	C3	C4	1.398(10)
N1	C8	1.492(8)	C6	C5	1.371(10)
N1	C7	1.486(8)	C18	C17	1.382(10)
N1	C14	1.481(9)	C18	C19	1.383(10)
N3	C9	1.357(9)	C24	C25	1.379(10)
N3	C13	1.346(9)	C17	C16	1.491(10)
N4	C28	1.340(8)	C21	C20	1.386(10)
N4	C24	1.350(9)	C5	C4	1.395(10)
N2	C23	1.477(9)	C13	C12	1.377(10)
N2	C15	1.476(9)	C19	C20	1.382(10)
N2	C16	1.505(8)	C12	C11	1.391(10)
C1	C2	1.404(9)	C25	C26	1.369(10)
C1	C6	1.407(9)			

Table S14d:
Bond Lengths for Complex 4

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Co2	2.6055(8)	C24	C23	1.503(7)
I2	Co2	2.5502(8)	C24	C25	1.375(7)
Co1	O1	2.140(3)	C22	C17	1.405(7)
Co1	O2	2.029(3)	C22	C21	1.377(7)
Co1	N4	2.151(4)	C25	C26	1.390(8)
Co1	N2	2.186(4)	C9	C8	1.496(8)
Co1	N3	2.146(4)	C9	C10	1.374(8)
Co1	N1	2.181(4)	C17	C16	1.490(8)
Co2	O1	1.959(3)	C17	C18	1.370(8)

Co2	O2	1.939(3)	C28	C27	1.365(8)
O1	C1	1.351(6)	C6	C5	1.399(7)
O2	C22	1.358(6)	C6	C7	1.492(8)
N4	C24	1.335(7)	C2	C3	1.392(7)
N4	C28	1.345(7)	C13	C12	1.384(7)
N2	C23	1.467(6)	C14	C15	1.501(7)
N2	C15	1.493(6)	C21	C20	1.381(8)
N2	C16	1.494(6)	C5	C4	1.369(8)
N3	C9	1.347(7)	C3	C4	1.364(9)
N3	C13	1.334(7)	C26	C27	1.363(8)
N1	C14	1.495(7)	C18	C19	1.382(8)
N1	C8	1.467(7)	C12	C11	1.371(9)
N1	C7	1.493(7)	C10	C11	1.366(9)
C1	C6	1.404(7)	C20	C19	1.374(9)
C1	C2	1.388(7)			

Bond angles for complexes 1-4

Table S15a:
Bond Angles for Complex 1

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	Co1	N1	87.60(5)	C29	N5	Co2	166.55(18)
O1	Co1	N2	112.35(6)	C30	N6	Co2	174.52(17)
O2	Co1	O1	75.96(5)	N5	C29	S1	179.0(2)
O2	Co1	N3	116.72(6)	N2	C23	C24	111.62(17)
O2	Co1	N1	156.72(6)	N4	C24	C23	115.77(16)
O2	Co1	N2	89.60(6)	N4	C24	C25	122.54(19)
O2	Co1	N4	86.57(6)	C25	C24	C23	121.64(19)
N3	Co1	O1	87.18(6)	O2	C22	C17	119.27(18)
N3	Co1	N1	78.10(6)	O2	C22	C21	120.8(2)
N3	Co1	N2	151.00(7)	C17	C22	C21	120.0(2)
N3	Co1	N4	90.88(6)	C22	C17	C16	119.56(18)
N2	Co1	N1	81.42(6)	C22	C17	C18	119.2(2)
N4	Co1	O1	159.27(6)	C18	C17	C16	121.2(2)
N4	Co1	N1	112.20(6)	N3	C9	C8	115.55(18)
N4	Co1	N2	78.08(6)	N3	C9	C10	122.3(2)
O1	Co2	N5	114.86(7)	C10	C9	C8	122.1(2)
O2	Co2	O1	83.52(6)	O1	C1	C2	122.06(18)
O2	Co2	N5	110.26(7)	O1	C1	C6	118.75(17)
O2	Co2	N6	115.48(7)	C2	C1	C6	119.18(18)
N6	Co2	O1	115.49(7)	N2	C15	C14	109.34(16)
N6	Co2	N5	113.76(8)	N1	C14	C15	109.79(16)
Co2	O1	Co1	98.21(5)	N6	C30	S2	178.9(2)
C1	O1	Co1	120.87(12)	N3	C13	C12	122.7(2)
C1	O1	Co2	128.15(12)	N1	C8	C9	111.16(16)
Co2	O2	Co1	101.31(6)	C26	C27	C28	119.0(2)
C22	O2	Co1	123.22(13)	N2	C16	C17	112.10(16)
C22	O2	Co2	128.55(13)	C3	C2	C1	120.4(2)
C9	N3	Co1	115.14(13)	C1	C6	C7	119.48(18)
C13	N3	Co1	126.64(15)	C5	C6	C1	119.40(19)
C13	N3	C9	117.91(19)	C5	C6	C7	120.89(19)
C14	N1	Co1	107.43(11)	C20	C21	C22	119.5(2)

C14	N1	C7	107.61(14)	N1	C7	C6	116.36(15)
C8	N1	Co1	105.85(11)	C4	C3	C2	120.9(2)
C8	N1	C14	111.72(16)	C27	C26	C25	118.9(2)
C8	N1	C7	110.92(15)	C6	C5	C4	121.1(2)
C7	N1	Co1	113.32(11)	C11	C10	C9	119.1(2)
C23	N2	Co1	110.63(12)	C26	C25	C24	118.8(2)
C23	N2	C16	109.28(16)	N4	C28	C27	122.5(2)
C15	N2	Co1	106.24(12)	C3	C4	C5	119.0(2)
C15	N2	C23	111.02(16)	C10	C11	C12	119.4(2)
C15	N2	C16	110.40(15)	C11	C12	C13	118.6(2)
C16	N2	Co1	109.23(12)	C19	C18	C17	120.5(3)
C24	N4	Co1	116.03(12)	C19	C20	C21	120.9(2)
C24	N4	C28	118.16(17)	C20	C19	C18	119.8(2)
C28	N4	Co1	123.47(14)	N7	C31	C32	179.6(6)

Table S15b:
Bond Angles for Complex 2

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O2	Co1	O1	77.18(9)	C13	N3	Co1	125.4(3)
O2	Co1	N1	158.09(10)	C13	N3	C9	119.0(3)
O2	Co1	N2	90.15(10)	O2	C22	C17	119.3(3)
O2	Co1	N4	88.00(11)	O2	C22	C21	121.1(3)
O2	Co1	N3	114.66(11)	C21	C22	C17	119.6(4)
O1	Co1	N1	87.24(10)	N2	C23	C24	112.0(3)
O1	Co1	N2	112.71(10)	N4	C24	C23	116.6(3)
O1	Co1	N4	161.38(10)	N4	C24	C25	122.0(3)
N2	Co1	N1	81.66(11)	C25	C24	C23	121.3(3)
N4	Co1	N1	109.89(11)	O1	C1	C6	119.2(3)
N4	Co1	N2	78.07(11)	O1	C1	C2	121.7(4)
N3	Co1	O1	86.23(10)	C6	C1	C2	119.1(4)
N3	Co1	N1	79.03(12)	N3	C9	C8	115.4(3)
N3	Co1	N2	152.18(12)	N3	C9	C10	121.1(4)
N3	Co1	N4	89.88(11)	C10	C9	C8	123.5(4)
Cl2	Co2	Cl1	113.92(5)	N4	C28	C27	124.0(4)
O2	Co2	Cl1	110.84(8)	N1	C7	C6	115.5(3)
O2	Co2	Cl2	115.12(8)	N1	C8	C9	111.2(3)
O1	Co2	Cl1	116.68(8)	N1	C14	C15	109.3(3)
O1	Co2	Cl2	113.42(8)	N2	C15	C14	109.3(3)
O1	Co2	O2	83.39(10)	N3	C13	C12	122.6(4)
Co2	O2	Co1	100.40(11)	C1	C6	C7	119.4(3)
C22	O2	Co1	122.0(2)	C1	C6	C5	119.6(4)
C22	O2	Co2	128.8(2)	C5	C6	C7	121.0(4)
Co2	O1	Co1	98.42(10)	C22	C17	C16	119.4(3)
C1	O1	Co1	120.9(2)	C18	C17	C22	119.1(4)
C1	O1	Co2	129.0(2)	C18	C17	C16	121.4(4)
C7	N1	Co1	113.3(2)	C17	C16	N2	112.1(3)
C8	N1	Co1	104.8(2)	C19	C18	C17	120.3(4)
C8	N1	C7	110.8(3)	C3	C2	C1	119.7(5)
C8	N1	C14	112.5(3)	C20	C21	C22	120.0(4)
C14	N1	Co1	107.0(2)	C28	C27	C26	117.7(4)
C14	N1	C7	108.4(3)	C26	C25	C24	119.4(4)
C23	N2	Co1	111.7(2)	C4	C5	C6	121.3(5)

C23	N2	C16	110.4(3)	C2	C3	C4	121.5(5)
C15	N2	Co1	106.2(2)	C11	C10	C9	119.2(4)
C15	N2	C23	109.9(3)	C11	C12	C13	118.0(4)
C15	N2	C16	111.0(3)	C5	C4	C3	118.8(4)
C16	N2	Co1	107.5(2)	C25	C26	C27	119.4(4)
C24	N4	Co1	116.6(2)	C20	C19	C18	120.4(4)
C24	N4	C28	117.4(3)	C12	C11	C10	120.1(4)
C28	N4	Co1	124.5(2)	C19	C20	C21	120.5(5)
C9	N3	Co1	114.4(3)				

Table S15c:
Bond Angles for Complex 3

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	Co1	N1	88.26(19)	C15	N2	C16	110.1(5)
O1	Co1	N2	111.07(19)	C16	N2	Co1	107.4(4)
O2	Co1	O1	77.60(17)	O1	C1	C2	121.4(6)
O2	Co1	N1	159.89(18)	O1	C1	C6	119.4(6)
O2	Co1	N3	114.4(2)	C2	C1	C6	119.2(6)
O2	Co1	N4	86.96(19)	N1	C8	C9	109.9(5)
O2	Co1	N2	90.06(19)	N1	C7	C6	116.9(6)
N3	Co1	O1	87.5(2)	N3	C9	C8	114.2(6)
N3	Co1	N1	78.7(2)	C10	C9	N3	123.1(6)
N3	Co1	N4	89.9(2)	C10	C9	C8	122.7(6)
N3	Co1	N2	152.5(2)	N2	C23	C24	112.7(6)
N4	Co1	O1	161.60(19)	N4	C28	C27	123.4(7)
N4	Co1	N1	109.1(2)	C9	C10	C11	119.0(7)
N4	Co1	N2	78.5(2)	O2	C22	C17	118.8(6)
N2	Co1	N1	81.7(2)	O2	C22	C21	121.9(6)
Br2	Co2	Br1	114.76(5)	C21	C22	C17	119.3(7)
O1	Co2	Br1	117.34(14)	N1	C14	C15	109.7(5)
O1	Co2	Br2	112.37(13)	C26	C27	C28	118.2(6)
O1	Co2	O2	84.09(19)	N2	C15	C14	109.3(5)
O2	Co2	Br1	107.89(13)	C3	C2	C1	120.4(7)
O2	Co2	Br2	116.82(13)	C2	C3	C4	120.4(7)
Co2	O1	Co1	98.07(19)	C1	C6	C7	118.8(6)
C1	O1	Co1	120.6(4)	C5	C6	C1	119.4(7)
C1	O1	Co2	128.0(4)	C5	C6	C7	121.6(6)
Co2	O2	Co1	99.6(2)	C17	C18	C19	121.9(7)
C22	O2	Co1	122.7(4)	N4	C24	C23	115.6(6)
C22	O2	Co2	127.4(4)	N4	C24	C25	122.1(6)
C8	N1	Co1	105.5(4)	C25	C24	C23	122.1(6)
C7	N1	Co1	113.0(4)	C22	C17	C16	119.1(6)
C7	N1	C8	110.7(5)	C18	C17	C22	118.3(7)
C14	N1	Co1	107.2(4)	C18	C17	C16	122.6(7)
C14	N1	C8	112.1(5)	C20	C21	C22	120.9(7)
C14	N1	C7	108.3(5)	C6	C5	C4	121.6(7)
C9	N3	Co1	115.6(4)	C17	C16	N2	111.5(5)
C13	N3	Co1	126.5(5)	N3	C13	C12	123.7(7)
C13	N3	C9	117.2(6)	C5	C4	C3	118.8(7)
C28	N4	Co1	124.6(5)	C20	C19	C18	119.6(7)
C28	N4	C24	117.4(6)	C13	C12	C11	117.4(7)
C24	N4	Co1	116.1(4)	C26	C25	C24	119.4(7)

C23	N2	Co1	111.4(4)	C10	C11	C12	119.6(7)
C23	N2	C16	110.3(5)	C25	C26	C27	119.4(7)
C15	N2	Co1	106.1(4)	C19	C20	C21	120.0(7)
C15	N2	C23	111.4(5)				

Table S15d:
Bond Angles for Complex 4

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	Co1	N4	157.33(15)	C7	N1	Co1	112.0(3)
O1	Co1	N2	116.31(15)	C7	N1	C14	107.8(4)
O1	Co1	N3	85.77(15)	O1	C1	C6	118.5(5)
O1	Co1	N1	88.96(15)	O1	C1	C2	121.7(5)
O2	Co1	O1	75.17(13)	C2	C1	C6	119.8(5)
O2	Co1	N4	88.39(15)	N4	C24	C23	115.1(5)
O2	Co1	N2	88.90(15)	N4	C24	C25	122.4(5)
O2	Co1	N3	118.24(16)	C25	C24	C23	122.2(5)
O2	Co1	N1	155.63(16)	O2	C22	C17	118.6(5)
N4	Co1	N2	78.13(16)	O2	C22	C21	121.0(5)
N4	Co1	N1	111.26(16)	C21	C22	C17	120.3(5)
N3	Co1	N4	88.51(17)	N2	C23	C24	113.1(4)
N3	Co1	N2	149.57(17)	C24	C25	C26	119.2(6)
N3	Co1	N1	77.98(17)	N3	C9	C8	115.8(5)
N1	Co1	N2	81.60(17)	N3	C9	C10	120.4(6)
I2	Co2	I1	115.39(3)	C10	C9	C8	123.7(6)
O1	Co2	I1	118.95(10)	C22	C17	C16	119.0(5)
O1	Co2	I2	113.87(10)	C18	C17	C22	118.3(5)
O2	Co2	I1	108.40(11)	C18	C17	C16	122.6(6)
O2	Co2	I2	113.77(11)	N4	C28	C27	124.0(6)
O2	Co2	O1	81.48(14)	C1	C6	C7	120.6(5)
Co2	O1	Co1	98.57(14)	C5	C6	C1	117.9(6)
C1	O1	Co1	122.1(3)	C5	C6	C7	121.1(5)
C1	O1	Co2	129.8(3)	C1	C2	C3	119.7(6)
Co2	O2	Co1	103.12(16)	N3	C13	C12	121.5(6)
C22	O2	Co1	124.6(3)	N1	C14	C15	109.9(4)
C22	O2	Co2	128.7(3)	N1	C8	C9	112.0(4)
C24	N4	Co1	116.2(4)	N2	C15	C14	110.0(4)
C24	N4	C28	117.1(5)	C22	C21	C20	119.9(6)
C28	N4	Co1	125.0(4)	C17	C16	N2	111.9(4)
C23	N2	Co1	110.3(3)	C4	C5	C6	122.2(6)
C23	N2	C15	110.7(4)	C4	C3	C2	121.3(6)
C23	N2	C16	110.9(4)	C27	C26	C25	118.7(6)
C15	N2	Co1	105.8(3)	C6	C7	N1	116.3(5)
C15	N2	C16	109.7(4)	C17	C18	C19	121.5(6)
C16	N2	Co1	109.4(3)	C26	C27	C28	118.6(6)
C9	N3	Co1	114.7(4)	C11	C12	C13	118.8(6)
C13	N3	Co1	125.4(4)	C11	C10	C9	120.2(6)
C13	N3	C9	119.8(5)	C19	C20	C21	120.2(6)
C14	N1	Co1	107.8(3)	C3	C4	C5	119.0(6)
C8	N1	Co1	106.9(3)	C20	C19	C18	119.6(6)
C8	N1	C14	111.6(4)	C10	C11	C12	119.2(6)
C8	N1	C7	110.8(4)				