

Supplementary Information

Magneto-structural studies on a number of doubly end-on cyanate and azide bridged dinuclear nickel(II) complexes with {N₃O} donor Schiff base ligands

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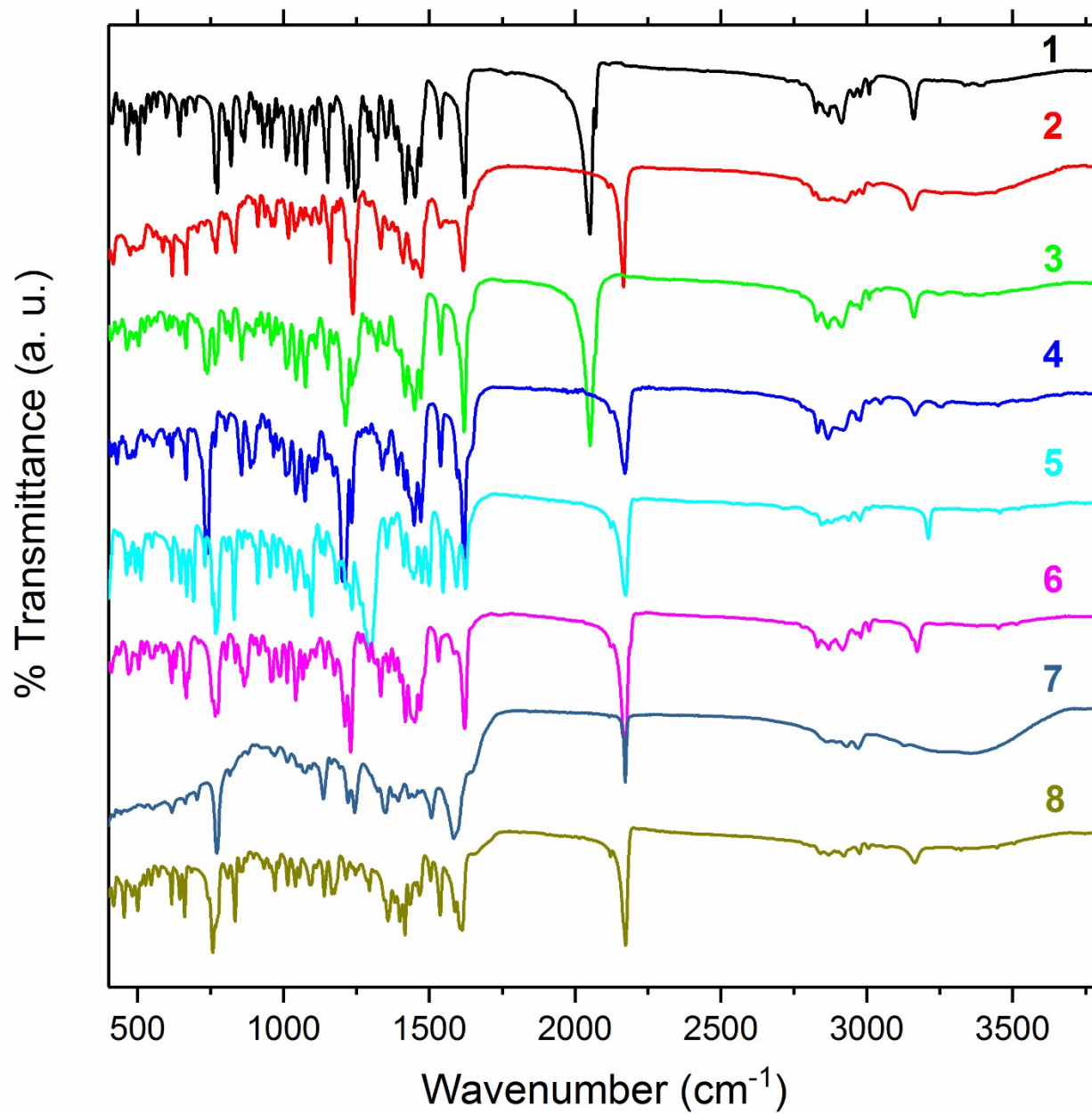


Fig. S1. IR spectra of complexes 1–8.

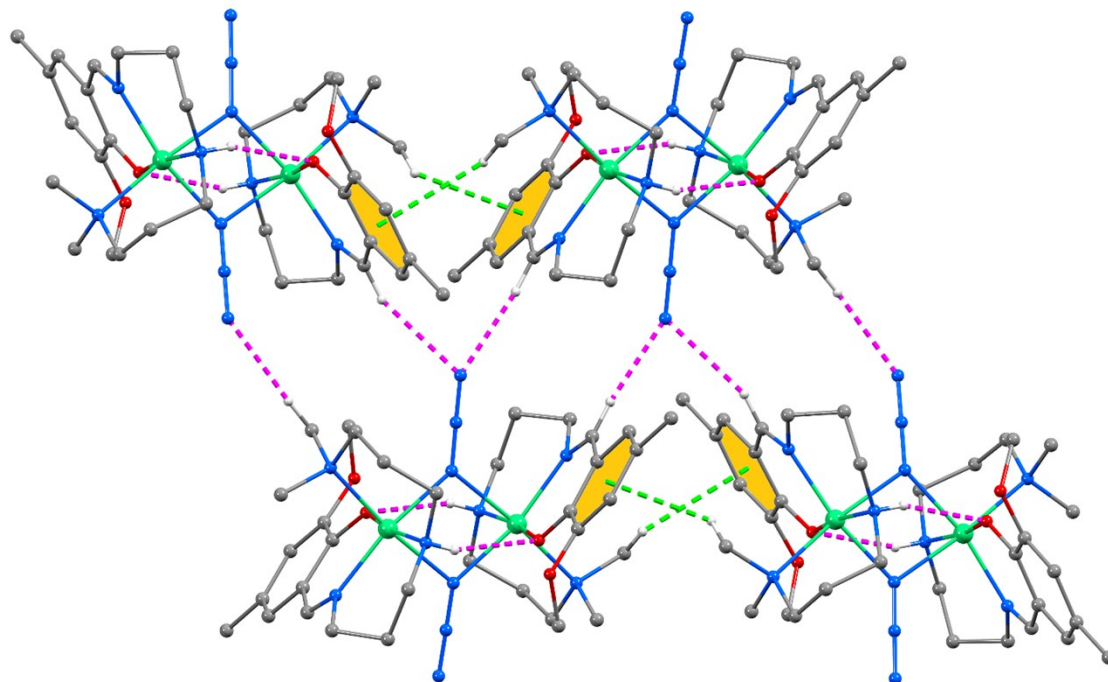


Fig. S2. Molecular packing in complex 1.

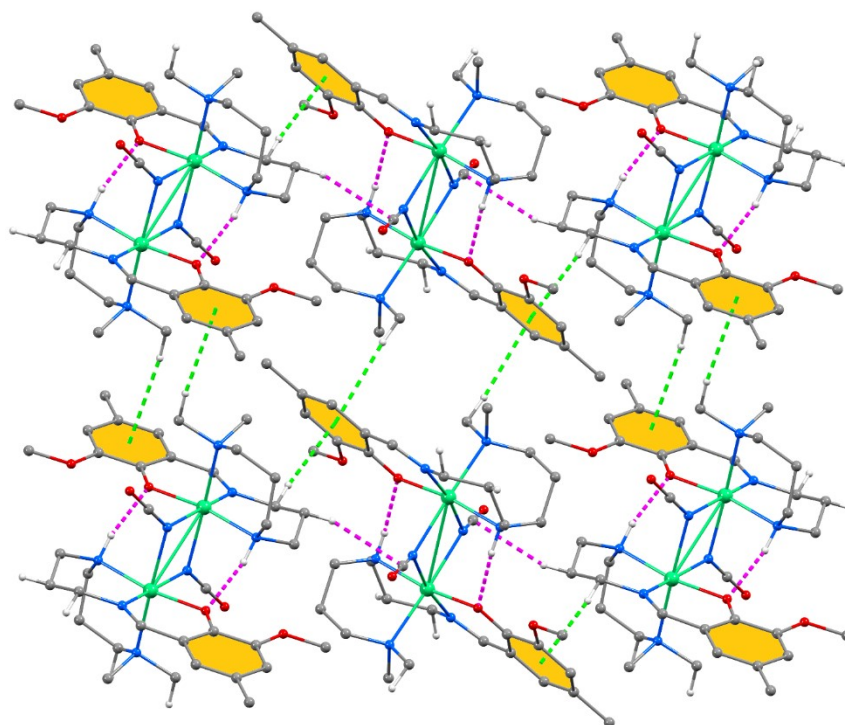


Fig. S3. Molecular packing in complex 2.

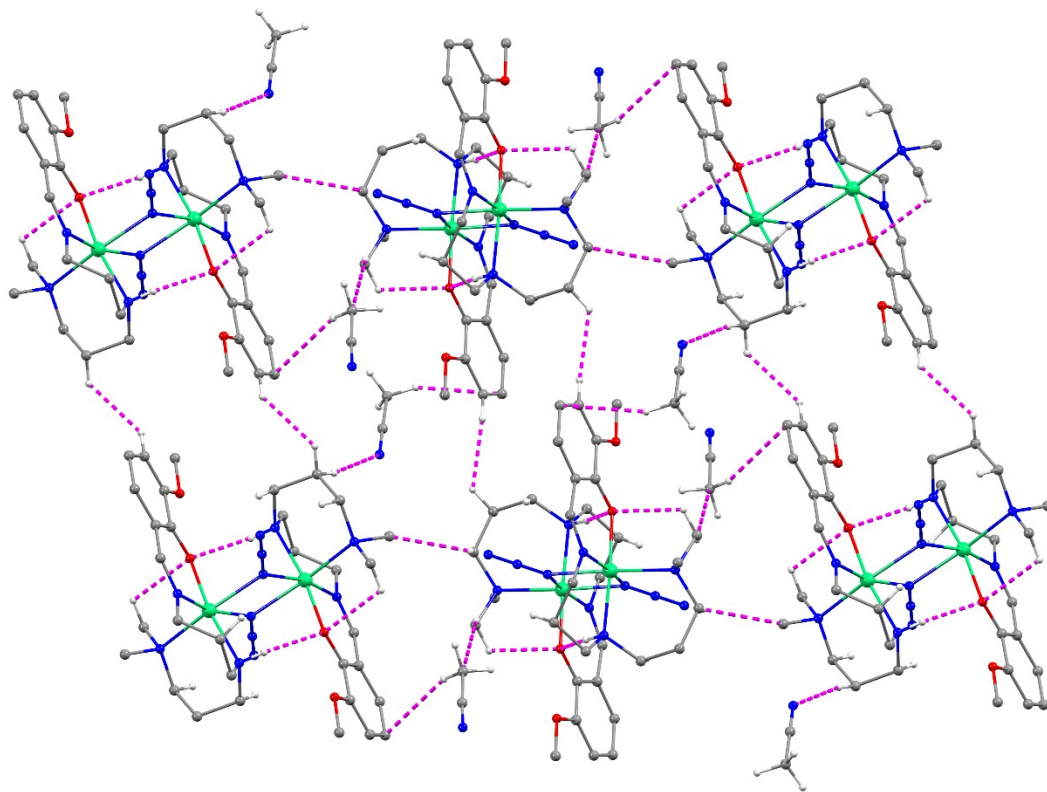


Fig. S4. Molecular packing in complex 3.

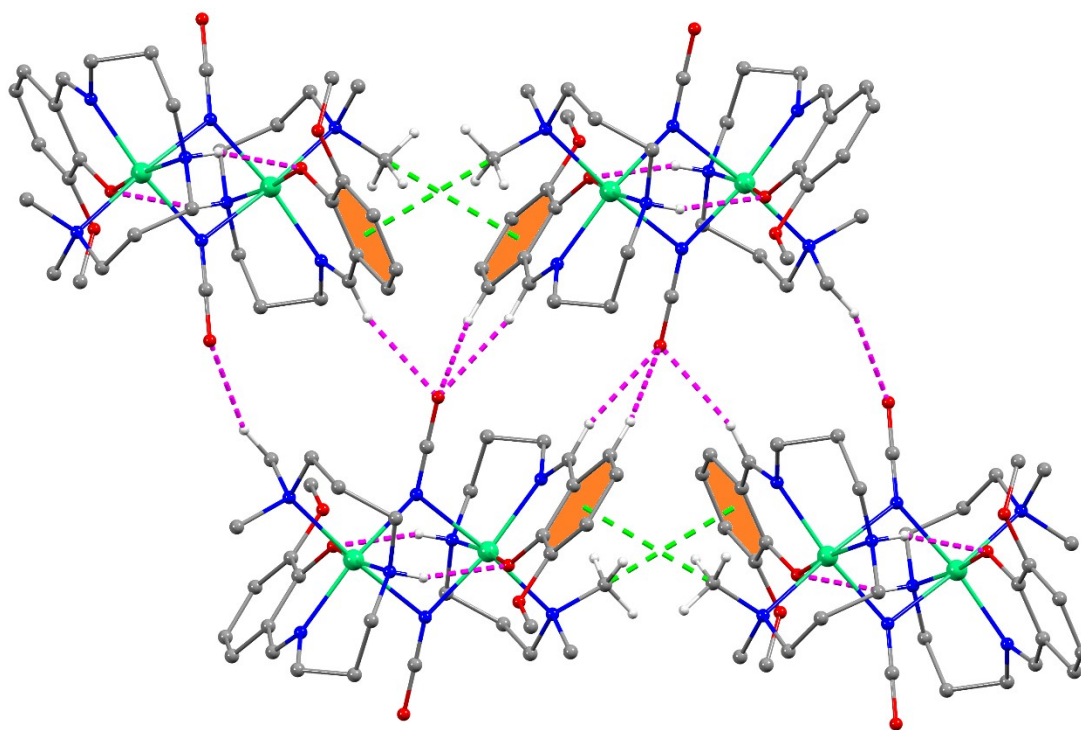


Fig. S5. Molecular packing in complex 4.

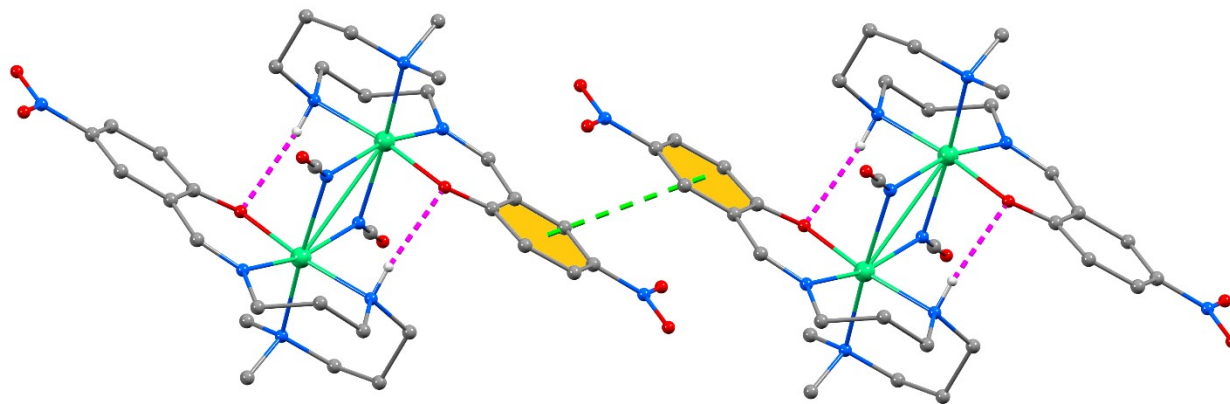


Fig. S6. Molecular packing in complex 5.

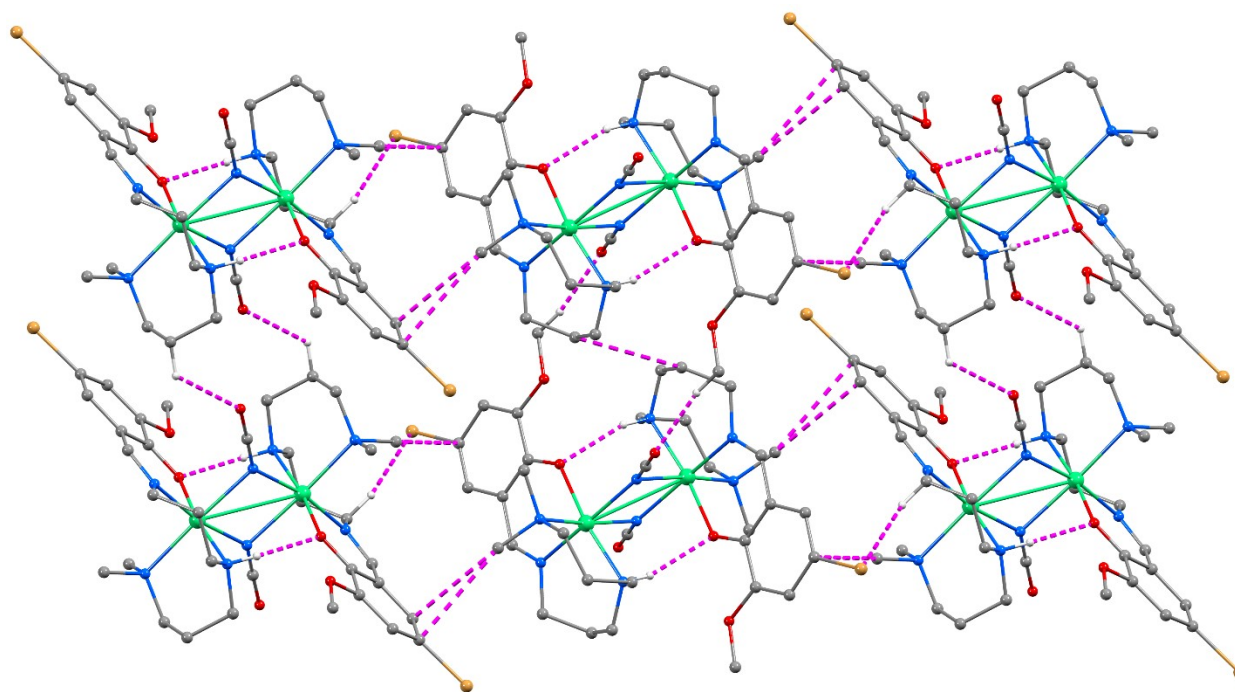


Fig. S7. Molecular packing in complex 6.

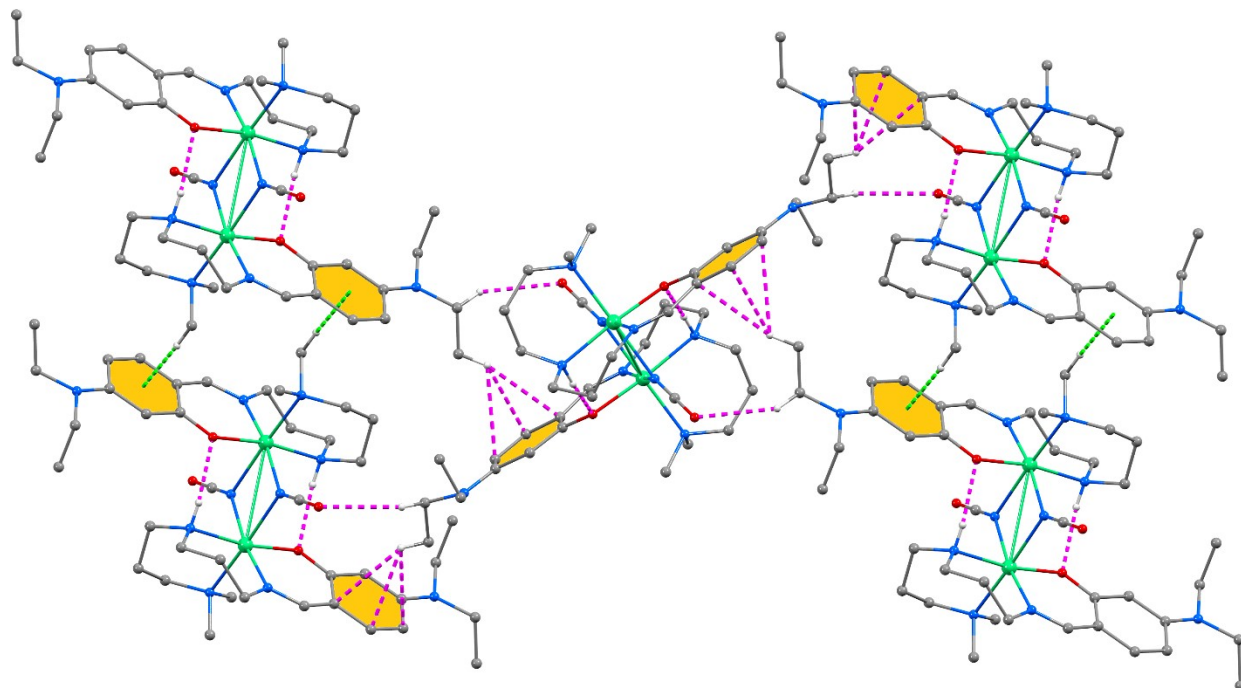


Fig. S8. Molecular packing in complex 7.

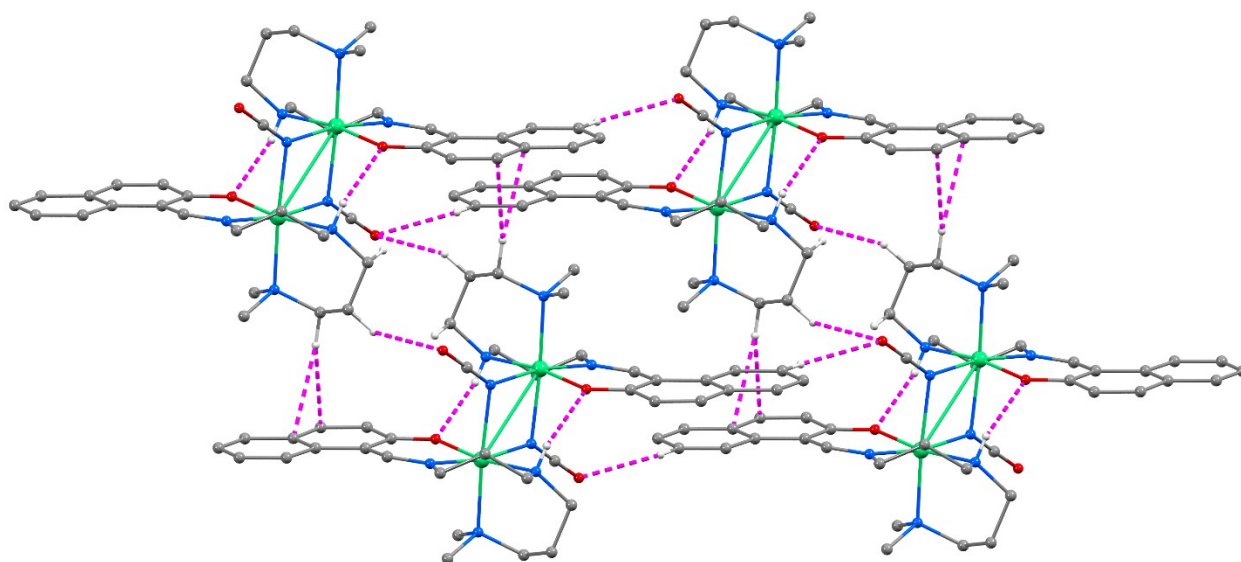


Fig. S9. Molecular packing in complex 8.

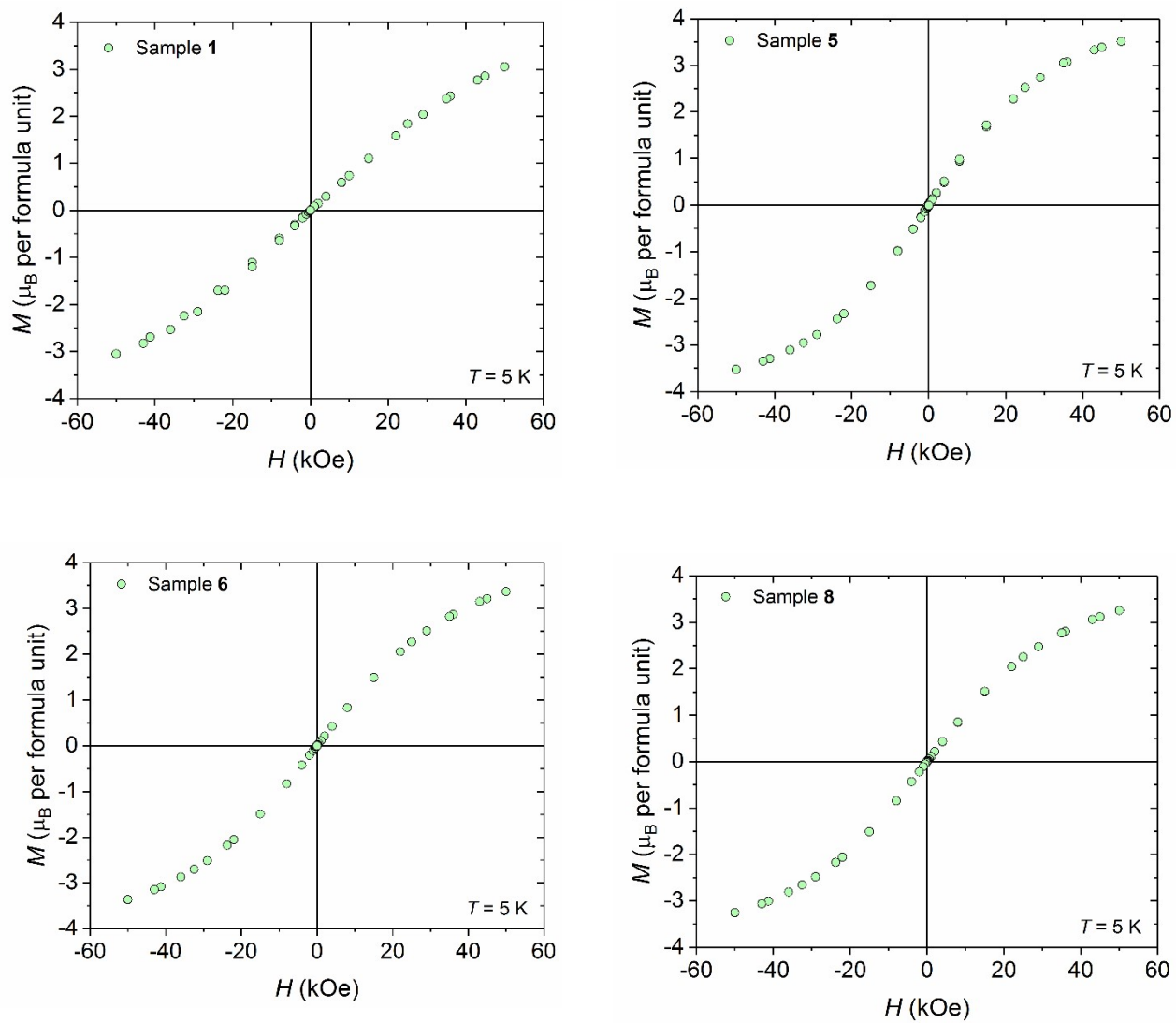


Fig. S10. Representative isothermal magnetization curves for complexes **1**, **5**, **6** and **8** at 5 K

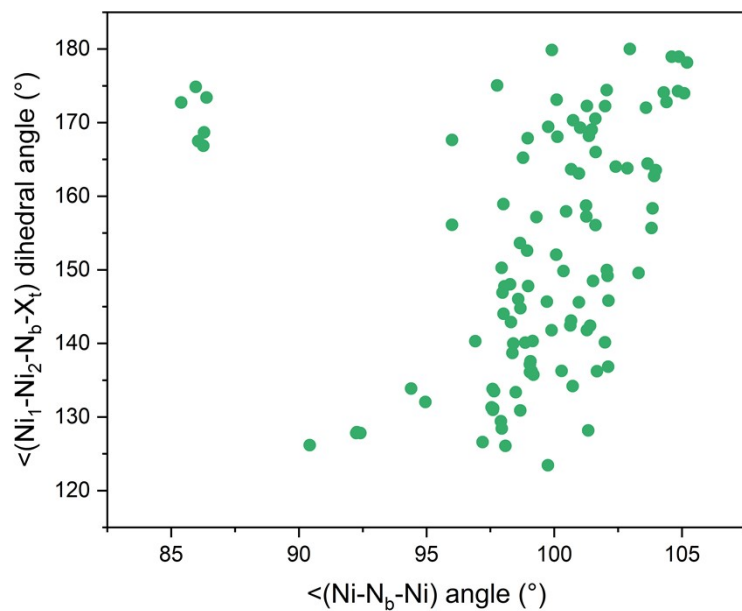


Fig. S11. The results of structural search in CSD for dinuclear Ni^{II} motives comprising two azide bridging ligands as a function of Ni-N_b-Ni angle and Ni1-Ni2-N_b-X_t dihedral angle.

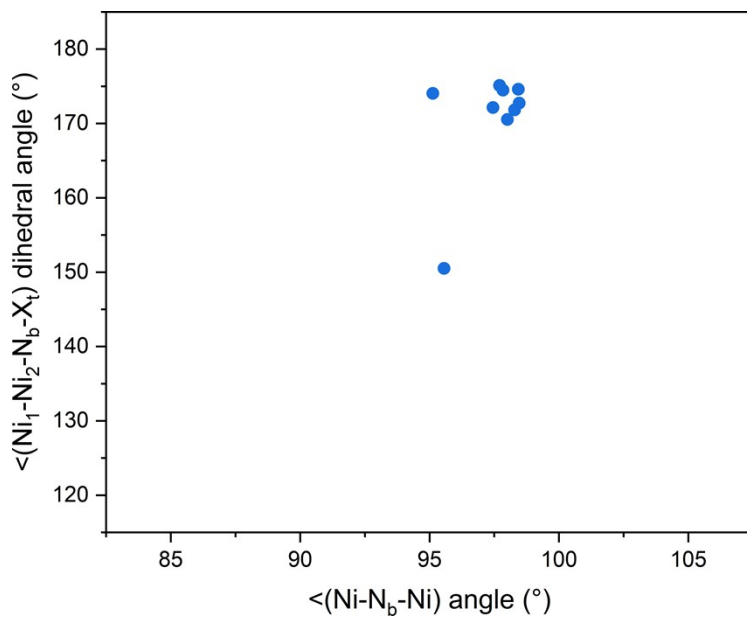


Fig. S12. The results of structural search in CSD for dinuclear Ni^{II} motives comprising two cyanate bridging ligands as a function of Ni-N_b-Ni angle and Ni1-Ni2-N_b-X_t dihedral angle.

Table S1 The evaluation of the magnetic exchange by the broken-symmetry DFT approach for **1-8**

Complex	$\langle(\text{Ni-Nb-Ni})_{\text{aver.}}\rangle$ ($^{\circ}$)	J_{B3LYP}^R (cm^{-1})	J_{B3LYP}^Y (cm^{-1})	J_{M062X}^R (cm^{-1})	J_{M062X}^Y (cm^{-1})
1	101.496	35.23	52.76	24.11	36.10
2	96.791	7.35	11.02	2.80	4.19
3	101.478	31.51	47.19	21.35	31.97
4A	98.235	8.75	13.11	3.87	5.81
4B	97.932	7.46	11.19	3.01	4.52
5	99.873	12.30	18.44	6.48	9.72
6A	99.00	9.81	14.70	4.48	6.72
6B	96.770	7.22	10.83	2.28	3.41
7	97.428	8.41	12.60	3.62	5.43
8	98.037	8.45	12.66	3.71	5.57