

Tuning magnetic exchange and relaxation dynamics in dinuclear Dy(III) single-molecule magnets via co-ligand modulation on a hydrazone-based Schiff base platform

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Table S1. Crystal data and structure refinement for Schiff base H₂L and complexes 1-4

| | | | | | |
|---|--|--|--|--|--|
| Identification code | H₂L | 1 | 2 | 3 | 4 |
| Empirical formula | C₁₅H₁₇N₃O₄ | C₃₄H₃₈Dy₂N₆O₁₃ | C₆₄H₆₀Cl₄Dy₂N₆O₁₂ | C₄₈H_{59.6}Dy₂N₈O_{22.8} | C₄₈H₅₄Dy₂N₈O₂₀ |
| Formula weight | 303.32 | 1063.70 | 1571.98 | 1438.43 | 1387.99 |
| Temperature/K | 297.15 | 163.15 | 150.15 | 100.15 | 212.15 |
| Crystal system | orthorhombic | monoclinic | monoclinic | triclinic | monoclinic |
| Space group | P2₁2₁2₁ | C2/c | P2₁/c | P-1 | P2₁/n |
| a/Å | 4.8688(3) | 17.5235(15) | 12.6969(4) | 9.6439(3) | 9.77060(10) |
| b/Å | 22.4405(12) | 14.8457(8) | 23.4074(9) | 11.8709(3) | 24.2648(3) |
| c/Å | 13.4798(8) | 16.8034(16) | 11.2438(4) | 13.3805(5) | 11.30730(10) |
| α/° | 90 | 90 | 90 | 75.396(3) | 90 |
| β/° | 90 | 111.712(12) | 111.660(4) | 72.866(3) | 94.6700(10) |
| γ/° | 90 | 90 | 90 | 70.625(3) | 90 |
| Volume/Å ³ | 1472.78(15) | 4061.3(6) | 3105.7(2) | 1360.53(8) | 2671.85(5) |
| Z | 4 | 4 | 2 | 1 | 2 |
| ρ _{calc} /cm ³ | 1.368 | 1.740 | 1.681 | 1.756 | 1.725 |
| μ/mm ⁻¹ | 0.840 | 20.040 | 14.865 | 2.814 | 15.511 |
| F(000) | 640.0 | 2080.0 | 1564.0 | 718.0 | 1380.0 |
| Radiation | CuKα (λ = 1.54184) | CuKα (λ = 1.54184) | CuKα (λ = 1.54184) | MoKα (λ = 0.71073) | CuKα (λ = 1.54184) |
| 2θ range for data collection/° | 7.65 to 149.978 | 8.06 to 136.98 | 7.492 to 158.992 | 4.602 to 50.696 | 7.286 to 145.07 |
| Reflections collected | 7009 | 13494 | 23672 | 21510 | 22539 |
| Independent reflections | 2814 [R_{int} = 0.0367, R_{sigma} = 0.0339] | 3677 [R_{int} = 0.0732, R_{sigma} = 0.0437] | 6455 [R_{int} = 0.0568, R_{sigma} = 0.0475] | 4942 [R_{int} = 0.0489, R_{sigma} = 0.0373] | 5161 [R_{int} = 0.0432, R_{sigma} = 0.0325] |
| Data/restraints/parameters | 2814/0/211 | 3677/92/281 | 6455/50/431 | 4942/61/423 | 5161/47/391 |
| Goodness-of-fit on F ² | 1.118 | 1.165 | 1.175 | 1.082 | 1.054 |
| Final R indexes [I ≥ 2σ(I)] | R₁ = 0.0459, wR₂ = 0.1370 | R₁ = 0.0617, wR₂ = 0.1793 | R₁ = 0.0506, wR₂ = 0.1433 | R₁ = 0.0331, wR₂ = 0.0698 | R₁ = 0.0280, wR₂ = 0.0695 |
| Final R indexes [all data] | R₁ = 0.0499, wR₂ = 0.1413 | R₁ = 0.0650, wR₂ = 0.1830 | R₁ = 0.0580, wR₂ = 0.1545 | R₁ = 0.0418, wR₂ = 0.0752 | R₁ = 0.0314, wR₂ = 0.0712 |
| Largest diff. peak/hole / e Å ⁻³ | 0.20/-0.20 | 2.21/-1.70 | 1.14/-1.36 | 2.88/-0.99 | 0.61/-0.74 |
| Flack parameter | 0.11(19) | | | | |

Table S2. Important bond distances in complexes 1–4.

| | 1 | 2 | 3 | 4 |
|----------------------|-----------|----------|----------|----------|
| Dy1–O1 | 2.313(5) | 2.346(4) | 2.309(3) | 2.312(2) |
| Dy1–O1 ¹ | 2.392(6) | 2.363(3) | 2.345(3) | 2.401(2) |
| Dy1–O3 | 2.271(6) | 2.300(4) | 2.277(3) | 2.254(2) |
| Dy1–O2 ¹ | 2.429(6) | 2.546(4) | 2.487(3) | 2.560(2) |
| Dy1–N1 | 2.440(6) | 2.465(4) | 2.473(4) | 2.502(2) |
| Dy1–O4 | 2.388(12) | 2.300(4) | 2.294(3) | 2.406(2) |
| Dy1–O5 | 2.414(12) | 2.282(4) | 2.373(3) | 2.693(2) |
| Dy1–O6 | 2.330(5) | 2.386(4) | 2.408(3) | 2.381(2) |
| Dy1–O7 | – | – | – | 2.487(2) |
| C10– O3 | 1.269(10) | 1.281(6) | 1.302(5) | 1.278(3) |
| Dy1–Dy1 ¹ | 3.709(1) | 3.799(1) | 3.730(1) | 3.805(1) |

Symmetry code: ¹1-X,+Y,3/2-Z**Table S3.** Shape analysis for Dy(III) centers in 1–3.

| Label | Shape | Symmetry | 1 | 2 | 3 |
|----------------|--|-----------------------|--------------|--------------|--------------|
| | | | Dy1 | Dy1 | Dy1 |
| OP-8 | Octagon | D _{8h} | 33.365 | 31.107 | 31.054 |
| HPY-8 | Heptagonal pyramid | C _{7v} | 21.541 | 23.662 | 24.175 |
| HBPY-8 | Hexagonal bipyramid | D _{6h} | 16.665 | 15.760 | 16.066 |
| CU-8 | Cube | Oh | 13.083 | 11.665 | 10.242 |
| SAPR-8 | Square antiprism | D _{4d} | 3.706 | 2.476 | 2.539 |
| TDD-8 | Triangular dodecahedron | D_{2d} | 2.405 | 1.770 | 0.804 |
| JGBF-8 | Johnson gyrobifastigium J26 | D _{2d} | 13.151 | 12.956 | 13.019 |
| JETBPY-8 | Johnson elongated triangular bipyramid J14 | D _{3h} | 26.683 | 26.924 | 28.723 |
| JBTPR-8 | Biaugmented trigonal prism J50 | C_{2v} | 2.467 | 1.255 | 1.970 |
| BTPR-8 | Biaugmented trigonal prism | C_{2v} | 2.046 | 0.973 | 1.607 |
| JSD-8 | Snub diphenoid J84 | D _{2d} | 3.901 | 3.438 | 2.737 |
| TT-8 | Triakis tetrahedron | Td | 13.505 | 12.076 | 10.732 |
| ETBPY-8 | Elongated trigonal bipyramid | D _{3h} | 23.298 | 23.779 | 23.865 |

Table S4. Shape analysis around Dy(III) centers in **4**.

| Label | Shape | Symmetry | 4 |
|----------------|--|-----------------------|--------------|
| EP-9 | Enneagon | D _{9h} | 33.736 |
| OPY-9 | Octagonal pyramid | C _{8v} | 21.792 |
| HBPY-9 | Heptagonal bipyramid | D _{7h} | 16.623 |
| JTC-9 | Johnson triangular cupola J3 | C _{3v} | 14.907 |
| JCCU-9 | Capped cube J8 | C _{4v} | 8.294 |
| CCU-9 | Spherical-relaxed capped cube | C _{4v} | 7.212 |
| JCSAPR-9 | Capped square antiprism J10 | C _{4v} | 2.876 |
| CSAPR-9 | Spherical capped square antiprism | C_{4v} | 2.102 |
| JTCTPR-9 | Tricapped trigonal prism J51 | D _{3h} | 2.231 |
| TCTPR-9 | Spherical tricapped trigonal prism | D _{3h} | 2.266 |
| JTDIC-9 | Tridiminishd icosahedron J63 | C _{3v} | 12.772 |
| HH-9 | Hula-hoop | C _{2v} | 8.841 |
| MFF-9 | Muffin | C_s | 1.791 |

Table S5. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **2** by Debye model with single relaxation process at $H_{dc} = 1.0$ kOe.

| T (K) | χ_s (emu/mol) | $\Delta\chi$ (emu/mol) | τ (s) | α |
|---------|-----------------------|---------------------------|------------|----------|
| 2 | 1.64959 | 3.99155 | 3.28E-04 | 0.4847 |
| 2.15 | 1.71594 | 3.87051 | 3.15E-04 | 0.47134 |
| 2.4 | 1.81291 | 3.66226 | 3.11E-04 | 0.44941 |
| 2.6 | 1.85417 | 3.51454 | 3.05E-04 | 0.43669 |
| 2.8 | 1.86656 | 3.38489 | 2.97E-04 | 0.42593 |
| 3 | 1.86922 | 3.26052 | 2.89E-04 | 0.41494 |
| 3.2 | 1.93009 | 3.07605 | 2.96E-04 | 0.39952 |
| 3.4 | 1.92163 | 2.96102 | 2.90E-04 | 0.39047 |
| 3.6 | 1.9398 | 2.818 | 2.88E-04 | 0.38013 |
| 3.8 | 1.93103 | 2.70632 | 2.81E-04 | 0.37114 |
| 4 | 1.96852 | 2.55018 | 2.87E-04 | 0.35772 |
| 4.2 | 1.93959 | 2.46695 | 2.75E-04 | 0.35153 |
| 4.4 | 1.93719 | 2.36051 | 2.70E-04 | 0.34308 |
| 4.6 | 1.93392 | 2.26013 | 2.64E-04 | 0.33793 |
| 4.8 | 1.91491 | 2.17796 | 2.54E-04 | 0.33116 |
| 5 | 1.92231 | 2.07412 | 2.49E-04 | 0.32775 |
| 5.5 | 1.90557 | 1.86141 | 2.33E-04 | 0.31211 |
| 6 | 1.89451 | 1.66668 | 2.20E-04 | 0.29795 |
| 6.5 | 1.87459 | 1.50485 | 2.06E-04 | 0.28726 |
| 7 | 1.87119 | 1.33949 | 2.00E-04 | 0.26827 |
| 7.5 | 1.85874 | 1.19873 | 1.93E-04 | 0.2512 |
| 8 | 1.80577 | 1.11075 | 1.74E-04 | 0.23899 |
| 8.5 | 1.77581 | 1.01163 | 1.62E-04 | 0.22673 |
| 9 | 1.74335 | 0.92598 | 1.47E-04 | 0.20904 |
| 9.5 | 1.71826 | 0.84226 | 1.36E-04 | 0.19439 |
| 10 | 1.67874 | 0.78043 | 1.18E-04 | 0.17941 |
| 10.5 | 1.65154 | 0.71394 | 1.02E-04 | 0.1719 |
| 11 | 1.54965 | 0.72891 | 7.26E-05 | 0.17752 |
| 11.5 | 1.60287 | 0.59631 | 7.08E-05 | 0.16721 |
| 12 | 1.56673 | 0.54483 | 5.36E-05 | 0.17591 |
| 12.5 | 1.63778 | 0.40608 | 5.94E-05 | 0.13307 |
| 13 | 1.63065 | 0.34958 | 5.01E-05 | 0.16316 |
| 13.5 | 1.51859 | 0.40012 | 2.52E-05 | 0.17195 |

Table S6. Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **3** by Debye model with single relaxation process at zero dc field.

| T (K) | χ_s (emu/mol) | $\Delta\chi$ (emu/mol) | τ (s) | α |
|---------|-----------------------|---------------------------|------------|----------|
| 2 | 1.76328 | 13.51411 | 2.62E-03 | 0.26719 |
| 2.15 | 1.69773 | 12.22466 | 2.49E-03 | 0.26728 |
| 2.4 | 1.62688 | 10.5898 | 2.32E-03 | 0.26391 |
| 2.6 | 1.55438 | 9.43585 | 2.20E-03 | 0.26265 |
| 2.8 | 1.48679 | 8.53446 | 2.12E-03 | 0.26298 |
| 3 | 1.43909 | 7.74322 | 2.04E-03 | 0.25873 |
| 3.2 | 1.38433 | 7.12722 | 1.97E-03 | 0.25807 |
| 3.4 | 1.34715 | 6.5853 | 1.91E-03 | 0.25491 |
| 3.6 | 1.30638 | 6.11464 | 1.85E-03 | 0.25301 |
| 3.8 | 1.2667 | 5.69992 | 1.79E-03 | 0.25183 |
| 4 | 1.23908 | 5.33176 | 1.73E-03 | 0.24408 |
| 4.2 | 1.20704 | 4.99746 | 1.68E-03 | 0.23967 |
| 4.4 | 1.17928 | 4.69069 | 1.62E-03 | 0.23549 |
| 4.6 | 1.15052 | 4.44604 | 1.56E-03 | 0.23184 |
| 4.8 | 1.12909 | 4.21583 | 1.48E-03 | 0.22621 |
| 5 | 1.11158 | 3.99322 | 1.41E-03 | 0.21944 |
| 5.5 | 1.07341 | 3.50463 | 1.19E-03 | 0.20017 |
| 6 | 1.04267 | 3.10697 | 9.31E-04 | 0.17832 |
| 6.5 | 1.02363 | 2.77885 | 6.69E-04 | 0.15643 |
| 7 | 1.00503 | 2.50035 | 4.25E-04 | 0.138 |
| 7.5 | 1.0166 | 2.23503 | 2.46E-04 | 0.12248 |
| 8 | 1.06439 | 1.96501 | 1.37E-04 | 0.10337 |

Table S7 Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **4** by Debye model with single relaxation process at zero and 1.0 kOe dc fields.

$H_{dc} = 0$ Oe

| T (K) | χ_s (emu/mol) | $\Delta\chi$ (emu/mol) | τ (s) | α |
|---------|-----------------------|---------------------------|------------|----------|
| 2 | 1.22645 | 15.0657 | 7.82E-04 | 0.13031 |
| 2.15 | 1.15276 | 13.80782 | 7.64E-04 | 0.13096 |
| 2.4 | 1.05866 | 12.17905 | 7.33E-04 | 0.13189 |
| 2.6 | 0.99422 | 11.03888 | 7.04E-04 | 0.13249 |
| 2.8 | 0.94071 | 10.08194 | 6.75E-04 | 0.13262 |
| 3 | 0.89751 | 9.2645 | 6.44E-04 | 0.13204 |
| 3.2 | 0.86092 | 8.57947 | 6.11E-04 | 0.13065 |
| 3.4 | 0.82805 | 7.98637 | 5.76E-04 | 0.12854 |
| 3.6 | 0.80314 | 7.45305 | 5.38E-04 | 0.12437 |
| 3.8 | 0.77985 | 6.97311 | 4.97E-04 | 0.11909 |
| 4 | 0.75812 | 6.53856 | 4.56E-04 | 0.11317 |
| 4.2 | 0.73526 | 6.15814 | 4.14E-04 | 0.10721 |
| 4.4 | 0.71072 | 5.82235 | 3.72E-04 | 0.10197 |
| 4.6 | 0.68926 | 5.52043 | 3.32E-04 | 0.09693 |
| 4.8 | 0.6651 | 5.25168 | 2.95E-04 | 0.09226 |
| 5 | 0.64807 | 4.99991 | 2.61E-04 | 0.08769 |
| 5.5 | 0.61101 | 4.45763 | 1.89E-04 | 0.0813 |
| 6 | 0.63437 | 3.96271 | 1.38E-04 | 0.07558 |
| 6.5 | 0.71528 | 3.50006 | 1.03E-04 | 0.06785 |
| 7 | 0.79548 | 3.09388 | 7.53E-05 | 0.06356 |
| 7.5 | 0.88092 | 2.7268 | 5.43E-05 | 0.05743 |
| 8 | 0.84817 | 2.51503 | 3.68E-05 | 0.05394 |
| 8.5 | 0.66009 | 2.49136 | 2.31E-05 | 0.05433 |

$H_{dc} = 1$ kOe

| T (K) | χ_s (emu/mol) | $\Delta\chi$ (emu/mol) | τ (s) | α |
|---------|-----------------------|---------------------------|------------|----------|
| 2 | 0.30397 | 13.29999 | 7.76E-02 | 0.31556 |
| 2.15 | 0.29801 | 12.78922 | 6.99E-02 | 0.31926 |
| 2.4 | 0.30902 | 11.64191 | 5.42E-02 | 0.30548 |
| 2.6 | 0.31103 | 10.63917 | 4.26E-02 | 0.29191 |
| 2.8 | 0.31733 | 9.72772 | 3.23E-02 | 0.27248 |
| 3 | 0.32121 | 8.96765 | 2.42E-02 | 0.2512 |
| 3.2 | 0.32062 | 8.3424 | 1.79E-02 | 0.23161 |
| 3.4 | 0.31998 | 7.86952 | 1.31E-02 | 0.21553 |
| 3.6 | 0.31871 | 7.40816 | 9.37E-03 | 0.19959 |
| 3.8 | 0.32412 | 6.97265 | 6.74E-03 | 0.18281 |
| 4 | 0.32856 | 6.54856 | 4.89E-03 | 0.16837 |

| | | | | |
|-----|---------|---------|----------|---------|
| 4.2 | 0.33144 | 6.194 | 3.59E-03 | 0.15846 |
| 4.4 | 0.33717 | 5.8581 | 2.65E-03 | 0.14992 |
| 4.6 | 0.34522 | 5.56477 | 1.98E-03 | 0.14224 |
| 4.8 | 0.35649 | 5.30943 | 1.50E-03 | 0.13758 |
| 5 | 0.3689 | 5.05915 | 1.14E-03 | 0.13321 |
| 5.5 | 0.42345 | 4.50628 | 6.05E-04 | 0.12299 |
| 6 | 0.51042 | 3.98102 | 3.39E-04 | 0.11326 |
| 6.5 | 0.6226 | 3.52696 | 2.01E-04 | 0.10409 |
| 7 | 0.75115 | 3.08838 | 1.22E-04 | 0.09048 |
| 7.5 | 0.79563 | 2.77219 | 7.31E-05 | 0.08693 |
| 8 | 0.85977 | 2.47068 | 4.56E-05 | 0.07761 |
| 8.5 | 0.65841 | 2.46402 | 2.61E-05 | 0.0754 |

Table S8. CASSCF calculated energies and g-factors for the eight Kramers doublets corresponding to the ${}^6\text{H}_{15/2}$ ground multiplet.

| Complex | KD | E (cm ⁻¹) | g _x | g _y | g _z |
|-----------|----|-----------------------|----------------|----------------|----------------|
| 1 | 1 | 0.0 | 0.059 | 0.139 | 19.084 |
| | 2 | 96.7 | 1.098 | 2.213 | 14.569 |
| | 3 | 155.6 | 3.576 | 3.997 | 11.387 |
| | 4 | 208.0 | 7.409 | 5.777 | 1.480 |
| | 5 | 240.5 | 1.452 | 1.931 | 17.084 |
| | 6 | 279.4 | 1.386 | 2.762 | 13.599 |
| | 7 | 322.9 | 0.693 | 1.651 | 16.964 |
| | 8 | 452.8 | 0.012 | 0.015 | 19.716 |
| 2 | 1 | 0.0 | 0.221 | 0.505 | 18.832 |
| | 2 | 38.1 | 0.200 | 0.715 | 18.088 |
| | 3 | 103.0 | 0.194 | 2.328 | 11.663 |
| | 4 | 114.9 | 2.366 | 5.274 | 10.144 |
| | 5 | 160.8 | 4.393 | 5.575 | 8.376 |
| | 6 | 200.2 | 0.882 | 1.440 | 14.881 |
| | 7 | 290.3 | 0.173 | 0.412 | 18.770 |
| | 8 | 357.0 | 0.057 | 0.124 | 19.661 |
| 3 | 1 | 0.0 | 0.053 | 0.097 | 19.336 |
| | 2 | 114.8 | 11.506 | 7.045 | 2.211 |
| | 3 | 152.7 | 8.058 | 4.126 | 0.064 |
| | 4 | 211.0 | 2.461 | 3.145 | 10.770 |
| | 5 | 271.3 | 0.888 | 1.887 | 13.601 |
| | 6 | 295.4 | 0.137 | 2.665 | 16.163 |
| | 7 | 309.2 | 1.248 | 1.987 | 14.738 |
| | 8 | 403.5 | 0.040 | 0.117 | 19.357 |
| 4a | 1 | 0.0 | 0.033 | 0.063 | 19.369 |
| | 2 | 99.1 | 0.409 | 0.535 | 15.992 |
| | 3 | 193.5 | 2.594 | 2.714 | 12.156 |

| | | | | | |
|-----------|---|-------|--------|-------|--------|
| | 4 | 274.0 | 8.893 | 6.667 | 3.390 |
| | 5 | 343.5 | 1.701 | 2.311 | 12.769 |
| | 6 | 375.6 | 11.061 | 7.100 | 0.458 |
| | 7 | 400.1 | 1.081 | 6.420 | 11.983 |
| | 8 | 487.3 | 0.102 | 0.214 | 19.415 |
| 4b | 1 | 0.0 | 0.026 | 0.047 | 19.348 |
| | 2 | 102.1 | 0.427 | 0.548 | 15.907 |
| | 3 | 196.5 | 2.800 | 2.934 | 11.882 |
| | 4 | 276.3 | 8.910 | 6.436 | 2.571 |
| | 5 | 339.9 | 1.853 | 3.080 | 12.290 |
| | 6 | 373.8 | 0.237 | 5.212 | 11.430 |
| | 7 | 397.7 | 1.146 | 5.947 | 12.357 |
| | 8 | 457.2 | 0.188 | 0.401 | 19.107 |

Table S9. Spin Hamiltonian parameters of the exchange coupled doublets calculated by the Lines model.

| | ΔE (cm ⁻¹) | g_z | |
|----------|--------------------------------|--------|--------|
| | | KD1 | KD2 |
| 1 | 2.451 | 0.000 | 38.129 |
| 2 | 1.844 | 36.046 | 0.000 |
| 3 | 2.401 | 38.667 | 0.000 |
| 4 | 2.634 | 38.713 | 0.563 |

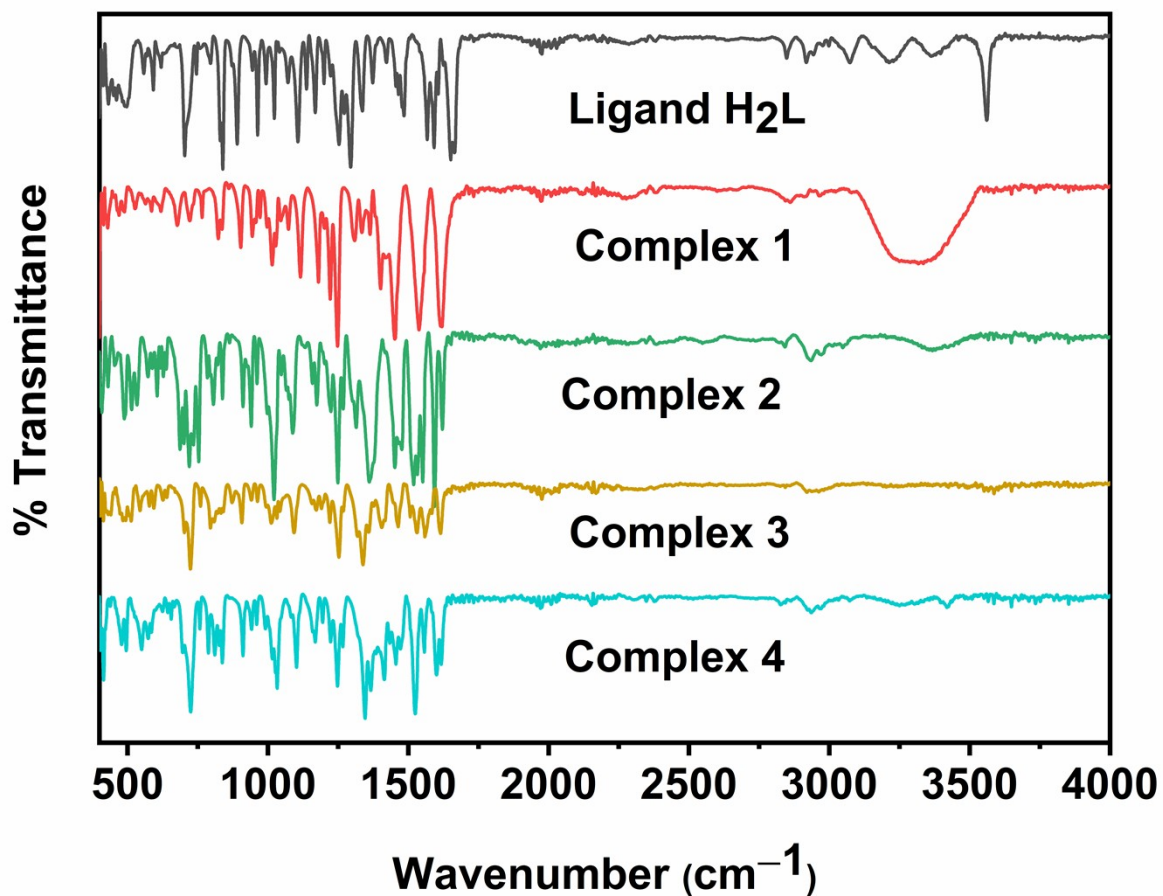


Fig. S1. IR data of Schiff base H₂L and complexes 1–4.

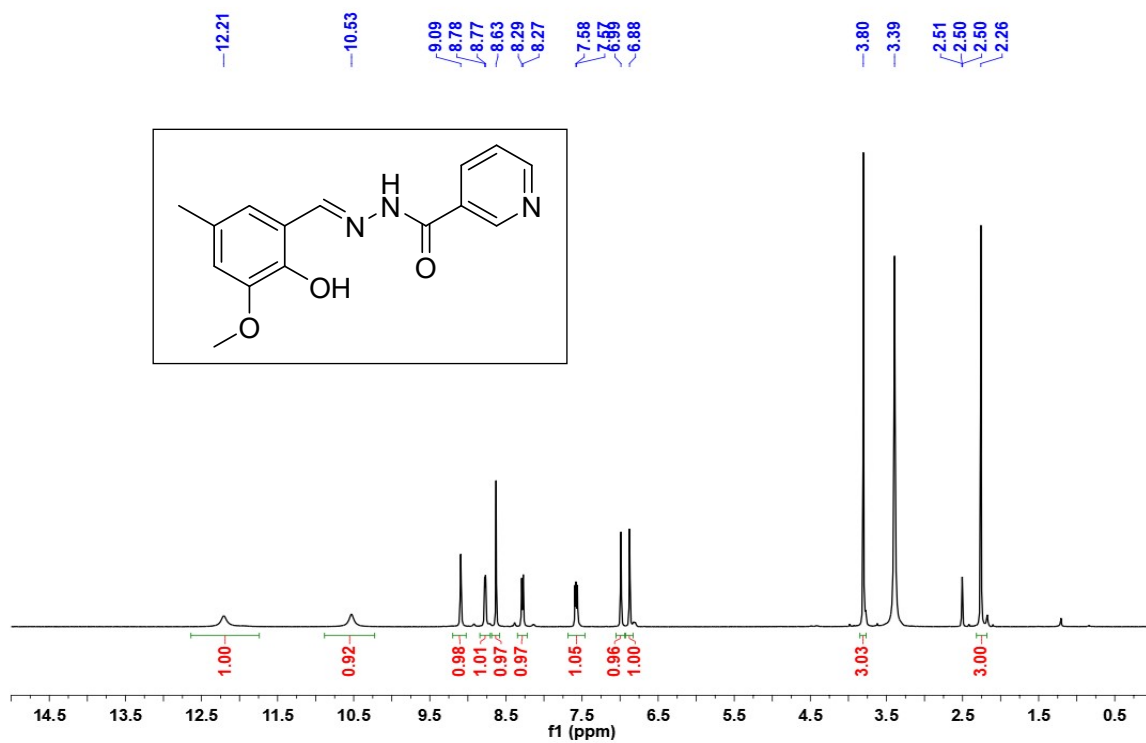


Fig. S2: ¹H NMR spectra of Schiff base H₂L in DMSO-d₆ at room temperature.

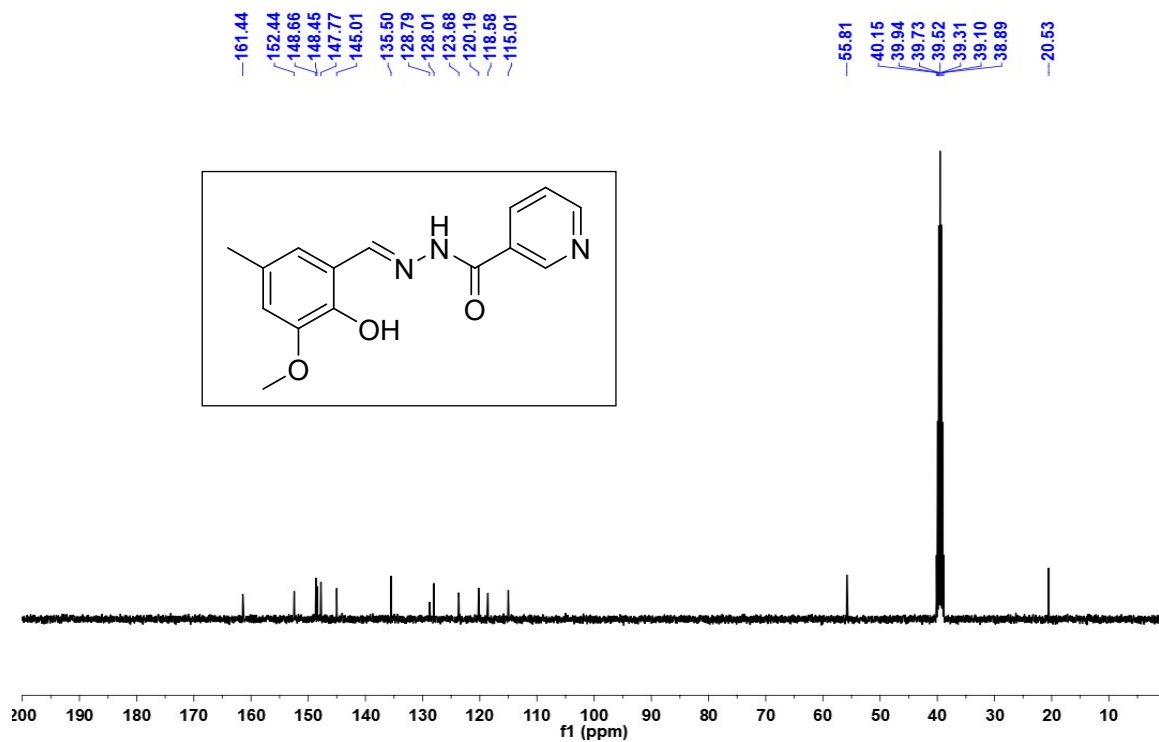


Fig. S3: ¹³C NMR spectra of Schiff H₂L in DMSO-d₆ at room temperature

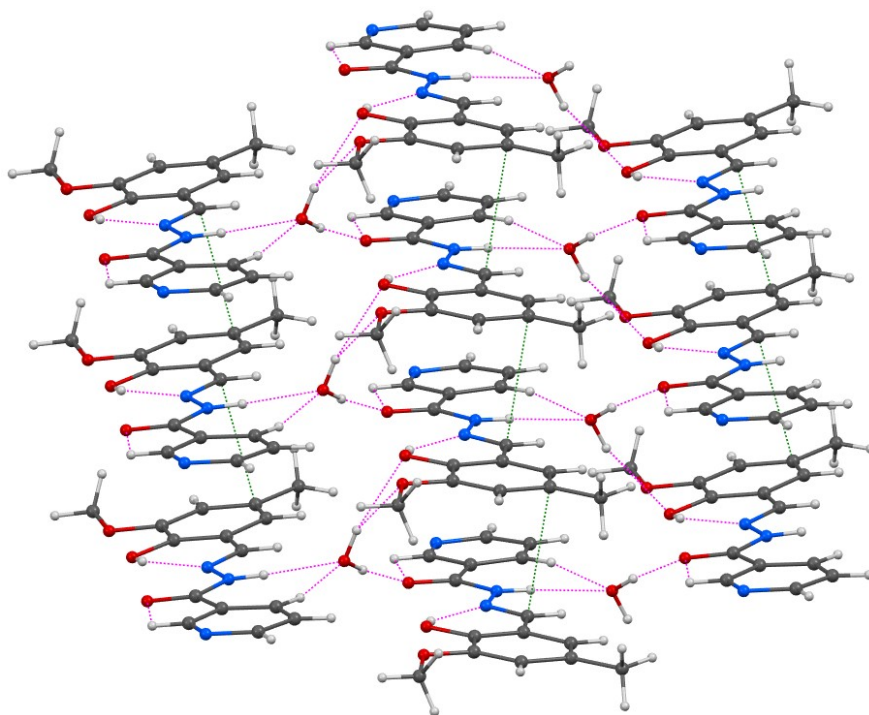


Fig. S4. The crystal packing of Schiff base H₂L showing hydrogen bonding and π - π stacking interactions.

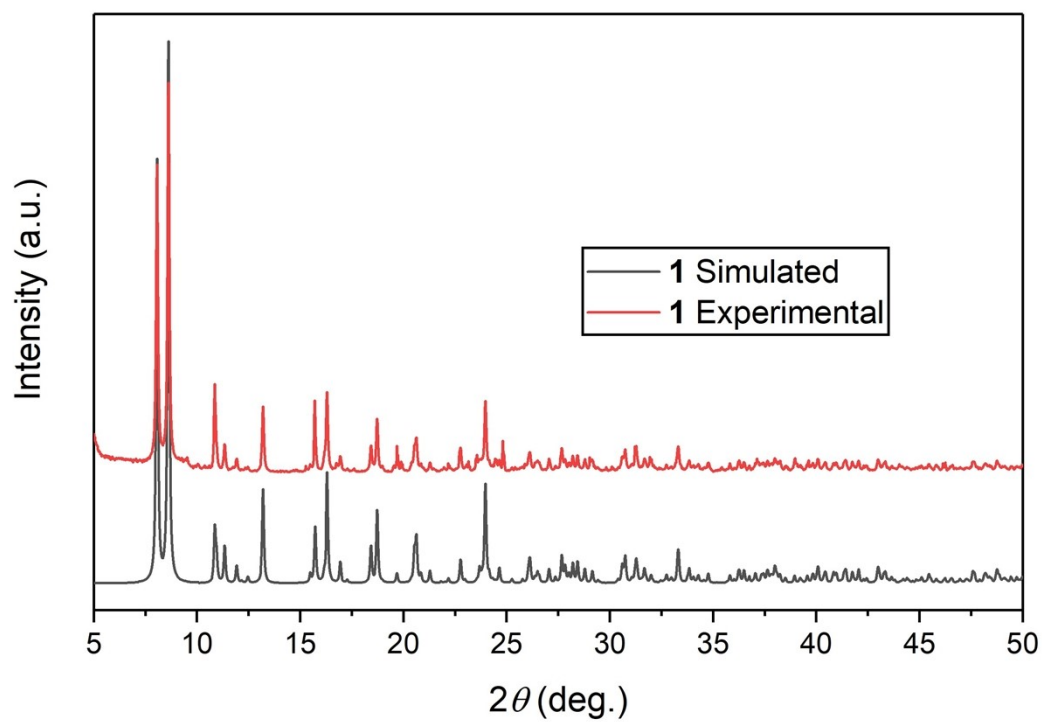


Fig. S5. PXRD data for complex 1.

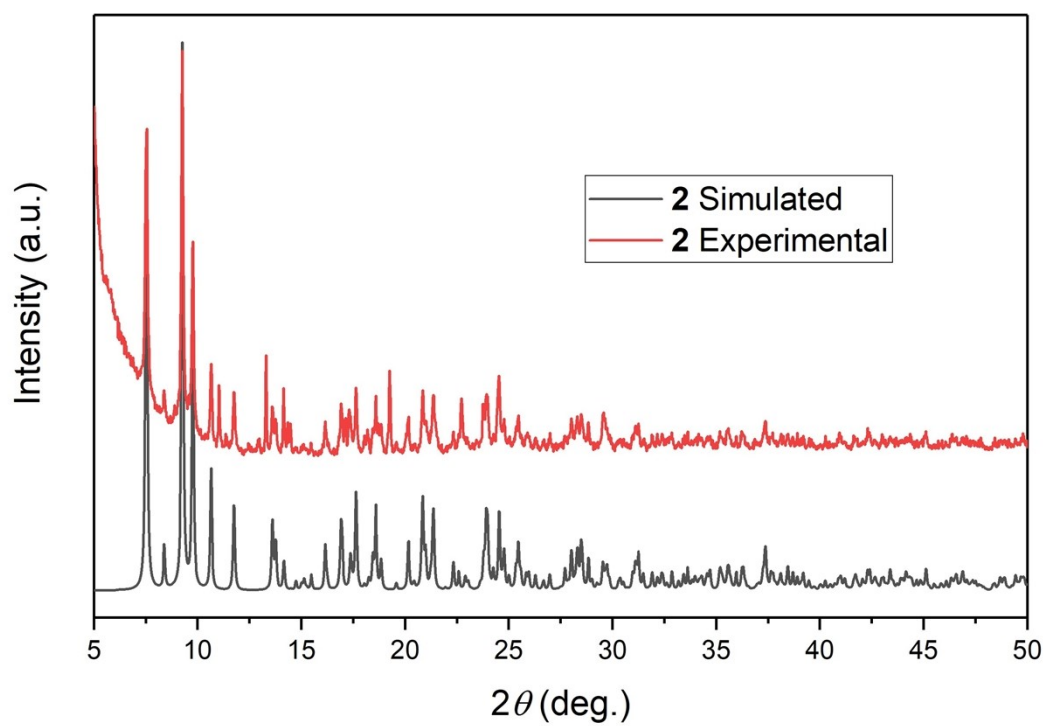


Fig. S6. PXRD data for complex 2.

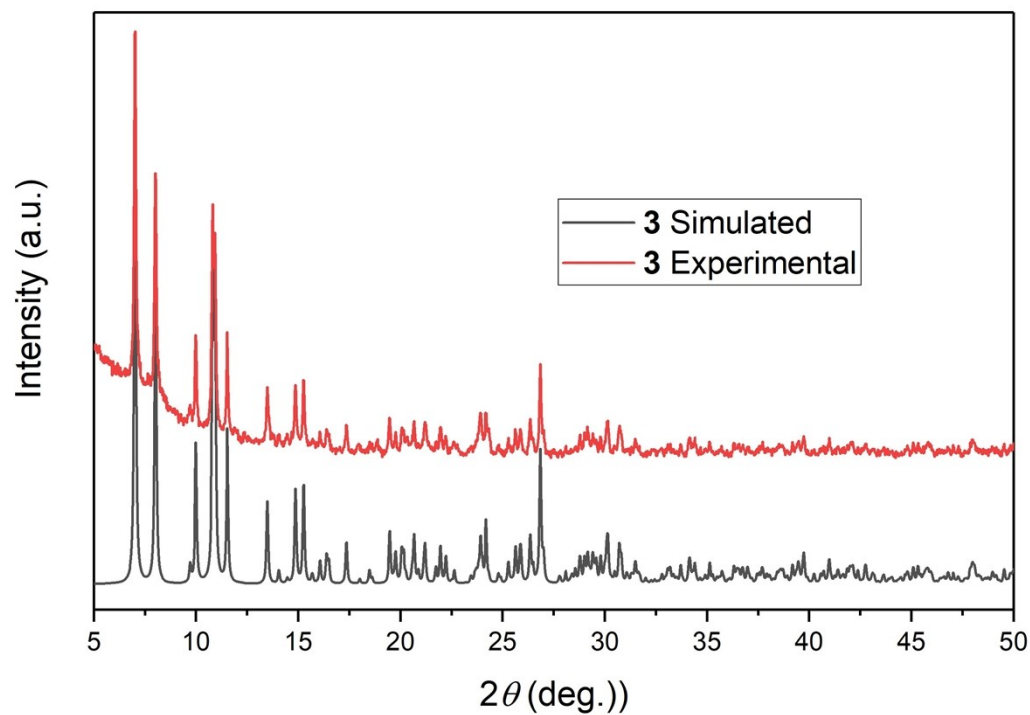


Fig. S7. PXRD data for complex 3.

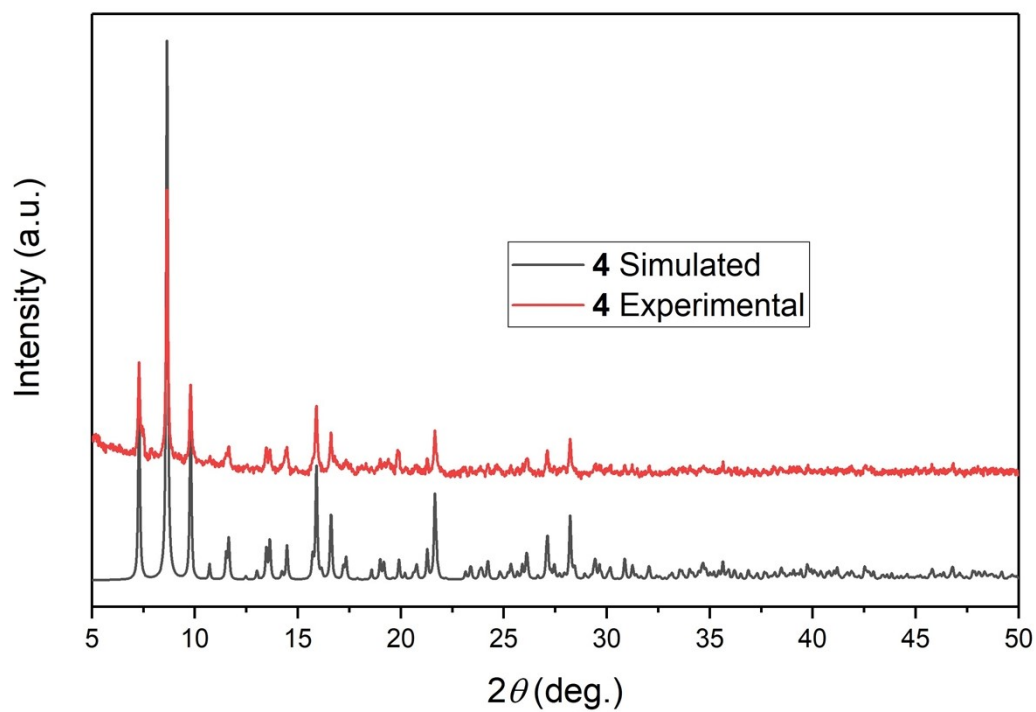


Fig. S8. PXRD data for complex 4.

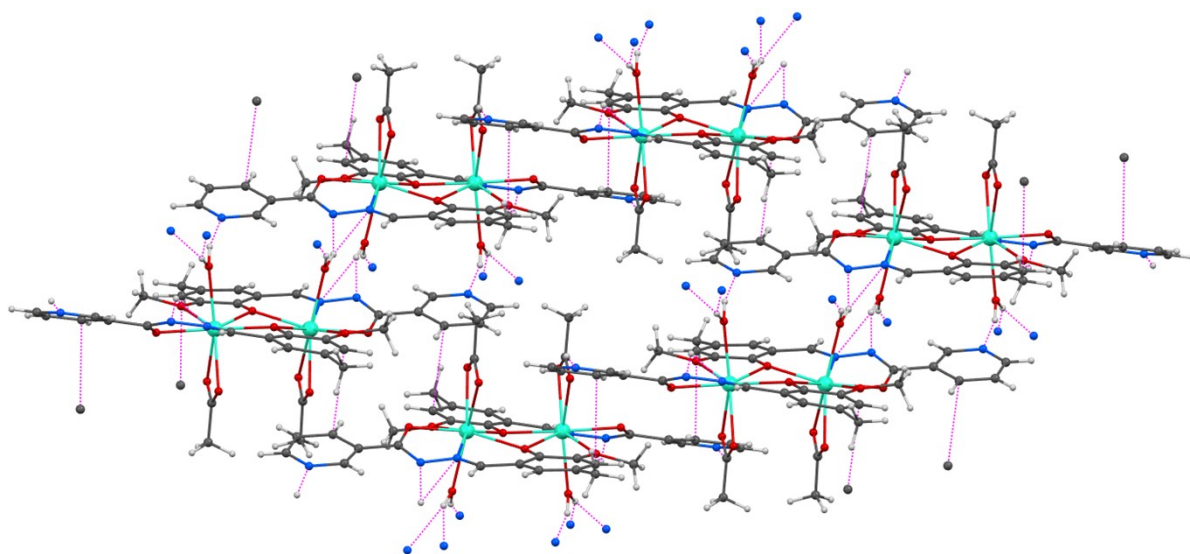


Fig. S9. The crystal packing of complex 1 showing different non-covalent interactions.

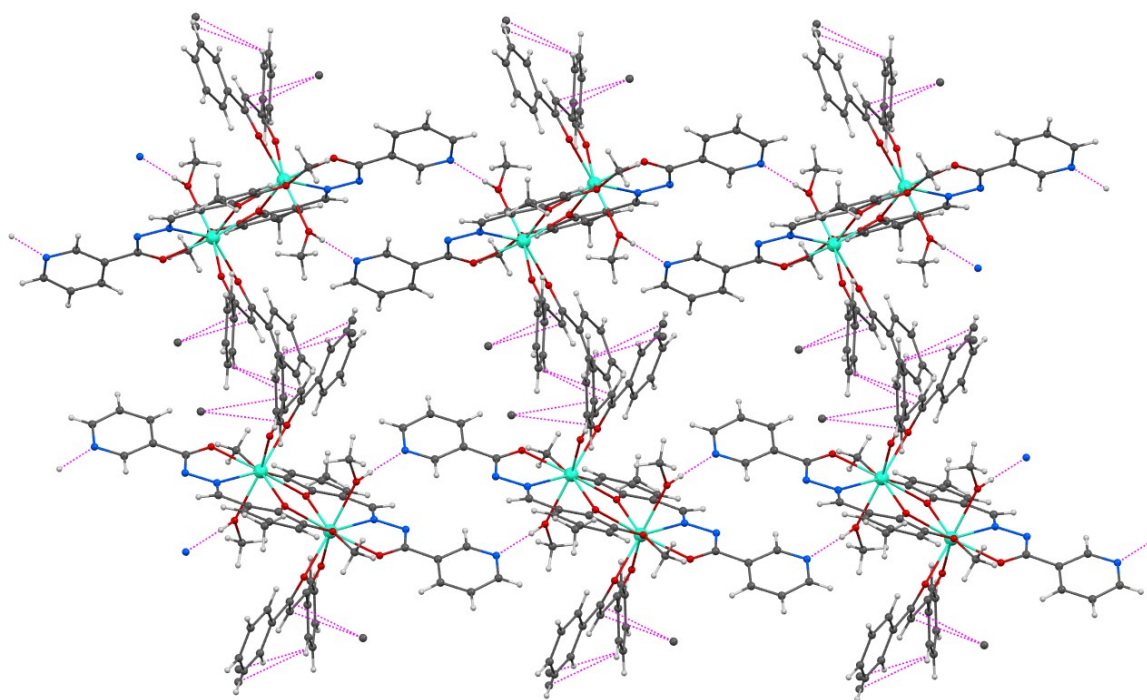


Fig. S10. The crystal packing of complex 2 showing different non-covalent interactions.

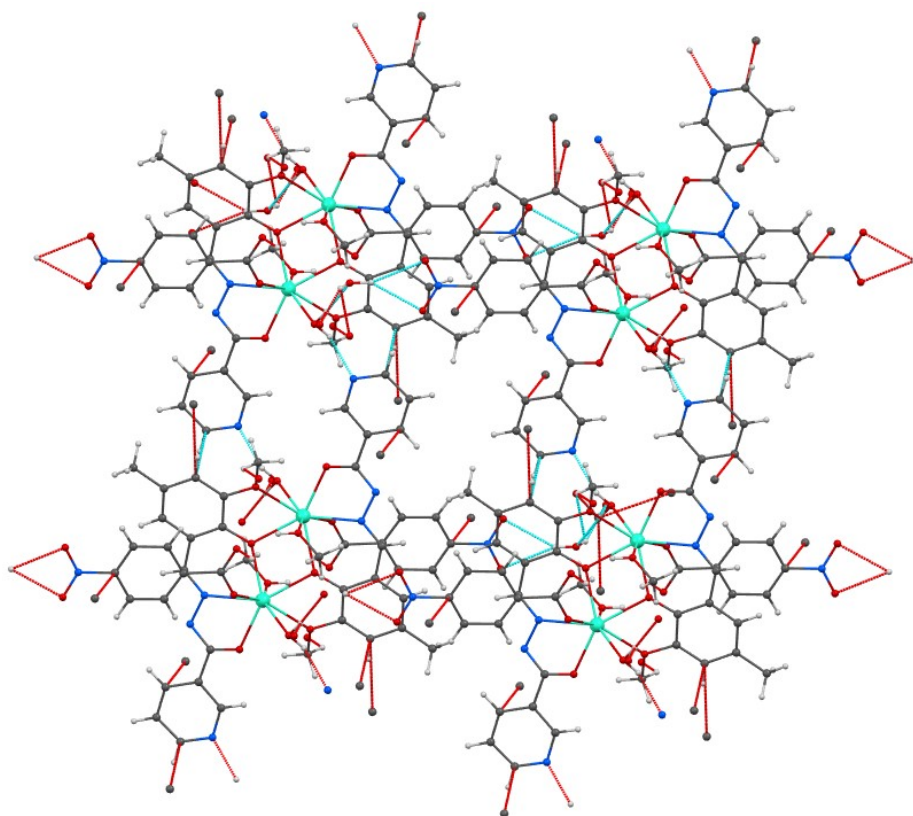


Fig. S11. The crystal packing of complex **3** showing different non-covalent interactions.

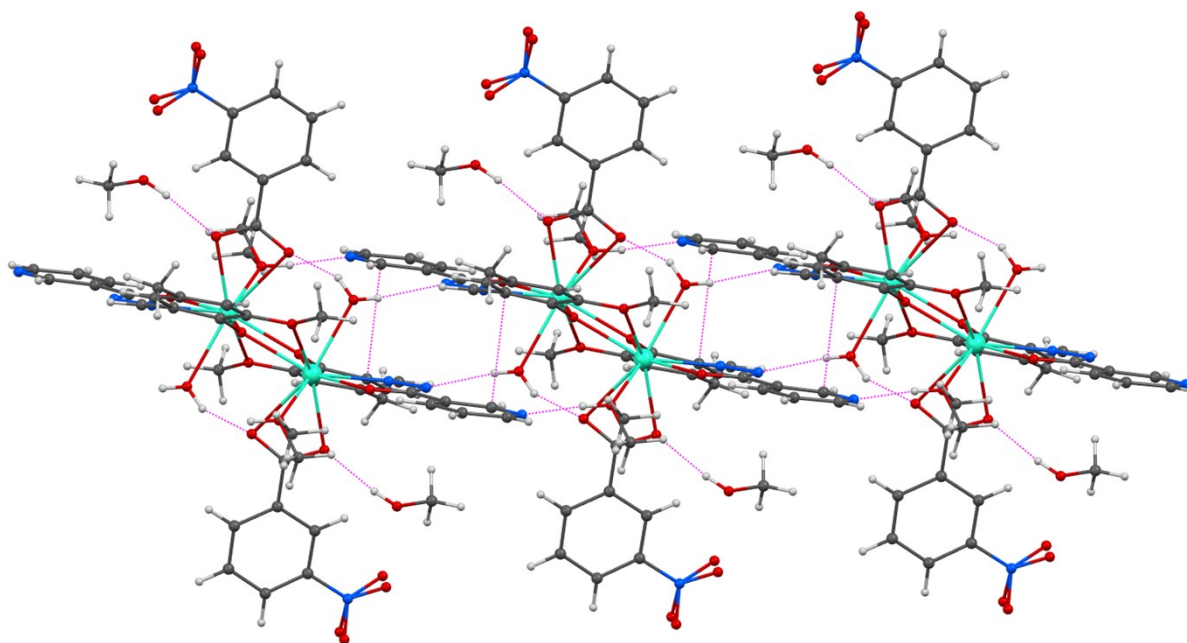


Fig. S12. The crystal packing of complex **4** showing different non-covalent interactions.

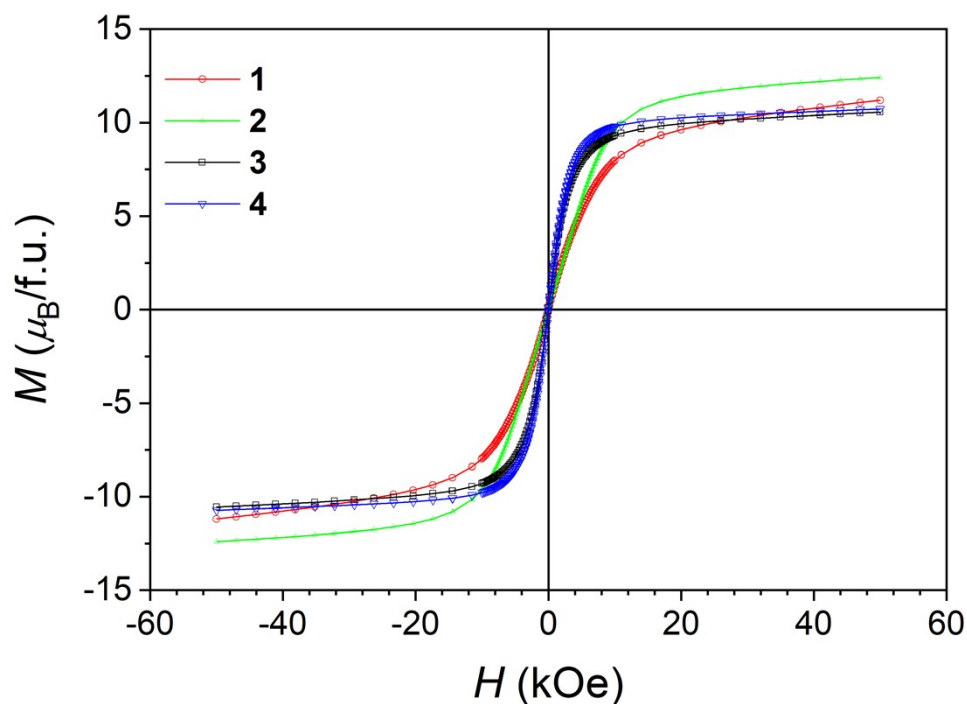


Fig. S13. Isothermal magnetization at temperature 2 K for complexes 1–4.

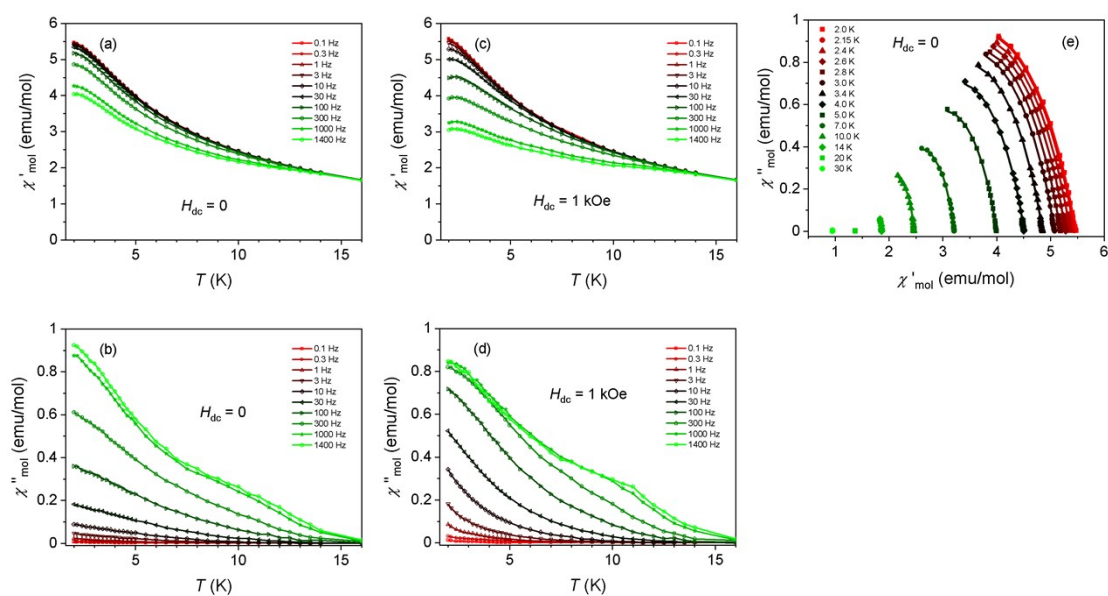


Fig. S14. The rest ac susceptibility plots for complex 2 those are not shown in Fig. 5

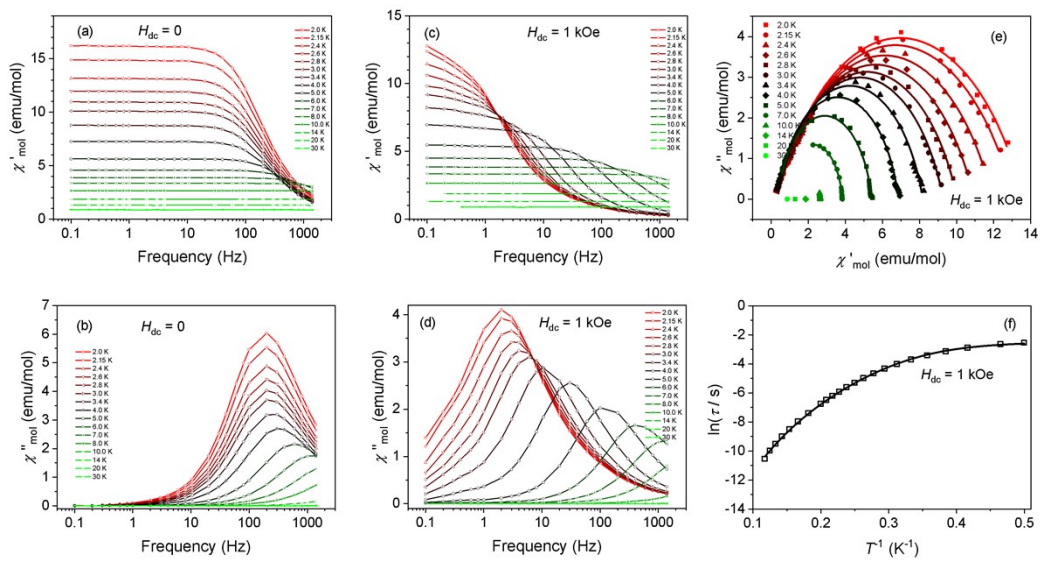


Fig. S15. The rest ac susceptibility plots for complex 4 those are not shown in Fig. 7

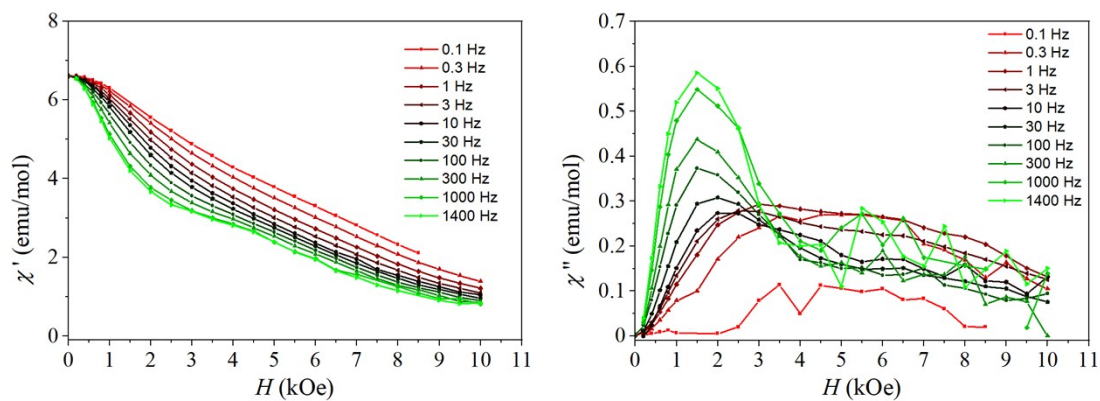


Fig. S16. Field dependence AC magnetic data for complex 1

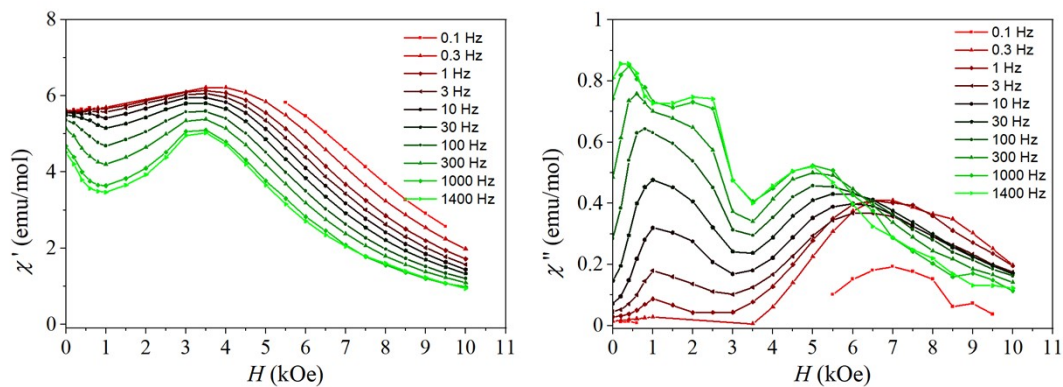


Fig. S17. Field dependence AC magnetic data for complex 2

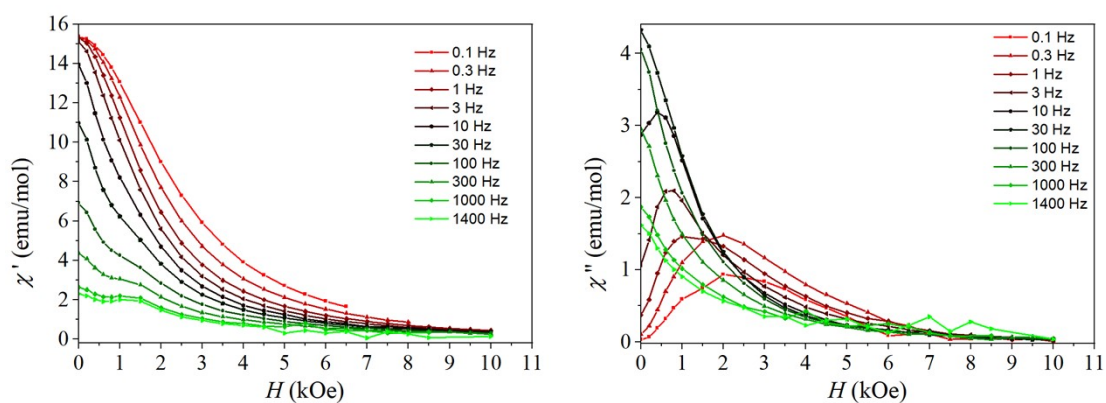


Fig. S18. Field dependence AC magnetic data for complex 3

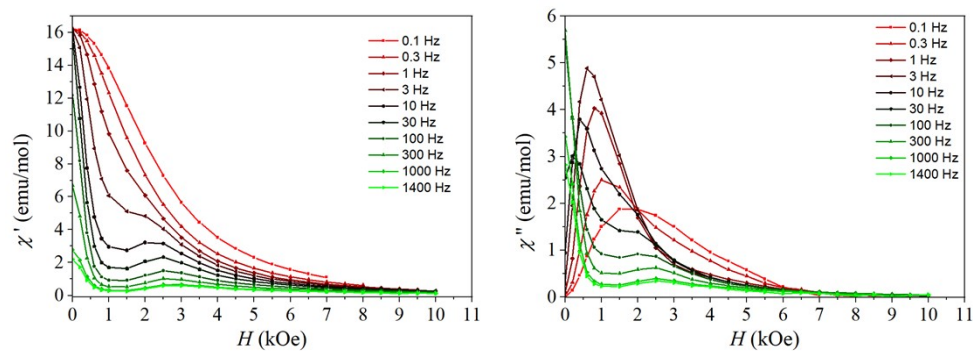


Fig. S19. Field dependence AC magnetic data for complex 4

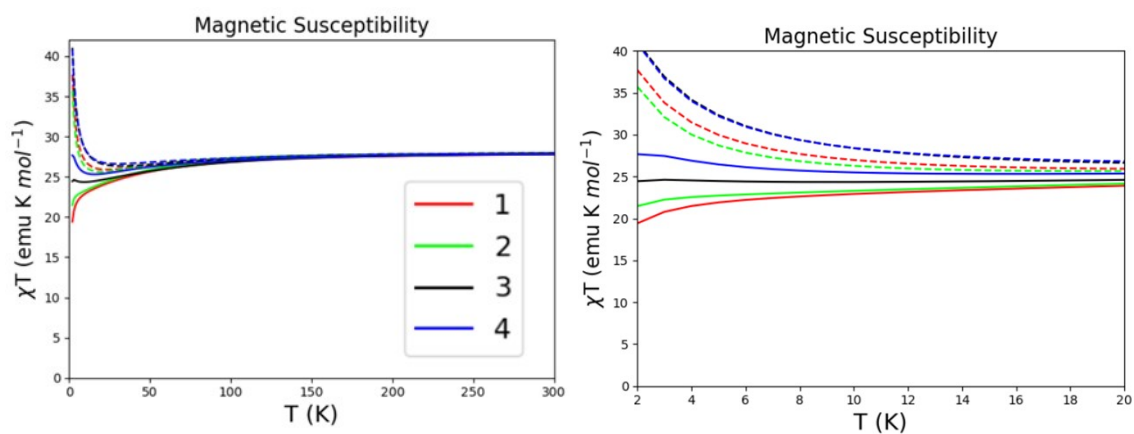


Fig S20. Temperature dependent magnetic susceptibility calculated for the dimeric systems based on Lines model simulations. Dashed lines correspond to simulations considering only

the dipolar term. Solid line considers the dipolar term and the exchange contribution calculated from *Broken Symmetry* DFT, scaled with factor of $5/7$.