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Supplementary Information

Unprecedented intramolecular pancake bonding in a {Dy_2} single-molecule magnet

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Experimental Section

General Procedures and Materials: All reactions were carried out under aerobic/ambient conditions, unless otherwise stated. All reagents and solvents were purchased from TCI, Alfa Aesar, or Strem Chemicals and used without further purification.

Synthesis of 3,6-bis(3,5-dimethyl-pyrazolyl)-1,2,4,5-tetrazine (bpytz): The **bpytz** ligand was prepared according to the literature.[1]

Synthesis of $[Dy^{III}_2(\mu\text{-bpytz})(TMHD)_6]\cdot 4(C_6H_6)$ (1): Upon stirring a solution of bpytz (0.125 mmol, 34 mg) and $Dy(TMHD)_3$ (0.125 mmol, 84 mg) in benzene (6 mL), a brown solution formed within minutes. Slow diffusion of acetonitrile (CH_3CN) afforded dark red crystals of **1** suitable for single crystal X-ray after 24h. Yield = 85%. Selected IR (cm^{-1}): 3233.69 (s), 1653.55 (s), 1580.16 (m), 1497.71 (m), 1436.65 (m), 1378.44 (s), 1251.30 (m), 1204.48 (m), 1118.05 (s), 1076.52 (m), 1040.94 (w), 780.98 (m), 682.95 (m), 671.21 (m). Anal. Calc. for $C_{96}H_{146}Dy_2N_8O_{12}$ (minus one C_6H_6 molecule): C, 59.77%; H, 7.63%; N, 5.81%; Found: C, 60.07%; H, 7.48%; N, 5.50%.

Synthesis of $[Dy^{III}_2(\mu\text{-bpytz}^{\bullet-})_2(TMHD)_4]$ (2):A dry degassed solution of bpytz (0.125 mmol, 34 mg), $CoCp_2$ (0.125 mmol, 21 mg) and $Dy(TMHD)_3$ (0.125 mmol, 84 mg) in benzene (6 mL) was stirred in a nitrogen-filled glovebox for several minutes resulting in a green solution, which was slowly diffused with CH_3CN. After two days, crystals suitable for single crystal X-ray crystallography of **2** were collected. Yield = 80%. Selected IR (cm^{-1}): 2745.26 (m), 1584.65 (s), 1497.12 (s), 1459.78 (m), 1442.21 (m), 1419.73 (m), 1375.12 (s), 1282.93 (s), 1095.83 (w), 1049.98 (b), 983.94 (m), 835.33 (m), 784.19 (m), 593.24 (w), 588.65 (m).Anal. Calc. for $C_{68}H_{104}Dy_2N_{16}O_8$: C, 51.09%; H, 6.56%; N, 14.02%; Found: C, 51.10%; H, 6.61%;N, 14.12%.

Synthesis of $[Y^{III}_2(\mu\text{-bpytz}^{\bullet-})_2(TMHD)_4]$ (3):A dry degassed solution of bpytz (0.125 mmol, 34 mg), $CoCp_2$ (0.125 mmol, 21 mg) and $Y(TMHD)_3$ (0.125 mmol, 80 mg) in benzene (6 mL) was stirred in a nitrogen-filled glovebox for several minutes resulting in a brown solution, which was slowly diffused with CH_3CN. After two days, crystals suitable for single crystal X-ray crystallography of **3** were collected. Yield = 80%. Selected IR (cm^{-1}): 2957.46 (m), 1571.44 (s), 1537.18 (m), 1501.92 (m), 1405.21 (vs), 1357.48 (s), 1289.12 (w), 1224.35 (m), 1176.54 (w), 1094.49 (m), 1036.25 (w), 983.56 (m), 867.09 (m), 788.00 (m), 746.30 (m), 664.48(w), 602.08(w).Anal. Calc. for $C_{68}H_{104}Y_2N_{16}O_8$: C, 56.27%; H, 7.22%; N, 15.44%; Found: C, 56.74%; H, 6.55%; N, 15.06%.

Infrared (IR) Spectroscopy: Infrared analyses were performed with a Nicolet 6700 FT-IR spectrometer equipped with an ATR in the 4000-400 cm^{-1} range.

X-ray crystallography: Suitable crystals were mounted on a glass fibre. A Bruker APEX-II CCD device was used to collect unit cell and intensity data using graphite Mo Kα radiation (λ = 0.71073). The data reduction included a correction for Lorentz and polarization effects, with an applied multiscan absorption correction (SADABS). The crystal structure was solved and refined using the SHELXTL v.6.12 program suite.[2] Direct methods yielded all non-hydrogen atoms, which were refined with anisotropic thermal parameters. All hydrogen atom positions were calculated geometrically and were riding on their respective atoms.

Powder X-ray diffraction: Powder X-ray diffraction for polycrystalline samples of **2** and **3** were carried out using a Rigaku Ultima IV X-ray powder diffractometer. The Parallel Beam mode was employed to collect the data (λ= 0.7173 Å).

Electron paramagnetic resonance spectroscopy (EPR): The X-band EPR spectra of **3** was recorded at ambient temperature using a Bruker EMX-200 spectrometer. The sample was dissolved in dry, degassed benzene.

Magnetic measurements: Magnetic susceptibility measurements were performed on a Quantum Design (SQUID) magnetometer MPMS-XL7, operating between 1.8 and 300 K and applied fields of up to 7 T. Direct current (dc) susceptibility measurements were performed on finely ground polycrystalline samples (25.5 and 14.8 for compounds **1** and **2**, respectively), fixed in a matrix of vacuum grease and wrapped in a polyethylene membrane. Alternating current (ac) magnetic susceptibility studies were performed under an applied dc field of 600 Oe for **1** and 1200 Oe for **2**, with frequency ranges spanning 0.1 – 1488 Hz.

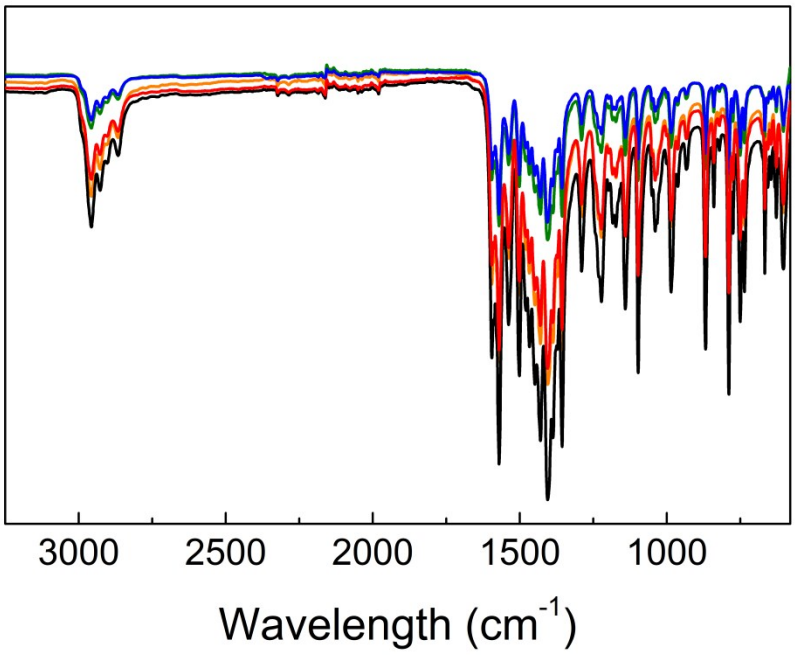

Figure S1. Solid-state infrared spectra of **2** measured over a period of 20 days, highlighting the stability of **2** under atmospheric conditions.

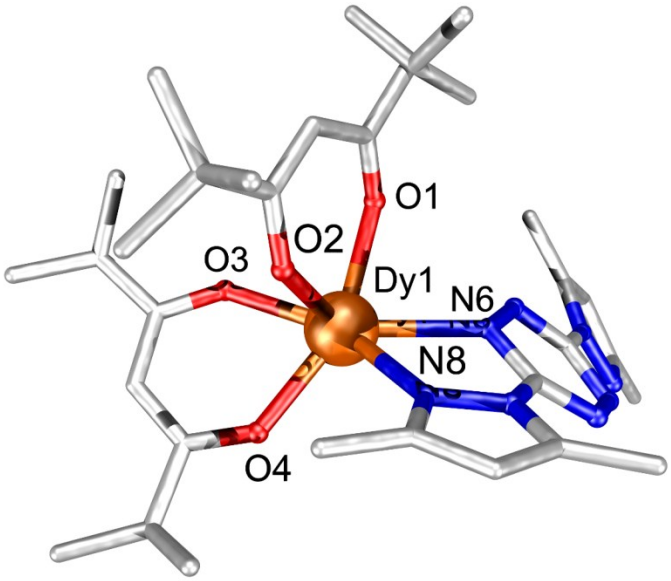

Figure S2. Asymmetric unit of the centrosymmetric complex **2** highlighting the coordination environment of the Dy^{III} ions. Hydrogen atoms and solvent molecules have been omitted for clarity. Colour code: Dy (orange), N (blue), O (red), C (grey).

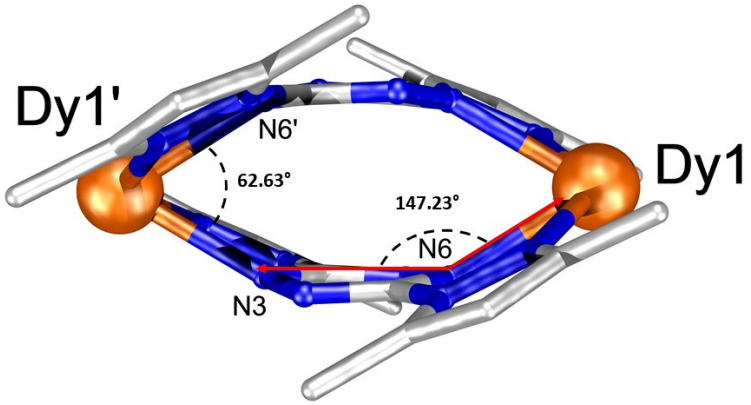

Figure S3. Molecular structure of **2** highlighting the N6'-Dy1'-N3 and Dy1-N6-N3 angles of pancake bonded $(bpytz^{\bullet-})_2$ bridge. TMHD co-ligands, hydrogen atoms and solvent molecules have been omitted for clarity. Colour code: C (grey), N (blue), Dy (orange).

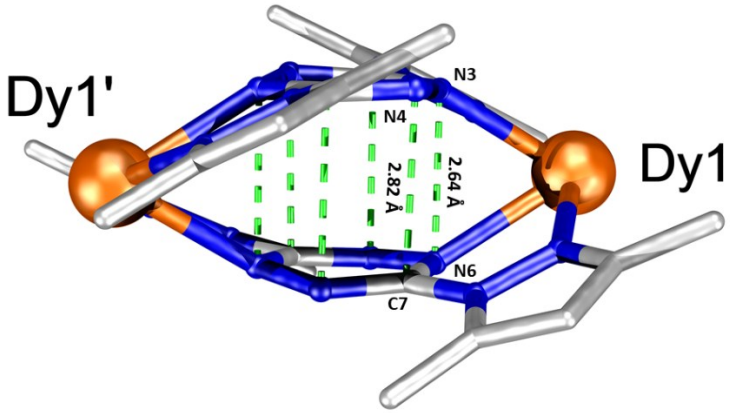

Figure S4. Intramolecular distances between the two reduced tetrazine rings in **2**. All C···N and N···N distances (green dashed lines) are 2.82 Å and 2.64 Å, respectively. TMHD co-ligands, hydrogen atoms and solvent molecules have been omitted for clarity. Colour code: C (grey), N (blue), Dy (orange).

Table S1. Crystallographic data for **1**, **2** and **3**.

	1	**2**	**3**
Empirical formula	$C_{102}H_{152}Dy_2N_8O_{12}$	$C_{68}H_{104}Dy_2N_{16}O_8$	$C_{68}H_{104}Y_2N_{16}O_8$
Formula weight	2007.31	1598.67	1451.47
Crystal system	Triclinic	Trigonal	Trigonal
Space group	$P\bar{1}$	$P3_221$	$P3_221$
a/Å	12.166(8)	17.4409(13)	17.4124(15)
b/Å	13.986(10)	17.4409(11)	17.4124(15)
c/Å	16.878(12)	22.8542(13)	22.0275(19)
α/ °	101.799(9)	90	90
β/ °	96.760(9)	90	90
γ/ °	103.238(9)	120	120
V/ Å^3	2695(3)	5814.5(10)	5783.8(11)
Z	1	3	3
T/K	200(2)	201(2)	200(2)
Radiation	Mo-K_α	Mo-K_α	Mo-K_α
Wavelength/ Å	0.71073	0.71073	0.71073
D_C/mg m^{-3}	1.237	1.370	1.250
μ/mm^{-1}	1.433	13.121	1.557
Reflections collected	97331	92658	9588
Goodness-of-fit on F^2	1.020	1.024	1.013
R1,wR2 (>2σ(I))[a]	0.0593, 0.0978	0.0381, 0.0668	0.0370, 0.0753

[a] $R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$. $wR_2 = (\Sigma[w(F_0^2 - F_c^2)^2]/\Sigma[w(F_0^2)^2])^{1/2}$.

Table S2. Selected distances (Å) for **1**, **2** and **3**.

1		**2**		**3**	
Dy(1)-O(1)	2.290(3)	Dy(1)-O(1)	2.277(3)	Y(1)-O(1)	2.271(2)
Dy(1)-O(2)	2.296(3)	Dy(1)-O(2)	2.307(3)	Y(1)-O(2)	2.293(2)
Dy(1)-O(3)	2.285(3)	Dy(1)-O(3)	2.292(4)	Y(1)-O(3)	2.278(2)
Dy(1)-O(4)	2.278(3)	Dy(1)-O(4)	2.286(3)	Y(1)-O(4)	2.276(2)
Dy(1)-O(5)	2.334(3)	Dy(1)-N(1)	2.553(4)	Y(1)-N(1)	2.546(3)
Dy(1)-O(6)	2.275(3)	Dy(1)-N(3)	2.516(3)	Y(1)-N(3)	2.515(2)
Dy(1)-N(1)	2.678(4)	Dy(1)-N(6)′	2.556(4)	Y(1)-N(6)′	2.552(3)
Dy(1)-N(3)	2.658(4)	Dy(1)-N(8)′	2.569(4)	Y(1)-N(8)′	2.558(3)
N(3)-N(4)	1.320(5)	N(3)-N(4)	1.386(6)	N(3)-N(4)	1.385(4)
C(6)-N(3)	1.334(5)	N(5)-N(6)	1.396(5)	N(5)-N(6)	1.389(4)
C(6)-N(4)	1.342(5)	C(6)-N(3)	1.340(7)	C(6)-N(3)	1.340(4)
C(6)-N(2)	1.382(5)	C(6)-N(4)	1.301(9)	C(6)-N(4)	1.317(6)
Dy(1)-Dy(1)′	8.007(4)	C(6)-N(2)	1.410(6)	C(6)-N(2)	1.409(4)
		Dy(1)-Dy(1)′	7.096(7)	Y(1)-Y(1)′	7.091(7)

Table S3. Selected angles (°) for **1**, **2** and **3**. Symmetry related atoms are indicated (′).

1		**2**		**3**	
O(1)-Dy(1)-O(2)	72.64(12)	O(1)-Dy(1)-O(2)	73.29(13)	O(1)-Y(1)-O(2)	73.48(9)
O(1)-Dy(1)-O(3)	78.48(12)	O(1)-Dy(1)-O(3)	86.82(13)	O(1)-Y(1)-O(3)	86.34(9)
O(1)-Dy(1)-O(4)	143.61(11)	O(1)-Dy(1)-O(4)	153.54(13)	O(1)-Y(1)-O(4)	153.76(8)
O(1)-Dy(1)-O(5)	137.68(10)	O(1)-Dy(1)-N(1)	81.82(13)	O(1)-Y(1)-N(1)	81.40(9)
O(1)-Dy(1)-O(6)	113.08(12)	O(1)-Dy(1)-N(3)	128.31(12)	O(1)-Y(1)-N(3)	128.26(9)
O(1)-Dy(1)-N(1)	65.79(11)	O(2)-Dy(1)-O(3)	77.82(15)	O(2)-Y(1)-O(3)	78.04(10)
O(1)-Dy(1)-N(3)	82.43(12)	O(2)-Dy(1)-O(4)	84.99(12)	O(2)-Y(1)-O(4)	85.20(9)
O(2)-Dy(1)-O(3)	83.49(12)	O(2)-Dy(1)-N(1)	144.02(14)	O(2)-Y(1)-N(1)	144.19(9)
O(2)-Dy(1)-O(4)	82.35(12)	O(2)-Dy(1)-N(3)	152.81(14)	O(2)-Y(1)-N(3)	152.53(10)
O(2)-Dy(1)-O(5)	145.31(11)	O(3)-Dy(1)-O(4)	73.71(12)	O(3)-Y(1)-O(4)	74.20(8)
O(2)-Dy(1)-O(6)	78.43(11)	O(3)-Dy(1)-N(1)	75.21(14)	O(3)-Y(1)-N(1)	75.23(9)
O(2)-Dy(1)-N(1)	123.25(12)	O(3)-Dy(1)-N(3)	115.67(13)	O(3)-Y(1)-N(3)	115.95(9)
O(2)-Dy(1)-N(3)	147.57(10)	O(4)-Dy(1)-N(1)	109.37(13)	O(4)-Y(1)-N(1)	109.54(9)
O(3)-Dy(1)-O(4)	72.69(11)	O(4)-Dy(1)-N(1)	77.23(12)	O(4)-Y(1)-N(1)	77.01(8)
O(3)-Dy(1)-O(5)	114.50(11)	N(1)-Dy(1)-N(3)	62.61(13)	N(1)-Y(1)-N(3)	62.80(9)
O(3)-Dy(1)-O(6)	153.97(11)	N(3)-Dy(1)'-N(6)′	62.81(1)	N(3)-Y(1)'-N(6)′	62.81(1)
O(3)-Dy(1)-N(1)	121.76(11)	N(6)′-Dy(1) -N(8)′	62.39(1)	N(6)′-Y(1) -N(8)′	62.39(1)
O(3)-Dy(1)-N(3)	71.23(11)	Dy(1)-N(3)-N(6)	149.90(2)	Y(1)-N(3)-N(6)	149.74(1)
O(4)-Dy(1)-O(5)	75.93(11)				
O(4)-Dy(1)-O(6)	86.38(12)				
O(4)-Dy(1)-N(1)	149.81(11)				
O(4)-Dy(1)-N(3)	108.03(13)				
O(5)-Dy(1)-O(6)	73.56(10)				
O(5)-Dy(1)-N(1)	73.90(11)				
O(5)-Dy(1)-N(3)	66.30(10)				
O(6)-Dy(1)-N(1)	84.02(11)				
O(6)-Dy(1)-N(3)	131.62(10)				
N(1)-Dy(1)-N(3)	60.15(11)				

Table S4. SHAPE Analysis of Dy1 metal ions for both compounds **1** and **2**. The second Dy metal ion in each dimer is related by symmetry and therefore identical.

SHAPE Geometry (Code)	Dy1, Compound 1	Dy1, Compound 2
Octagon (OP-8)	29.38	31.41
Heptagonal pyramid (HPY-8)	21.48	20.75
Hexagonal bipyramid (HBPY-8)	14.18	13.06
Cube (CU-8)	8.002	7.882
Square antiprism (SAPR-8)	1.317	1.107
Triangular dodecahedron (TDD-8)	1.794	2.368
Johnson gyrobifastigium J26 (JGBF-8)	15.39	15.41
Johnson elongated triangular bipyramid J14 (JETBPY-8)	25.21	28.18
Biaugmented trigonal prism J50 (JBTPR-8)	2.906	3.114
Biaugmented trigonal prism (BTPR-8)	2.773	2.531
Snub diphenoid J84 (JSD-8)	4.874	5.514
Triakis tetrahedron (TT-8)	8.853	8.708
Elongated trigonal bipyramid (ETBPY-8)	22.16	24.63

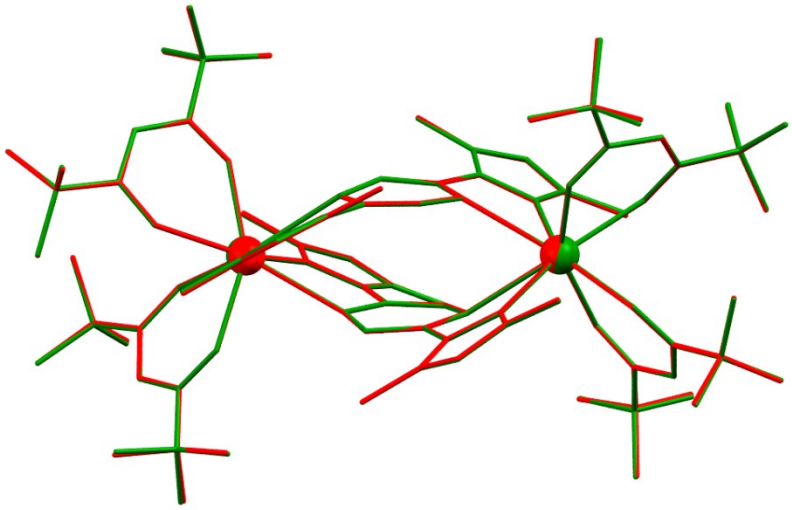

Figure S5. Structural overlay of **2** (red) and **3** (green) (RMS=0). H-atoms and disordered conformers have been omitted for clarity.

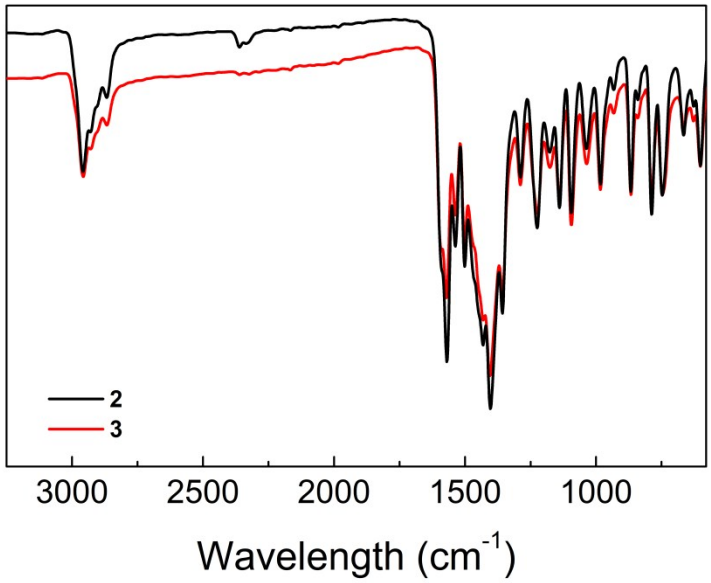

Figure S6. FT-IR spectra on crystals of **2** (black) and **3** (red).

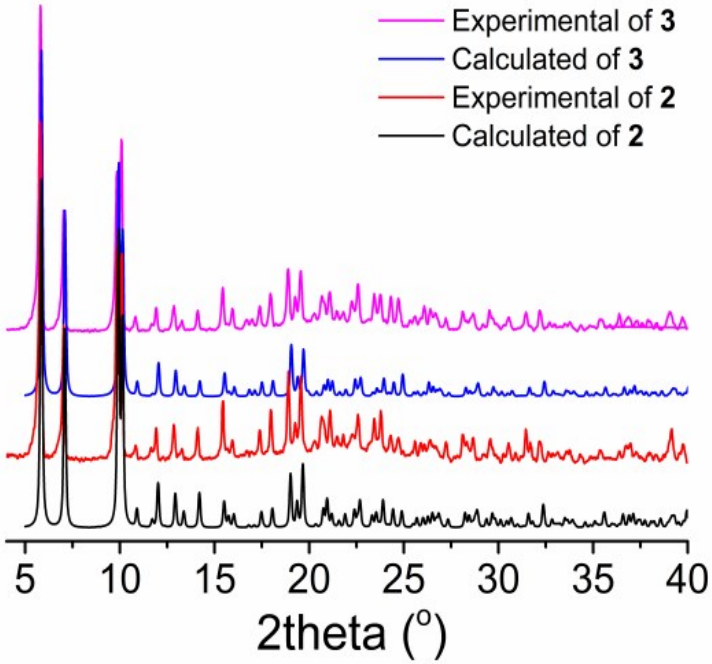

Figure S7. Powder X-ray diffraction pattern of **2** (calculated, black and experimental, red) and **3** (calculated, blue and experimental, magenta).

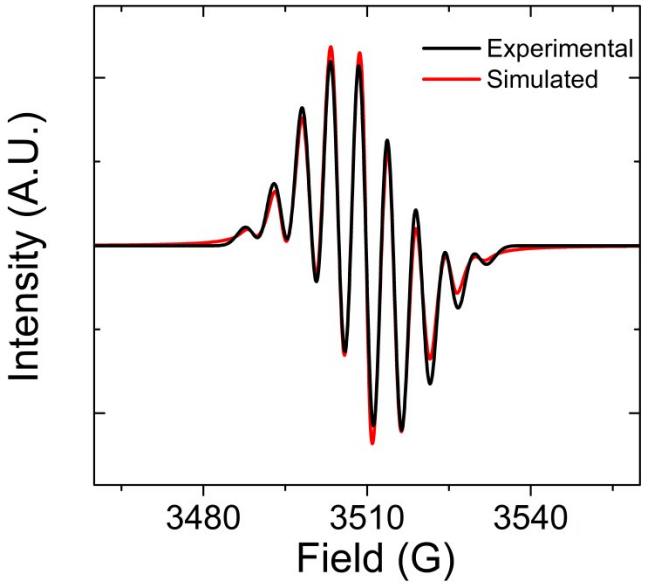

Figure S8. Experimental (black) and simulated (red) EPR spectra of **3** in benzene (g = 2.0013; SW = 10 mT; LW = 0.380 mT; a_N = 0.507 mT).

Computational details

To analyse the nature of the pancake bond in **2** and **3**, the unrestricted broken symmetry density functional theory (BS-DFT)[3-6] calculations were performed for **3** and the smaller Y-model system **4** at the B3LYP/def2-TZVP[7-12], CAM-B3LYP/def2-TZVP[10-13], PBE1PBE/def2-TZVP[10-12,14,15], LC-ωPBE/def2-TZVP[10-12,16-18], M06/def2-TZVP[10-12,19], and ωB97XD/def2-TZVP[11-13,20] levels of theory without and with dispersion correction in conjunction with damping function[21,22] as well as carrying out the complete active space self-consistent field CASSCF/def2-TZVP calculations for **4** (Figure S9).[23-25]

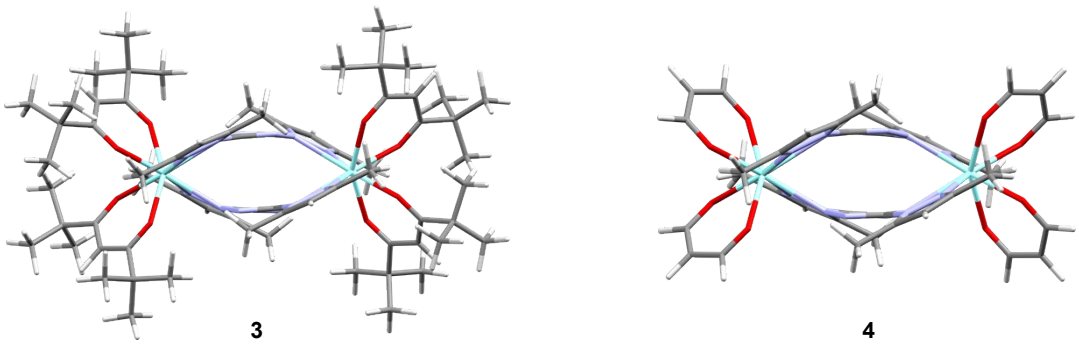

Figure S9. Frozen geometries adapted from the crystal structure of $[Y^{III}_2(\mu\text{-bpytz}^{\bullet-})_2(THMD)_4]$ for **3** and **4** with optimized hydrogen atoms at the LC-ωPBE/def2-TZVP level of theory.

In particular, we determined the singlet diradical character, unpaired electron density, formal bond order (p_{NO}) and vertical and adiabatic radical-radical exchange coupling constant ($J_{rad\text{-}rad}$) in these systems. The vertical $J_{vert\text{-}rad\text{-}rad}$ was calculated using the Yamaguchi projection

$$J_{vert-rad-rad} = \frac{2(E_{LS} - E_{HS})}{\langle S^2 \rangle_{HS} - \langle S^2 \rangle_{LS}}, \quad (1)$$

in which E_{LS} and E_{HS} are the energies of the low spin (LS) and high spin (HS) state, respectively, and $\langle S^2 \rangle_{HS}$ and $\langle S^2 \rangle_{LS}$ are the expectation values of the $\hat{S}^2$ operator evaluated in the Kohn-Sham determinant.[26-28] The adiabatic $J_{adia\text{-}rad\text{-}rad}$ was evaluated using the following equation

$$J_{adia-rad-rad} = \frac{2(E_{LS}^{LS} - E_{HS}^{LS})}{\langle S^2 \rangle_{HS}^{LS} - \langle S^2 \rangle_{LS}^{LS}} + E_{HS}^{LS} - E_{HS}^{HS}, \quad (2)$$

for the fully optimized geometries of **3** and **4**. In equation 2, the superscripts and subscripts indicate the optimized geometry and state, respectively, in which the energy or $\langle S^2 \rangle$ were evaluated in.[29,30] The geometry of **3** was only optimized at the LC-ωPBE-D3/def2-TZVP level of theory, whereas the geometry of **4** was optimized with all above mentioned exchange-correlation functionals. With every used functional, frequency analysis was also performed for the optimized geometry of **4** to ensure that it correspond to a true minimum on the potential energy hypersurface (no imaginary frequencies). Due to the size of the system no frequency analysis was performed for **3**. Because $J_{vert\text{-}rad\text{-}rad}$ and $J_{adia\text{-}rad\text{-}rad}$ corresponds to the vertical and adiabatic singlet-triplet gaps, respectively, they were also used to determine the ground state of **3** and **4**.[29,30]

The CASSCF/def2-TZVP calculations were carried out for the frozen and fully optimized geometry, both obtained from the LC-ωPBE-D3/def2-TZVP calculations, of **4** by using eight different active space: CAS(2,2), CAS(4,4), CAS(6,6), CAS(8,8), CAS(10,10), CAS(12,12), CAS(14,14) and CAS(16,16), that is, the size of active space was systematically increased by including more π-orbitals of π-dimerized bpytz$^{\bullet-}$ radicals into the active space. The π-orbital orbitals were chosen into the active space based on their natural orbital occupation numbers (NOONs) that were obtained at the second order Møller-Plesset perturbation theory level. NOONs are the eigenvalues of the one-particle electron density matrix and they converge towards values that they adopt in the exact wave function when enough high level of theory is used.[31,32] Because of this NOONs at the CASSCF level of theory can be used as a benchmark of the singlet diradical character: In a perfect diradical two natural orbitals are each occupied exactly by one electron. Thus, a suitable index for the singlet diradical character (SDR) is obtained by comparing the occupation number of the acceptor orbital n_{ACC} to the reference value of one electron:

$$SDR = \frac{n_{acc}}{1} \times 100\%. \quad (3)$$

The p_{NO} was computed employing following equation

$$p_{NO} = \frac{NEBO - NEABO}{2}, \quad (4)$$

where NEBO and NEABO are the NOONs of the frontier bonding and antibonding orbitals, respectively.[33] The total number of effectively unpaired electrons (N_u) between monomers was obtained with the following equation

$$N_U = \sum_{i=1}^{N} n_i^2 (2 - n_i)^2, \quad (5)$$

in which n_i refers to the *i*-th NOON and N to the number of natural orbitals.[34,35] N_u measures the total number of effectively unpaired electrons between radical ligands and it can be used as a benchmark for the singlet diradical character like the equation 3 at the CASSCF level. All above mentioned calculations were performed with Gaussian[36] and Orca[37] quantum chemistry codes.

To calculate the magnetic properties of complexes **1** and **2**, the multi-reference *ab inito* calculations were carried out with MOLCAS quantum chemistry program package versions 8.2 and 8.0.[38] The geometries of **1** and **2** were extracted from the crystal structures and the positions of hydrogen atoms were optimized at the PBE/def2-TZVP[10,11,39,40] level of theory prior the CASSCF calculations using Turbomole program package.[41] The core electrons of Y ions were modelled by effective core potential (ECP).[12] The positions of heavier elements were kept frozen during the optimizations of hydrogen atoms. To avoid convergence problems in optimizations, Dy^{III} ions were replaced with Y^{III} ions. In the CASSCF/SO-RASSI calculations, the spin-orbit states of each Dy^{III} ions were calculated separately while other one was replaced with Y^{III} ion. Due to the inversion symmetry Dy^{III} ions are equivalent, the CASSCF/SO-RASSI calculations were performed only for one Dy^{III} ion in both complexes. ANO-RCC-VTZP basis set for Dy^{III} ion and ANO-RCC-VDZP basis set for all other atoms (H, C, N, O, F, Y) were used in the CASSCF/SO-RASSI calculations.[42,43] In case of **1** the ANO-RCC-VDZP basis set of H was replaced with the ANO-RCC-VDZ basis due to the basis set limit of MOLCAS. The scalar relativistic effects were treated employing the exact two component (X2C) transformation.[44-46] The Cholesky decomposition was used for two electron integrals with the threshold value of 10^{-8} to speed up the calculations. In the SA-CASSCF calculations all 21 sextet, 224 quartet and 490 doublet states, originating from the active space of 9 electrons and seven 4f-orbitals, were solved. From these states, the lowest 21 spin sextets, 128 spin quartets and 130 spin doublets (corresponding to an energy cut-off of ~ 50 000 cm^{-1}) were mixed by spin-orbit coupling using the SO-RASSI method.[47] The local magnetic properties (***g***-tensors, transition magnetic moments, and orientation of magnetic axis) were extracted from the RASSI wave functions using the SINGLE_ANISO routine.[48-50] The exchange interaction between Dy^{III} ions was modelled using the Lines model as implemented in the POLY_ANISO routine and using the following effective Heisenberg Hamiltonian:[51-53]

$$H_{12}^{exch} = -J_{12}S_1S_2, \quad (1)$$

in which J_{12} is the exchange coupling constant between interacting Dy^{III} centres and S_1 and S_2 are local spin-operators (S=5/2) on Dy^{III} sites 1 and 2, respectively, in the absence of spin-orbit coupling. For both complexes, the exchange coupling parameter was obtained by fitting the calculated susceptibility and magnetization data to the experimental data. In the fitting procedure, the exchange parameter was increased in increments of 0.001 cm^{-1}, and 2 spin-orbit eigenstates from both Dy^{III} centres were included in the exchange interaction. During the fitting procedure the dipolar coupling between Dy^{III} centres was taken into account as implemented in the POLY_ANISO routine.

Table S5. Calculated vertical BS-DFT energies and $\langle S^2 \rangle$ values for high (HS) and low (LS) states of **3** and **4** as well as the calculated vertical radical-radical coupling constants ($J_{vert\text{-}rad\text{-}rad}$) for **3** and **4**. The dispersion correction does not have effect on the calculated $J_{vert\text{-}rad\text{-}rad}$ as the same geometry is used for HS and LS states.

3					
Functional	E_{HS} **[au]**	E_{LS} **[au]**	$\langle S^2 \rangle_{HS}$	$\langle S^2 \rangle_{LS}$	$J_{vert\text{-}rad\text{-}rad}$ **[cm^{-1}]**
LC-ωPBE-D3	-4208.016338	-4208.024700	2.0699	0.9329	-3228.4558
4					
Functional	E_{HS} **[au]**	E_{LS} **[au]**	$\langle S^2 \rangle_{HS}$	$\langle S^2 \rangle_{LS}$	$J_{vert\text{-}rad\text{-}rad}$ **[cm^{-1}]**
B3LYP	-2951.844752	-2951.857974	2.0353	0.5844	-4000.1989
B3LYP-D3	-2952.154105	-2952.167327	2.0353	0.5844	-4000.1989
CAM-B3LYP	-2950.447209	-2950.457051	2.0548	0.8417	-3561.1382

CAM-B3LYP-D3	-2950.618181	-2950.628023	2.0548	0.8417	-3561.1418
PBE1PBE	-2948.545256	-2948.557543	2.0445	0.6817	-3957.6683
PBE1PBE-D3	-2948.716953	-2948.729241	2.0445	0.6817	-3957.6683
LC-ωPBE	-2949.915524	-2949.923949	2.0699	0.9319	-3249.7066
LC-ωPBE-D3	-2950.108066	-2950.116491	2.0699	0.9319	-3249.7104
M06	-2949.925472	-2949.938121	2.0346	0.6288	-3949.5077
ωB97XD	-2950.964734	-2950.974894	2.0463	0.8166	-3626.5075

Table S6. Calculated centroid-centroid (*r*) distances between two bpytz$^{\bullet-}$ radicals for the gas-phase optimized geometries of **3** and **4** as well as the deviation of calculated values from the experimental distance r_{exp} (2.774 Å). The experimental distance was taken from the crystal structure of **3**.

3				
Functional	r_{HS} **(Å)**	r_{HS} **– r$_{exp}$(Å)**	r_{LS} **(Å)**	r_{LS} **– r$_{exp}$(Å)**
LC-ωPBE-D3	2.943	0.169	2.880	0.106
4				
Functional	r_{HS} **(Å)**	r_{HS} **– r$_{exp}$(Å)**	r_{LS} **(Å)**	r_{LS} **– r$_{exp}$(Å)**
B3LYP	3.086	0.312	2.965	0.191
B3LYP-D3	2.992	0.218	2.874	0.100
CAM-B3LYP	3.035	0.261	2.956	0.182
CAM-B3LYP-D3	2.999	0.225	2.924	0.150
PBE1PBE	3.019	0.245	2.896	0.122
PBE1PBE-D3	2.973	0.199	2.854	0.080
LC-ωPBE	2.997	0.223	2.927	0.153
LC-ωPBE-D3	2.951	0.177	2.886	0.112
M06	3.009	0.235	2.893	0.119
ωB97XD	3.004	0.230	2.934	0.160

Table S7. Calculated adiabatic BS-DFT energies and $\langle S^2 \rangle$ values as well as the calculated adiabatic radical-radical coupling constants ($J_{adia\text{-}rad\text{-}rad}$) for **3** and **4**.

3						
Functional	E_{HS}^{LS} **[au]**	E_{LS}^{LS} **[au]**	E_{HS}^{HS} **[au]**	$\langle S^2 \rangle_{HS}^{LS}$	$\langle S^2 \rangle_{LS}^{LS}$	$J_{vert\text{-}rad\text{-}rad}$ **[cm^{-1}]**
LC-ωPBE-D3	-4208.049048	-4208.053834	-4208.0499	2.0613	0.9873	-1767.5020
4						
Functional	E_{HS}^{LS} **[au]**	E_{LS}^{LS} **[au]**	E_{HS}^{HS} **[au]**	$\langle S^2 \rangle_{HS}^{LS}$	$\langle S^2 \rangle_{LS}^{LS}$	$J_{vert\text{-}rad\text{-}rad}$ **[cm^{-1}]**
B3LYP	-2951.875208	-2951.883692	-2951.877452	2.0337	0.7547	-2419.0379
B3LYP-D3	-2952.178038	-2952.187584	-2952.180909	2.0333	0.7131	-2543.6395
CAM-B3LYP	-2950.477204	-2950.482747	-2950.478271	2.0492	0.9352	-1950.0831
CAM-B3LYP-D3	-2950.646774	-2950.652226	-2950.647876	2.0490	0.9367	-1909.7952
PBE1PBE	-2948.572366	-2948.581483	-2948.574931	2.0408	0.7765	-2602.2870
PBE1PBE-D3	-2948.742747	-2948.752139	-2948.745552	2.0405	0.7658	-2618.3204
LC-ωPBE	-2949.947539	-2949.952426	-2949.948392	2.0612	0.9853	-1806.5623

LC-ωPBE-D3	-2950.139532	-2950.144374	-2950.140422	2.0610	0.9857	-1781.3528
M06	-2949.955877	-2949.964473	-2949.958339	2.0316	0.7717	-2454.3605
ωB97XD	-2950.994768	-2951.000035	-2950.995860	2.0418	0.9304	-1840.6649

Table S8. Calculated NOONs at the CASSCF/def2-TZVP level of theory for the frozen geometry of **4**. The positions of hydrogen atoms were optimized at the LC-ωPBE-D3/def2-TZVP level of theory.

NO	CAS(2,2)	CAS(4,4)	CAS(6,6)	CAS(8,8)	CAS(10,10)	CAS(12,12)	CAS(14,14)	CAS(16,16)
220	-	-	-	-	-	-	-	1.97
221	-	-	-	-	-	-	1.94	1.96
222	-	-	-	-	-	1.97	1.94	1.96
223	-	-	-	-	1.95	1.96	1.94	1.94
224	-	-	-	1.97	1.95	1.95	1.94	1.94
225	-	-	1.99	1.96	1.93	1.93	1.92	1.94
226	-	1.99	1.96	1.96	1.92	1.92	1.92	1.94
227	1.57	1.62	1.62	1.64	1.52	1.53	1.49	1.64
228	0.43	0.40	0.39	0.38	0.49	0.49	0.51	0.38
229	-	0.00	0.03	0.03	0.08	0.07	0.08	0.06
230	-	-	0.01	0.03	0.08	0.07	0.08	0.06
231	-	-	-	0.03	0.05	0.06	0.06	0.06
232	-	-	-	-	0.04	0.04	0.06	0.06
233	-	-	-	-	-	0.00	0.06	0.03
234	-	-	-	-	-	-	0.06	0.03
235	-	-	-	-	-	-	-	0.03

Table S9. Calculated NOONs at the CASSCF/def2-TZVP level of theory for the optimized geometry of **4**. The geometry was optimized at the LC-ωPBE-D3/def2-TZVP level of theory.

NO	CAS(2,2)	CAS(4,4)	CAS(6,6)	CAS(8,8)	CAS(10,10)	CAS(12,12)	CAS(14,14)	CAS(16,16)
220	-	-	-	-	-	-	-	1.97
221	-	-	-	-	-	-	1.99	1.96
222	-	-	-	-	-	1.97	1.97	1.96
223	-	-	-	-	1.99	1.97	1.94	1.94
224	-	-	-	1.97	1.97	1.96	1.94	1.94
225	-	-	1.98	1.96	1.96	1.94	1.94	1.94
226	-	1.99	1.97	1.96	1.96	1.93	1.94	1.94
227	1.45	1.47	1.51	1.53	1.52	1.44	1.51	1.53
228	0.55	0.53	0.50	0.48	0.50	0.58	0.50	0.48
229	-	0.00	0.02	0.03	0.04	0.06	0.06	0.06
230	-	-	0.02	0.03	0.03	0.05	0.06	0.06

231	-	-	-	0.03	0.03	0.05	0.06	0.06
232	-	-	-	-	0.00	0.04	0.06	0.06
233	-	-	-	-	-	0.00	0.02	0.03
234	-	-	-	-	-	-	0.01	0.03
235	-	-	-	-	-	-	-	0.03

Table S10. Calculated p_{NO} and N_u values for the frozen geometry of **4** with different active spaces. The positions of hydrogen atoms were optimized at the LC-ωPBE-D3/def2-TZVP level of theory.

	CAS(2,2)	CAS(4,4)	CAS(6,6)	CAS(8,8)	CAS(10,10)	CAS(12,12)	CAS(14,14)	CAS(16,16)
p_{NO}	0.57	0.61	0.62	0.63	0.52	0.52	0.49	0.63
N_u	0.91	0.79	0.77	0.74	1.19	1.19	1.36	0.86

Table S11. Calculated p_{NO} and N_u values for the optimized geometry of **4** with different active spaces. The geometry was optimized at the LC-ωPBE-D3/def2-TZVP level of theory.

	CAS(2,2)	CAS(4,4)	CAS(6,6)	CAS(8,8)	CAS(10,10)	CAS(12,12)	CAS(14,14)	CAS(16,16)
p_{NO}	0.45	0.47	0.51	0.53	0.51	0.43	0.50	0.52
N_u	1.26	1.21	1.11	1.07	1.12	1.41	1.22	1.18

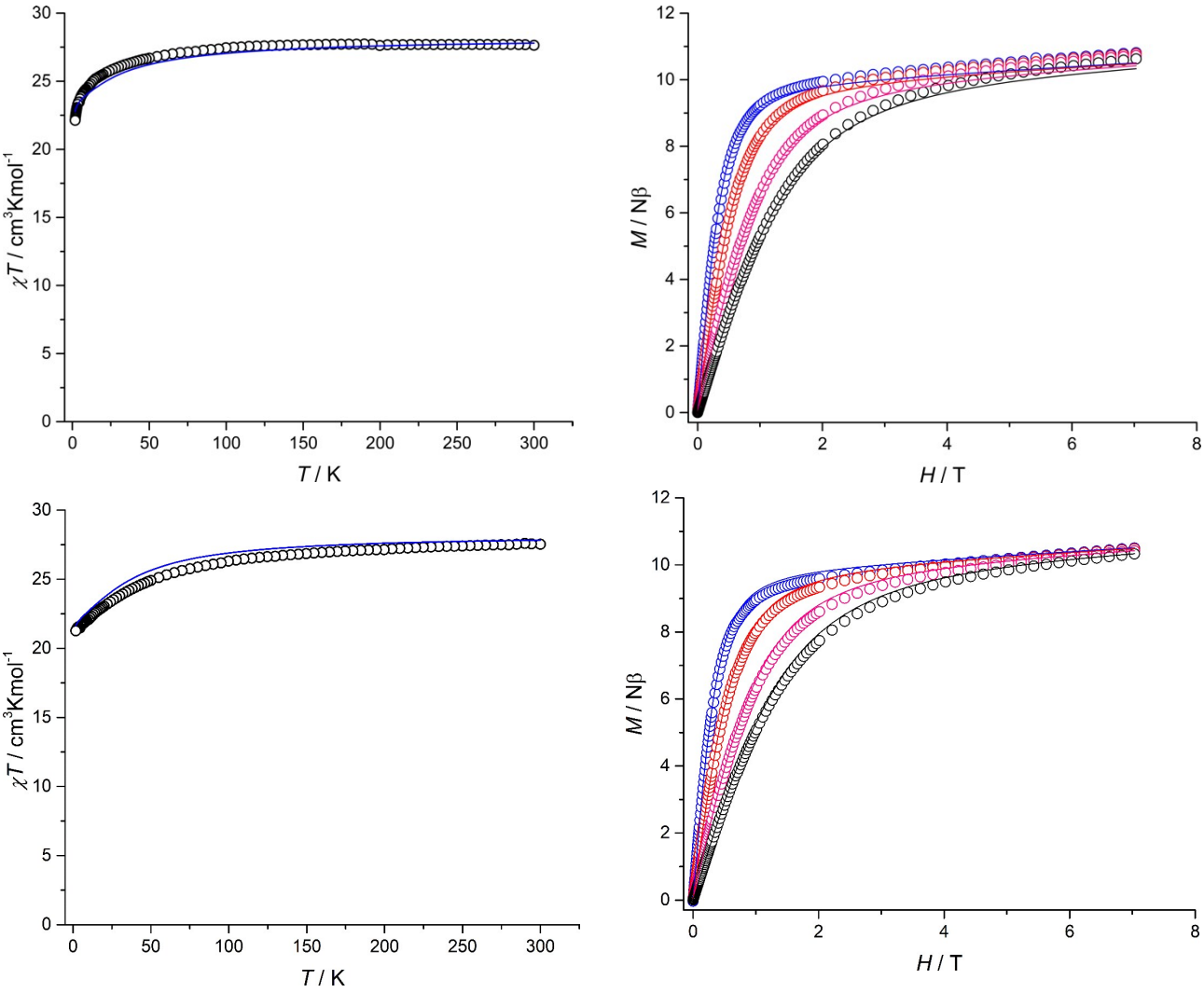

Figure S10. Experimental (black circles) and calculated (blue line) plots of $\chi_M T$ as function of temperature for **1** (up, left) and **2** (down, left). The plots of *M* as a function of magnetic field at 1.8 K (blue), 3 K (red), 5 K (pink) and 7 K (black) for **1** (up, right; circles = experimental values, lines = calculated data) and **2** (down, right; circles = experimental values, lines = calculated data). Calculated plots were obtained by including 2 spin-orbit eigenstates from both Dy centres into the exchange interaction and using the Lines parameter 0.006 cm^{-1} and 0.016 cm^{-1} for **1** and **2**, respectively.

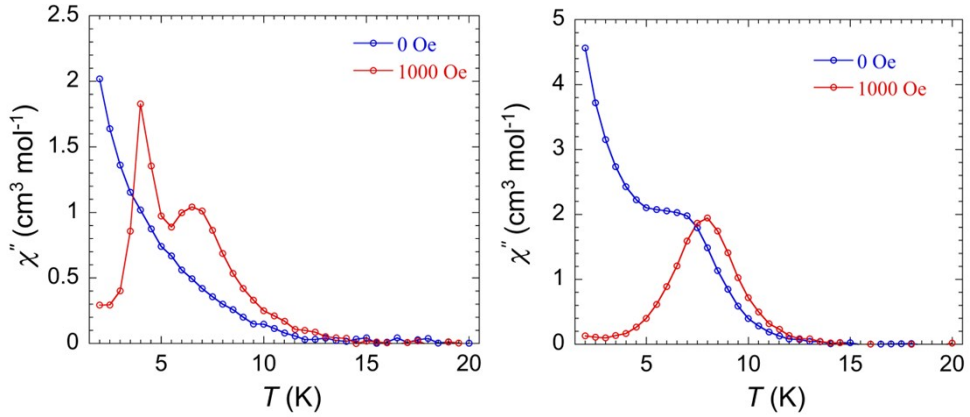

Figure S11. AC susceptibility measurement performed at variable temperature under zero and applied dc field of 1000 Oe for **1** (left) and **2** (right).

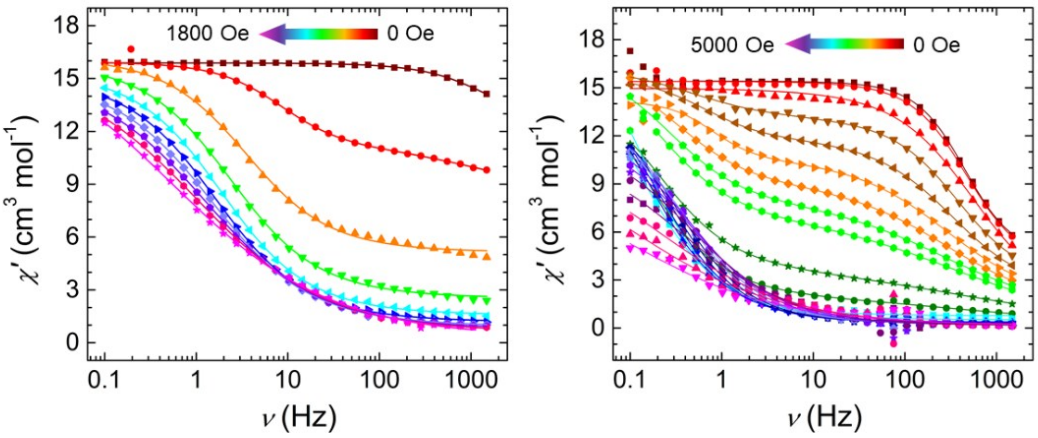

Figure S12. In-phase (χ') field-dependent susceptibility measurements performed at 2 K and magnetic fields ranging from 0 to 1800 Oe for **1** (left) and from 0 to 5000 Oe for **2** (right). The solid lines represent best fits obtained from either a generalized or double Debye model.

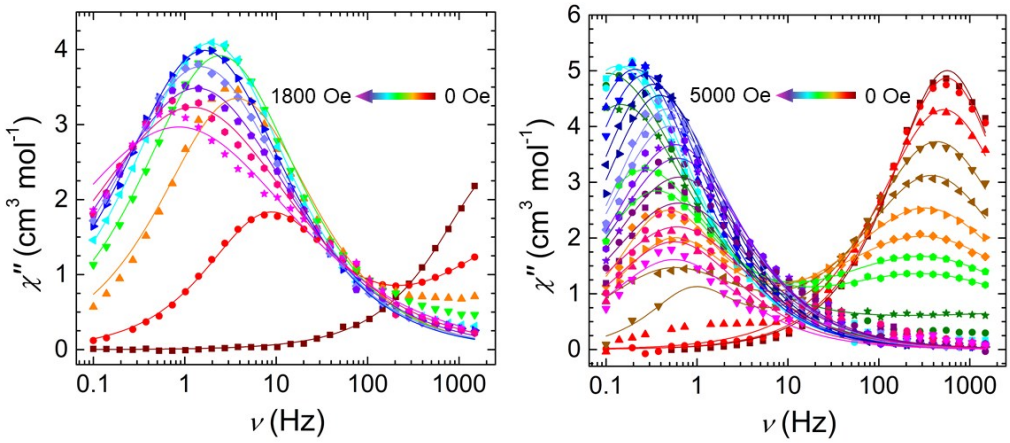

Figure S13. Out-of-phase (χ'') field-dependent susceptibility measurements performed at 2 K and magnetic fields ranging from 0 to 1800 Oe for **1** (left) and from 0 to 5000 Oe for **2** (right). The solid lines represent best fits obtained from either a generalized or double Debye model.

Table S12. Best fit parameters to the generalized/double Debye model for the field dependent ac susceptibility measurements of **1**.

***H* (Oe)**	τ(High Frequency Process)	τ(Low Frequency Process)	α(High Frequency Process)	α(Low Frequency Process)	χ_S(High Frequency Process)	χ_S(Low Frequency Process)	χ_T(High Frequency Process)	χ_T(Low Frequency Process)
0	5.27E-05	-	0.20304	-	0.00117	-	6.73138	-
200	1.53E-05	-	0.43931	-	1.00E-03	-	6.88802	-
400	-	0.01902	-	0.20802	-	0.00319	-	4.85111
600	-	0.04277	-	0.3065	-	0.01101	-	11.0657
800	-	0.06533	-	0.32322	-	0.06658	-	13.3959
1000	-	0.08306	-	0.32394	-	0.01382	-	13.93531
1200	-	0.09816	-	0.34532	-	0.05034	-	14.17599
1400	-	0.10673	-	0.37409	-	0.31914	-	14.40903
1600	-	0.11689	-	0.41699	-	0.00169	-	14.147
1800	-	0.18592	-	0.5144	-	1.86	-	16.661

Table S13. Best fit parameters to the generalized / double Debye model for the field dependent ac susceptibility measurements of **2**.

***H* (Oe)**	τ(High Frequency Process)	τ(Low Frequency Process)	α(High Frequency Process)	α(Low Frequency Process)	χ_S(High Frequency Process)	χ_S(Low Frequency Process)	χ_T (High Frequency Process)	χ_T(Low Frequency Process)
0	2.81E-04	-	0.15437	-	0.00716	-	12.79238	-
50	2.84E-04	-	0.17317	-	0.01426	-	12.84383	-
100	3.07E-04	-	0.25074	-	0.00426	-	12.90081	-
150	3.64E-04	0.17489	0.27536	0	0.02623	2.5396	11.67411	4.55254
200	4.09E-04	0.31509	0.30554	0.28589	0.01056	9.3229	10.18987	13.71204
250	4.79E-04	0.30129	0.37614	0.18161	14.92369	0.70917	24.35437	5.69191
300	5.07E-04	0.34277	0.46092	0.1247	0.10618	2.84482	9.04685	8.45951
350	5.07E-04	0.46542	0.48443	0.20886	1.58381	2.24486	9.22945	9.75524
400	4.71E-04	0.62038	0.5114	0.2549	1.23144	1.37689	7.76866	10.72311
600	6.28E-07	1.11096	0.84612	0.27814	1	1.00416	13.13016	13.99585
800	-	1.52949	-	0.36454	-	1.56165	-	19.74122
1000	-	1.18965	-	0.29754	-	4.24407	-	20.75935
1200	-	0.9498	-	0.25692	-	4.80649	-	20.19469
1400	-	0.76312	-	0.23469	-	2.30467	-	16.9713
1600	-	0.59849	-	0.21466	-	1.08863	-	14.98694
1800	-	0.48108	-	0.20289	-	2.24737	-	15.40817
2000	-	0.40441	-	0.20497	-	2.04866	-	14.70635
2200	-	0.33668	-	0.19951	-	0.71651	-	12.58752
2400	-	0.31173	-	0.23719	-	0.02799	-	11.76638
2600	-	0.27558	-	0.24691	-	0.01171	-	10.95986
2800	-	0.26155	-	0.26701	-	0.01011	-	10.58242
3000	-	0.24956	-	0.28229	-	0.14314	-	9.92782
3500	-	0.25317	-	0.30082	-	2.1923	-	10.77922
4000	-	0.26528	-	0.30127	-	2.67077	-	9.86872
4500	-	0.28246	-	0.24892	-	1.9642	-	7.73989
5000	-	0.2855	-	0.24187	-	0.23264	-	4.9993

Table S14. Best fit parameters and uncertainties to the generalized Debye model for the temperature dependent ac susceptibility measurements of **1**.

T (K)	τ	τ^{err}	α	α^{err}	χ_S	χ_S^{err}	χ_T	χ_T^{err}
1.9	7.88E-02	1.83E-03	3.38E-01	7.46E-03	2.61E+00	4.78E-02	1.67E+01	1.05E-01
1.99989	6.65E-02	1.39E-03	3.25E-01	7.04E-03	2.51E+00	4.36E-02	1.59E+01	8.76E-02
2.499953	2.46E-02	3.65E-04	2.63E-01	5.98E-03	2.04E+00	3.41E-02	1.27E+01	4.36E-02
2.999912	7.85E-03	1.16E-04	2.74E-01	5.82E-03	1.54E+00	3.59E-02	1.07E+01	2.94E-02
3.500006	2.68E-03	4.89E-05	3.59E-01	5.69E-03	1.01E+00	4.62E-02	9.37E+00	2.30E-02
3.998925	1.29E-03	6.22E-05	4.05E-01	1.18E-02	1.20E+00	1.09E-01	8.37E+00	3.62E-02
4.499843	1.07E-03	4.45E-05	3.20E-01	1.28E-02	2.17E+00	7.82E-02	7.40E+00	2.53E-02
4.999772	7.11E-04	1.66E-05	2.86E-01	7.41E-03	2.26E+00	4.15E-02	6.72E+00	1.10E-02
5.999911	2.44E-04	8.82E-06	2.89E-01	8.44E-03	1.86E+00	5.98E-02	5.64E+00	7.58E-03

Table S15. Best fit parameters and uncertainties to the generalized Debye model for the temperature dependent ac susceptibility measurements of **2**.

T (K)	τ	τ^{err}	α	α^{err}	χ_S	χ_S^{err}	χ_T	χ_T^{err}
1.899736	1.19E+00	5.26E-02	2.70E-01	8.75E-03	0.64811	0.02722	17.175	0.34026
1.999834	9.51E-01	3.59E-02	2.62E-01	8.50E-03	0.6121	0.027652	16.311	0.27761
2.197286	7.28E-01	4.17E-02	2.71E-01	1.39E-02	0.50408	0.049688	15.807	0.39966
2.399995	3.47E-01	1.03E-02	2.16E-01	1.08E-02	0.51848	0.040327	13.142	0.17535
2.599967	2.04E-01	4.98E-03	1.96E-01	1.02E-02	0.53649	0.040327	12.026	0.12386
2.799965	1.20E-01	1.64E-03	1.91E-01	5.95E-03	0.42127	0.023656	10.982	0.06013
2.999946	7.20E-02	1.42E-03	1.67E-01	9.35E-03	0.44287	0.038166	10.046	0.070211
3.500046	2.47E-02	2.23E-04	1.54E-01	4.44E-03	0.28121	0.018759	8.6414	0.023224
3.99912	1.03E-02	7.50E-05	1.33E-01	3.70E-03	0.29165	0.015591	7.5612	0.014438
4.499553	4.93E-03	4.78E-05	1.16E-01	5.05E-03	0.24844	0.021315	6.7331	0.015591
4.999649	2.56E-03	1.75E-05	1.17E-01	3.57E-03	0.2164	0.015519	6.121	0.009002
5.499788	1.45E-03	7.30E-06	1.01E-01	2.68E-03	0.20271	0.011954	5.5809	0.005581
5.999833	8.48E-04	7.02E-06	1.01E-01	4.32E-03	0.18363	0.020415	5.1488	0.007453
6.999737	3.17E-04	3.27E-06	1.10E-01	4.55E-03	0.12206	0.026428	4.4287	0.005149
8.000051	1.29E-04	1.97E-06	1.05E-01	4.60E-03	0.22432	0.036006	3.8886	0.002938

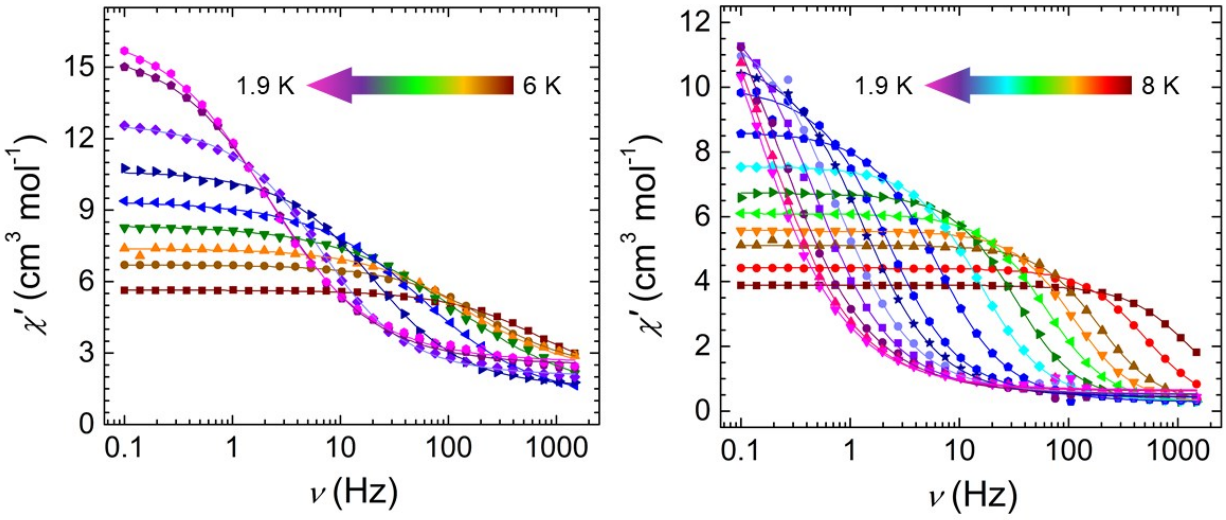

Figure S14. In-phase (χ') frequency-dependent susceptibility measurements performed at a constant magnetic field of 600 Oe for **1** (left) and 1200 Oe for **2** (right). The solid lines represent best fits obtained from a generalized Debye model.

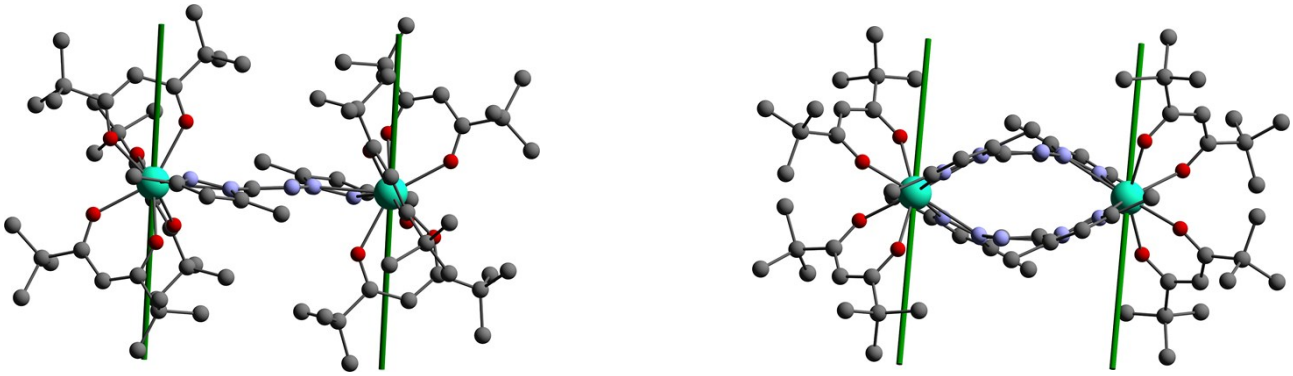

Figure S15. Orientations of the main axes of the ***g***-tensors in the ground Kramers' doublets for **1** (left) and **2** (right). Hydrogen atoms are omitted for clarity.

Table S16. Calculated energies and ***g***-tensors for the eight lowest KDs in **1** as well as the angle (θ) between the principal magnetic axes of ground KD and each excited KD.

KD	E / cm^{-1}	g_x	g_y	g_z	θ
1	0.000	0.048	0.084	19.376	-
2	73.744	0.203	0.289	16.965	20.595
3	174.177	1.371	1.558	13.844	171.351
4	240.734	3.245	5.167	9.488	166.670
5	323.009	2.836	5.136	10.549	90.538
6	430.867	0.885	1.891	16.138	77.806
7	549.580	0.318	0.732	16.219	96.655
8	653.053	0.112	0.319	18.324	86.709

Table S17. Calculated energies and ***g***-tensors for the eight lowest KDs in **2** as well as the angle (θ) between the principal magnetic axes of ground KD and each excited KD.

KD	E / cm^{-1}	g_x	g_y	g_z	θ
1	0.000	0.035	0.037	18.667	-
2	80.468	0.326	1.083	14.099	16.504
3	126.562	2.834	4.529	12.407	100.448
4	171.838	2.553	3.076	8.264	65.464
5	249.809	0.184	0.229	12.036	70.011
6	367.991	0.204	0.266	14.208	74.897
7	451.513	0.242	0.258	17.471	115.515
8	522.905	0.038	0.054	19.150	75.185

Table S18. Percentage composition of the SO-RASSI wave functions for each M_J state of the ground multiplet (J = 15/2) in **1**.

M_J	KD1		KD2		KD3		KD4		KD5		KD6		KD7		KD8	
-15/2	0.0	91.1	1.5	0.0	6.0	0.0	0.0	0.6	0.0	0.4	0.2	0.0	0.1	0.0	0.0	0.0
-13/2	0.0	0.1	69.1	0.1	20.4	0.2	2.1	2.6	2.7	1.0	0.0	1.0	0.6	0.2	0.1	0.0
-11/2	0.0	8.4	12.7	0.0	49.6	0.1	0.4	14.3	0.4	7.0	4.2	0.4	1.6	0.2	0.6	0.1
-9/2	0.0	0.1	14.8	0.0	2.6	0.4	13.0	38.8	15.5	0.1	4.0	4.6	2.7	1.7	0.9	0.8
-7/2	0.0	0.2	0.7	0.0	14.7	0.0	0.4	3.5	12.0	36.2	7.4	12.3	7.3	2.1	1.1	2.0
-5/2	0.0	0.1	0.4	0.0	3.0	0.2	2.4	9.4	5.7	0.7	40.1	4.5	20.1	6.2	1.3	5.9
-3/2	0.0	0.1	0.3	0.0	1.2	0.3	1.7	7.0	2.9	3.1	1.1	10.9	15.8	29.4	3.2	23.0
-1/2	0.0	0.0	0.3	0.0	0.5	0.7	1.2	2.7	0.8	11.3	5.8	3.6	9.5	2.6	36.8	24.2
1/2	0.0	0.0	0.0	0.3	0.7	0.5	2.7	1.2	11.3	0.8	3.6	5.8	2.6	9.5	24.2	36.8
3/2	0.1	0.0	0.0	0.3	0.3	1.2	7.0	1.7	3.1	2.9	10.9	1.1	29.4	15.8	23.0	3.2
5/2	0.1	0.0	0.0	0.4	0.2	3.0	9.4	2.4	0.7	5.7	4.5	40.1	6.2	20.1	5.9	1.3
7/2	0.2	0.0	0.0	0.7	0.0	14.7	3.5	0.4	36.2	12.0	12.3	7.4	2.1	7.3	2.0	1.1
9/2	0.1	0.0	0.0	14.8	0.4	2.6	38.8	13.0	0.1	15.5	4.6	4.0	1.7	2.7	0.8	0.9
11/2	8.4	0.0	0.0	12.7	0.1	49.6	14.3	0.4	7.0	0.4	0.4	4.2	0.2	1.6	0.1	0.6
13/2	0.1	0.0	0.1	69.1	0.2	20.4	2.6	2.1	1.0	2.7	1.0	0.0	0.2	0.6	0.0	0.1
15/2	91.1	0.0	0.0	1.5	0.0	6.0	0.6	0.0	0.4	0.0	0.0	0.2	0.0	0.1	0.0	0.0

Table S19. Percentage composition of the SO-RASSI wave functions for each M_J state of the ground multiplet (J = 15/2) in **2**.

M_J	KD1		KD2		KD3		KD4		KD5		KD6		KD7		KD8	
-15/2	0.0	79.8	0.0	0.6	3.9	0.1	0.1	5.4	0.3	2.6	2.1	0.2	0.0	4.6	0.0	0.3
-13/2	0.0	4.1	1.3	52.1	0.5	5.1	9.2	0.3	6.6	2.6	4.2	1.7	0.4	11.2	0.4	0.2
-11/2	0.0	11.8	0.0	0.9	3.7	1.6	6.4	13.8	15.5	9.4	5.3	12.5	1.9	16.1	0.7	0.6
-9/2	0.0	1.7	0.6	22.3	0.6	1.3	0.1	0.0	11.6	1.7	10.3	19.5	4.3	19.0	2.9	4.2
-7/2	0.0	1.0	0.2	11.7	5.3	1.7	7.6	13.4	2.4	0.8	2.5	11.1	10.0	10.3	19.4	2.6
-5/2	0.0	1.2	0.1	0.4	24.0	4.3	0.6	9.5	14.6	3.1	0.2	0.8	2.6	8.5	17.6	12.4
-3/2	0.0	0.3	0.8	6.2	6.6	7.6	24.6	3.3	0.9	8.3	2.1	10.1	0.3	5.9	20.8	2.2
-1/2	0.1	0.0	0.3	2.4	17.7	16.2	1.9	3.8	3.6	16.0	8.2	9.3	1.7	3.3	4.1	11.4
1/2	0.0	0.1	2.4	0.3	16.2	17.7	3.8	1.9	16.0	3.6	9.3	8.2	3.3	1.7	11.4	4.1
3/2	0.3	0.0	6.2	0.8	7.6	6.6	3.3	24.6	8.3	0.9	10.1	2.1	5.9	0.3	2.2	20.8
5/2	1.2	0.0	0.4	0.1	4.3	24.0	9.5	0.6	3.1	14.6	0.8	0.2	8.5	2.6	12.4	17.6
7/2	1.0	0.0	11.7	0.2	1.7	5.3	13.4	7.6	0.8	2.4	11.1	2.5	10.3	10.0	2.6	19.4
9/2	1.7	0.0	22.3	0.6	1.3	0.6	0.0	0.1	1.7	11.6	19.5	10.3	19.0	4.3	4.2	2.9
11/2	11.8	0.0	0.9	0.0	1.6	3.7	13.8	6.4	9.4	15.5	12.5	5.3	16.1	1.9	0.6	0.7
13/2	4.1	0.0	52.1	1.3	5.1	0.5	0.3	9.2	2.6	6.6	1.7	4.2	11.2	0.4	0.2	0.4
-15/2	79.8	0.0	0.6	0.0	0.1	3.9	5.4	0.1	2.6	0.3	0.2	2.1	4.6	0.0	0.3	0.0

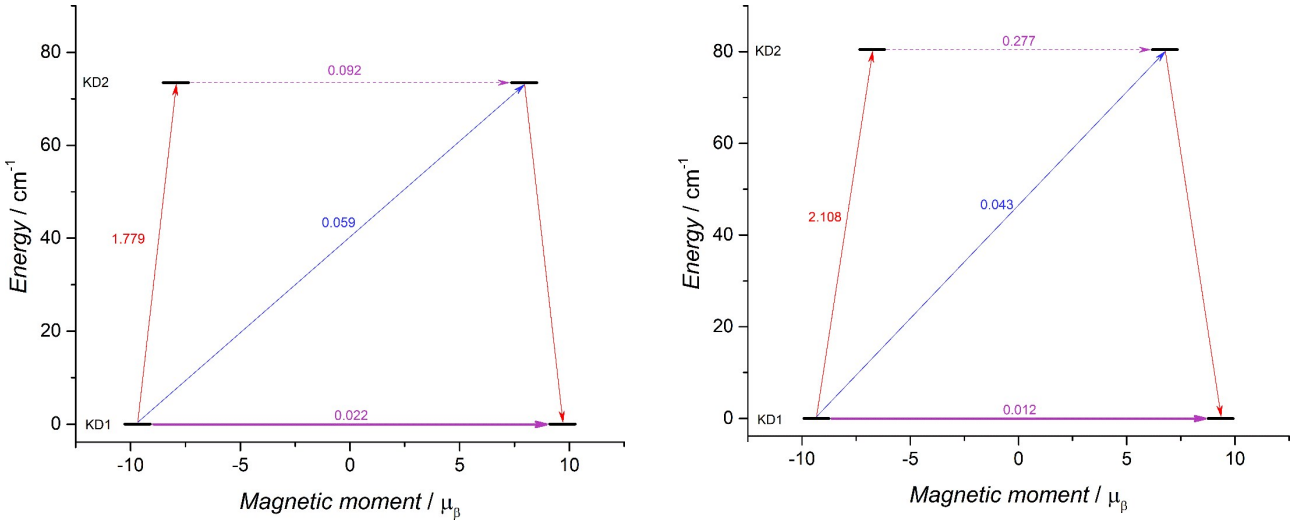

Figure S16. Qualitative relaxation barrier for **1** (left) and **2** (right). The numbers show the transition probabilities between KDs. Red, blue, and purple lines show the transition probabilities for the direct vertical transitions, Orbach process, and QTM, respectively. The most plausible relaxation pathways for the studied systems are presented by the solid bold purple arrow.

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XYZ coordinates of optimized geometries

3 low-spin state at the LC-ωPBE-D3/def2-TZVP level

Y	-3.49065	0.00718	-0.01227
C	-4.20409	-3.94274	0.03148
H	-4.83598	-3.08213	-0.15905
H	-4.73007	-4.63801	0.68567
H	-4.00927	-4.46204	-0.90705
C	-2.92364	-3.52386	0.65126
C	-1.93147	-4.36752	1.18154
H	-1.96151	-5.44244	1.25690
C	-0.91482	-3.55421	1.59437
C	0.37244	-3.91296	2.23443
H	1.20666	-3.69353	1.57239
H	0.36245	-4.97497	2.47328
H	0.53551	-3.34121	3.14613
C	-0.61725	-1.08455	1.43282
C	0.60681	1.09857	1.43708
C	-0.38913	3.92723	2.23045
H	-0.38116	4.98941	2.46862
H	-0.55930	3.35611	3.14123
H	-1.21808	3.70719	1.56204
C	0.90323	3.56825	1.60090
C	1.92338	4.38149	1.19668
H	1.95296	5.45638	1.27256
C	2.91978	3.53783	0.67448
C	4.20549	3.95674	0.06574
H	4.83922	3.09618	-0.11890
H	4.72544	4.65243	0.72430
H	4.01878	4.47563	-0.87465
C	-4.96228	-2.33997	-3.73852
C	-6.04056	-3.37979	-3.43942
H	-7.03587	-2.93473	-3.44310
H	-5.88179	-3.83935	-2.46304
H	-6.01586	-4.16826	-4.19446
C	-3.59491	-3.00287	-3.75143
H	-2.80942	-2.27153	-3.94151
H	-3.56261	-3.76633	-4.53127
H	-3.37196	-3.46762	-2.79441
C	-5.21904	-1.71018	-5.10504
H	-6.22028	-1.28849	-5.18247
H	-5.11423	-2.46910	-5.88305
H	-4.50094	-0.91414	-5.30807
C	-5.00950	-1.27252	-2.64353
C	-6.11340	-0.41384	-2.59641
H	-6.92024	-0.59623	-3.28521
C	-6.17577	0.71212	-1.78289
C	-7.36750	1.66592	-1.87482
C	-6.87633	2.90338	-2.62341
H	-6.01437	3.33658	-2.11989
H	-7.66852	3.65343	-2.67048
H	-6.58367	2.64886	-3.64371
C	-8.56343	1.07896	-2.61008
H	-8.34856	0.90267	-3.66460
H	-9.39725	1.78151	-2.55988

H	-8.88900	0.13869	-2.16226
C	-7.79500	2.05359	-0.46342
H	-8.16768	1.18821	0.08601
H	-8.59237	2.79780	-0.50886
H	-6.96249	2.46381	0.10256
C	-7.37416	-1.65683	1.83105
C	-8.57437	-1.07252	2.56140
H	-8.36409	-0.89558	3.61675
H	-9.40637	-1.77699	2.50796
H	-8.90030	-0.13308	2.11212
C	-6.88366	-2.89357	2.58125
H	-6.01830	-3.32440	2.08154
H	-7.67430	-3.64550	2.62421
H	-6.59637	-2.63893	3.60305
C	-7.79488	-2.04473	0.41767
H	-8.16695	-1.17984	-0.13293
H	-8.59098	-2.79053	0.45938
H	-6.95916	-2.45308	-0.14490
C	-6.18394	-0.70067	1.74442
C	-6.12808	0.42621	2.55707
H	-6.93889	0.60762	3.24143
C	-5.02653	1.28769	2.60872
C	-4.98791	2.35703	3.70223
C	-6.06517	3.39514	3.39364
H	-7.05995	2.94889	3.39082
H	-5.89983	3.85325	2.41766
H	-6.04685	4.18487	4.14754
C	-5.25345	1.72975	5.06822
H	-4.53630	0.93451	5.27764
H	-6.25496	1.30770	5.13992
H	-5.15424	2.49030	5.84537
C	-3.62132	3.02130	3.72331
H	-3.59507	3.78621	4.50195
H	-3.39226	3.48449	2.76701
H	-2.83650	2.29101	3.92013
N	-2.54555	-2.26665	0.74563
N	-1.32437	-2.29062	1.32201
N	-1.36608	0.00794	1.39371
N	-0.69122	1.18241	1.48513
N	0.68042	-1.16840	1.48957
N	1.35587	0.00607	1.40280
N	1.31476	2.30464	1.33156
N	2.54073	2.28062	0.76534
O	-4.04875	-1.23399	-1.83936
O	-5.26094	1.06383	-0.99019
O	-5.26435	-1.05130	0.95674
O	-4.06150	1.25050	1.80968
Y	3.49064	0.00718	0.01227
C	4.20420	-3.94271	-0.03173
H	4.83607	-3.08209	0.15881
H	4.73016	-4.63793	-0.68600
H	4.00947	-4.46209	0.90678
C	2.92369	-3.52384	-0.65139
C	1.93152	-4.36750	-1.18165
H	1.96158	-5.44242	-1.25705
C	0.91483	-3.55420	-1.59441

C	-0.37244	-3.91295	-2.23444
H	-1.20664	-3.69356	-1.57237
H	-0.36243	-4.97495	-2.47333
H	-0.53555	-3.34117	-3.14611
C	0.61725	-1.08454	-1.43281
C	-0.60682	1.09857	-1.43707
C	0.38912	3.92724	-2.23044
H	0.38116	4.98943	-2.46858
H	0.55927	3.35613	-3.14123
H	1.21808	3.70718	-1.56205
C	-0.90323	3.56825	-1.60088
C	-1.92337	4.38149	-1.19662
H	-1.95294	5.45639	-1.27247
C	-2.91976	3.53783	-0.67441
C	-4.20544	3.95674	-0.06561
H	-4.83918	3.09619	0.11903
H	-4.72541	4.65246	-0.72413
H	-4.01869	4.47560	0.87479
C	4.96225	-2.33994	3.73856
C	6.04043	-3.37986	3.43941
H	7.03577	-2.93489	3.44301
H	5.88155	-3.83943	2.46305
H	6.01571	-4.16830	4.19448
C	3.59483	-3.00272	3.75158
H	2.80942	-2.27130	3.94170
H	3.56252	-3.76615	4.53144
H	3.37177	-3.46748	2.79460
C	5.21917	-1.71013	5.10504
H	6.22044	-1.28851	5.18238
H	5.11435	-2.46902	5.88308
H	4.50114	-0.91402	5.30810
C	5.00950	-1.27252	2.64354
C	6.11339	-0.41384	2.59642
H	6.92022	-0.59622	3.28523
C	6.17576	0.71212	1.78289
C	7.36750	1.66592	1.87483
C	6.87630	2.90341	2.62334
H	6.01436	3.33659	2.11977
H	7.66849	3.65346	2.67041
H	6.58360	2.64893	3.64364
C	8.56340	1.07899	2.61015
H	8.34848	0.90274	3.66467
H	9.39722	1.78154	2.55996
H	8.88898	0.13870	2.16239
C	7.79505	2.05352	0.46342
H	8.16774	1.18812	-0.08595
H	8.59242	2.79774	0.50886
H	6.96256	2.46373	-0.10260
C	7.37415	-1.65684	-1.83105
C	8.57431	-1.07259	-2.56152
H	8.36397	-0.89574	-3.61687
H	9.40631	-1.77706	-2.50807
H	8.90027	-0.13312	-2.11234
C	6.88359	-2.89364	-2.58111
H	6.01827	-3.32443	-2.08131
H	7.67423	-3.64557	-2.62407

H	6.59623	-2.63907	-3.60291
C	7.79496	-2.04463	-0.41766
H	8.16707	-1.17969	0.13284
H	8.59105	-2.79043	-0.45937
H	6.95927	-2.45294	0.14500
C	6.18394	-0.70067	-1.74442
C	6.12807	0.42621	-2.55707
H	6.93888	0.60761	-3.24144
C	5.02653	1.28770	-2.60871
C	4.98790	2.35701	-3.70224
C	6.06513	3.39517	-3.39364
H	7.05993	2.94894	-3.39079
H	5.89976	3.85328	-2.41768
H	6.04681	4.18489	-4.14755
C	5.25350	1.72973	-5.06821
H	4.53637	0.93446	-5.27764
H	6.25501	1.30770	-5.13988
H	5.15428	2.49026	-5.84538
C	3.62130	3.02125	-3.72337
H	3.59505	3.78615	-4.50201
H	3.39220	3.48445	-2.76707
H	2.83651	2.29094	-3.92020
N	2.54557	-2.26664	-0.74567
N	1.32438	-2.29061	-1.32203
N	1.36608	0.00795	-1.39371
N	0.69121	1.18242	-1.48513
N	-0.68042	-1.16839	-1.48957
N	-1.35587	0.00608	-1.40280
N	-1.31476	2.30465	-1.33154
N	-2.54073	2.28062	-0.76531
O	4.04874	-1.23399	1.83937
O	5.26094	1.06382	0.99019
O	5.26435	-1.05130	-0.95673
O	4.06150	1.25050	-1.80967

3 high-spin state at the LC-ωPBE-D3/def2-TZVP level

Y	-3.46797	0.00024	-0.00028
C	-4.17124	-3.96234	0.03254
H	-4.80496	-3.10188	-0.15303
H	-4.69564	-4.66316	0.68207
H	-3.97477	-4.47526	-0.90921
C	-2.89239	-3.54342	0.65555
C	-1.89721	-4.38683	1.18158
H	-1.92324	-5.46226	1.25073
C	-0.88362	-3.57215	1.59866
C	0.40430	-3.92767	2.23895
H	1.23878	-3.68851	1.58443
H	0.40459	-4.99322	2.46143
H	0.55678	-3.36862	3.16043
C	-0.60081	-1.09812	1.46252
C	0.60028	1.09843	1.46249
C	-0.40536	3.92818	2.23785
H	-0.40590	4.99386	2.45976
H	-0.55835	3.36961	3.15952
H	-1.23942	3.68858	1.58295

C	0.88301	3.57249	1.59858
C	1.89704	4.38711	1.18243
H	1.92310	5.46254	1.25171
C	2.89255	3.54369	0.65711
C	4.17199	3.96260	0.03532
H	4.80562	3.10207	-0.15027
H	4.69606	4.66289	0.68570
H	3.97639	4.47615	-0.90626
C	-4.97046	-2.33163	-3.72332
C	-6.04699	-3.37093	-3.41601
H	-7.04157	-2.92425	-3.40708
H	-5.87795	-3.83415	-2.44308
H	-6.03181	-4.15678	-4.17403
C	-3.60418	-2.99609	-3.75029
H	-2.81911	-2.26503	-3.94329
H	-3.57917	-3.75635	-4.53351
H	-3.37471	-3.46516	-2.79708
C	-5.23925	-1.69900	-5.08617
H	-6.24134	-1.27779	-5.15457
H	-5.14067	-2.45635	-5.86651
H	-4.52331	-0.90218	-5.29373
C	-5.00649	-1.26730	-2.62492
C	-6.10542	-0.40269	-2.57060
H	-6.91639	-0.57907	-3.25606
C	-6.15874	0.72068	-1.75328
C	-7.34723	1.67929	-1.83508
C	-6.85477	2.91961	-2.57798
H	-5.98866	3.34606	-2.07588
H	-7.64418	3.67308	-2.61639
H	-6.56805	2.67053	-3.60131
C	-8.54814	1.10108	-2.56910
H	-8.33767	0.92938	-3.62527
H	-9.37885	1.80683	-2.51229
H	-8.87611	0.15991	-2.12497
C	-7.76759	2.05921	-0.41945
H	-8.14041	1.19130	0.12596
H	-8.56279	2.80620	-0.45659
H	-6.93122	2.46305	0.14545
C	-7.34497	-1.68151	1.83693
C	-8.54549	-1.10480	2.57274
H	-8.33376	-0.93314	3.62867
H	-9.37550	-1.81143	2.51688
H	-8.87509	-0.16387	2.12928
C	-6.85044	-2.92176	2.57856
H	-5.98446	-3.34704	2.07526
H	-7.63906	-3.67603	2.61746
H	-6.56280	-2.67297	3.60171
C	-7.76678	-2.06103	0.42161
H	-8.14122	-1.19315	-0.12274
H	-8.56120	-2.80882	0.45934
H	-6.93076	-2.46369	-0.14463
C	-6.15745	-0.72178	1.75409
C	-6.10464	0.40183	2.57112
H	-6.91535	0.57761	3.25703
C	-5.00672	1.26780	2.62421
C	-4.97137	2.33306	3.72173

C	-6.04843	3.37146	3.41326
H	-7.04277	2.92422	3.40473
H	-5.87956	3.83372	2.43983
H	-6.03372	4.15815	4.17042
C	-5.23999	1.70170	5.08518
H	-4.52364	0.90548	5.29366
H	-6.24186	1.28006	5.15397
H	-5.14189	2.45992	5.86474
C	-3.60545	2.99826	3.74822
H	-3.58086	3.75919	4.53080
H	-3.37620	3.46665	2.79462
H	-2.82002	2.26775	3.94185
N	-2.51881	-2.28564	0.75568
N	-1.29706	-2.30864	1.33185
N	-1.35867	-0.01729	1.43880
N	-0.70193	1.17075	1.51333
N	0.70140	-1.17044	1.51322
N	1.35813	0.01760	1.43863
N	1.29655	2.30897	1.33197
N	2.51877	2.28592	0.75677
O	-4.04256	-1.23707	-1.82425
O	-5.23825	1.06597	-0.96408
O	-5.23725	-1.06635	0.96426
O	-4.04321	1.23818	1.82301
Y	3.46797	0.00023	0.00028
C	4.17128	-3.96234	-0.03249
H	4.80500	-3.10187	0.15305
H	4.69567	-4.66316	-0.68202
H	3.97484	-4.47524	0.90928
C	2.89240	-3.54344	-0.65546
C	1.89722	-4.38687	-1.18145
H	1.92326	-5.46231	-1.25058
C	0.88361	-3.57221	-1.59853
C	-0.40431	-3.92775	-2.23880
H	-1.23878	-3.68858	-1.58426
H	-0.40460	-4.99331	-2.46124
H	-0.55681	-3.36872	-3.16028
C	0.60080	-1.09817	-1.46248
C	-0.60028	1.09838	-1.46254
C	0.40537	3.92810	-2.23800
H	0.40590	4.99377	-2.45994
H	0.55834	3.36950	-3.15966
H	1.23942	3.68851	-1.58310
C	-0.88301	3.57243	-1.59871
C	-1.89703	4.38707	-1.18257
H	-1.92308	5.46250	-1.25188
C	-2.89254	3.54367	-0.65722
C	-4.17197	3.96260	-0.03543
H	-4.80560	3.10209	0.15019
H	-4.69604	4.66289	-0.68581
H	-3.97635	4.47618	0.90614
C	4.97044	-2.33148	3.72342
C	6.04690	-3.37085	3.41612
H	7.04151	-2.92423	3.40711
H	5.87779	-3.83412	2.44321
H	6.03172	-4.15667	4.17417

C	3.60413	-2.99586	3.75049
H	2.81911	-2.26474	3.94349
H	3.57911	-3.75608	4.53375
H	3.37458	-3.46496	2.79732
C	5.23934	-1.69880	5.08622
H	6.24145	-1.27764	5.15456
H	5.14075	-2.45610	5.86661
H	4.52345	-0.90193	5.29378
C	5.00649	-1.26720	2.62497
C	6.10542	-0.40260	2.57061
H	6.91639	-0.57895	3.25608
C	6.15874	0.72074	1.75324
C	7.34723	1.67936	1.83502
C	6.85474	2.91972	2.57783
H	5.98865	3.34613	2.07569
H	7.64416	3.67319	2.61621
H	6.56800	2.67070	3.60117
C	8.54812	1.10120	2.56910
H	8.33762	0.92956	3.62528
H	9.37883	1.80694	2.51227
H	8.87610	0.15999	2.12503
C	7.76762	2.05919	0.41937
H	8.14045	1.19125	-0.12597
H	8.56282	2.80619	0.45648
H	6.93126	2.46300	-0.14557
C	7.34497	-1.68159	-1.83686
C	8.54554	-1.10485	-2.57255
H	8.33390	-0.93314	-3.62849
H	9.37554	-1.81150	-2.51666
H	8.87513	-0.16395	-2.12903
C	6.85047	-2.92180	-2.57859
H	5.98446	-3.34709	-2.07537
H	7.63909	-3.67608	-2.61746
H	6.56292	-2.67295	-3.60174
C	7.76666	-2.06117	-0.42153
H	8.14107	-1.19333	0.12290
H	8.56108	-2.80898	-0.45923
H	6.93059	-2.46385	0.14463
C	6.15745	-0.72184	-1.75406
C	6.10464	0.40174	-2.57112
H	6.91536	0.57749	-3.25703
C	5.00673	1.26770	-2.62425
C	4.97138	2.33292	-3.72182
C	6.04838	3.37138	-3.41334
H	7.04274	2.92417	-3.40476
H	5.87946	3.83366	-2.43994
H	6.03368	4.15803	-4.17054
C	5.24007	1.70151	-5.08523
H	4.52376	0.90526	-5.29371
H	6.24196	1.27991	-5.15396
H	5.14198	2.45970	-5.86482
C	3.60543	2.99806	-3.74838
H	3.58084	3.75896	-4.53100
H	3.37612	3.46649	-2.79482
H	2.82004	2.26751	-3.94202
N	2.51881	-2.28566	-0.75561

N	1.29706	-2.30869	-1.33177
N	1.35867	-0.01734	-1.43880
N	0.70193	1.17069	-1.51337
N	-0.70140	-1.17050	-1.51318
N	-1.35813	0.01755	-1.43863
N	-1.29655	2.30892	-1.33205
N	-2.51877	2.28589	-0.75685
O	4.04256	-1.23700	1.82430
O	5.23825	1.06600	0.96403
O	5.23724	-1.06639	-0.96422
O	4.04321	1.23812	-1.82306

4 low-spin state at the B3LYP/def2-TZVP level

Y	4.39317	14.40634	10.12623
C	1.55913	11.50025	10.38961
H	1.32959	12.55719	10.28397
H	0.70479	10.98334	10.82847
H	1.72443	11.09000	9.39093
C	2.76792	11.29633	11.23874
C	3.03902	10.18627	12.06485
H	2.39703	9.34026	12.24376
C	4.27827	10.39636	12.62162
C	5.03086	9.54665	13.58554
H	5.92855	9.12707	13.13325
H	4.38219	8.73739	13.91990
H	5.35821	10.11821	14.45467
C	5.92157	12.27009	12.30968
C	8.09132	13.52389	12.63706
C	8.50637	16.52237	13.45908
H	8.99600	17.42433	13.82543
H	7.81144	16.16469	14.21958
H	7.90864	16.76622	12.58176
C	9.54826	15.50555	13.14598
C	10.91614	15.64163	13.13385
H	11.46739	16.54026	13.35404
C	11.45008	14.37981	12.80077
C	12.89159	14.04202	12.62257
H	13.08493	13.00461	12.88199
H	13.50604	14.69423	13.24451
H	13.18951	14.19047	11.58225
C	2.95338	13.36699	7.31363
C	2.65409	14.62696	6.79120
H	2.14426	14.68581	5.83981
C	2.99876	15.81420	7.44048
C	1.55071	15.44320	11.53510
C	2.09855	16.51349	12.24520
H	1.44171	17.12797	12.84479
C	3.46204	16.81424	12.22355
N	3.77669	12.15991	11.28917
N	4.69814	11.60183	12.13235
N	5.89641	13.58402	12.03309
N	7.05303	14.25656	12.32635
N	6.95148	11.54223	12.65736
N	8.15867	12.18565	12.72723
N	9.30944	14.19532	12.83736

N	10.46907	13.49998	12.62931
O	3.53341	13.12221	8.40305
O	3.60089	15.92059	8.54053
O	2.17397	14.62971	10.80451
O	4.35645	16.20806	11.57875
Y	10.28049	11.00708	11.90094
C	9.18013	7.10078	11.63834
H	10.21112	7.42874	11.74086
H	9.15666	6.10172	11.20131
H	8.74461	7.04158	12.63823
C	8.39887	8.04570	10.78952
C	7.30098	7.72577	9.96461
H	6.88854	6.74697	9.78651
C	6.86354	8.90406	9.40771
C	5.75031	9.13120	8.44511
H	4.93905	9.69938	8.89842
H	5.37286	8.16489	8.11157
H	6.08071	9.70011	7.57542
C	7.66600	11.26373	9.71842
C	7.66730	13.76970	9.39158
C	10.05638	15.62805	8.56907
H	10.59291	16.50307	8.20307
H	10.09351	14.84784	7.80806
H	10.56654	15.23148	9.44594
C	8.65505	16.02222	8.88279
C	8.08897	17.27491	8.89528
H	8.59148	18.20165	8.67498
C	6.72925	17.10635	9.22843
C	5.71580	18.18566	9.40676
H	4.72185	17.83638	9.14015
H	5.97739	19.04693	8.79076
H	5.68973	18.51212	10.44874
C	10.10186	9.23996	14.71356
C	11.34269	9.61121	15.23564
H	11.64894	9.19942	16.18705
C	12.19819	10.50312	14.58568
C	12.59814	9.06607	10.48601
C	13.24994	10.07666	9.77623
H	14.10954	9.81596	9.17485
C	12.82868	11.40781	9.80076
N	8.64312	9.35090	10.73830
N	7.69871	9.87013	9.89569
N	8.81634	11.89883	9.99573
N	8.82077	13.23679	9.70267
N	6.52095	11.79183	9.37023
N	6.47470	13.15898	9.30076
N	7.63978	15.16030	9.19133
N	6.45784	15.81682	9.39972
O	9.59953	9.61950	13.62415
O	11.98858	11.07730	13.48550
O	11.58318	9.19805	11.21842
O	11.85751	11.87810	10.44793
H	13.15028	10.73178	15.08750
H	9.49979	8.54418	15.31730
H	13.00968	8.04996	10.39244
H	13.40434	12.11982	9.19023

H	2.65212	12.49741	6.71016
H	2.72063	16.75271	6.93805
H	0.46478	15.29158	11.62665
H	3.78934	17.66914	12.83439

4 high-spin state at the B3LYP/def2-TZVP level

Y	-3.47788	0.00001	-0.00000
C	-4.35949	3.95766	-0.45810
H	-5.09581	3.16338	-0.54830
H	-4.71325	4.84518	-0.98424
H	-4.26404	4.20883	0.60055
C	-3.04178	3.53040	-1.01026
C	-2.06944	4.35866	-1.60863
H	-2.14650	5.41631	-1.79660
C	-1.00235	3.55329	-1.92877
C	0.27774	3.91112	-2.60038
H	1.12776	3.79172	-1.93001
H	0.22131	4.94703	-2.93362
H	0.46993	3.27354	-3.46411
C	-0.63250	1.09494	-1.56246
C	0.63247	-1.09495	-1.56244
C	-0.27781	-3.91117	-2.60022
H	-0.22140	-4.94710	-2.93342
H	-0.47006	-3.27363	-3.46397
H	-1.12781	-3.79174	-1.92981
C	1.00231	-3.55332	-1.92870
C	2.06941	-4.35867	-1.60858
H	2.14647	-5.41633	-1.79654
C	3.04181	-3.53038	-1.01034
C	4.35958	-3.95762	-0.45831
H	5.09582	-3.16325	-0.54838
H	4.71342	-4.84500	-0.98464
H	4.26419	-4.20901	0.60029
C	-4.91434	1.59652	2.53483
C	-5.89960	0.64546	2.80797
H	-6.60042	0.84013	3.60764
C	-6.00795	-0.55321	2.10004
C	-6.00779	0.55320	-2.10022
C	-5.89947	-0.64553	-2.80805
H	-6.60026	-0.84023	-3.60774
C	-4.91427	-1.59662	-2.53479
N	-2.61096	2.27432	-0.97174
N	-1.36255	2.29594	-1.53140
N	-1.37212	-0.01412	-1.48707
N	-0.67684	-1.19565	-1.57972
N	0.67681	1.19564	-1.57975
N	1.37210	0.01411	-1.48707
N	1.36253	-2.29595	-1.53138
N	2.61096	-2.27431	-0.97178
O	-4.03058	1.52951	1.64174
O	-5.27010	-0.93636	1.15504
O	-5.26996	0.93640	-1.15522
O	-4.03054	-1.52959	-1.64168
Y	3.47786	-0.00000	-0.00001
C	4.35966	3.95757	0.45830

H	5.09592	3.16324	0.54860
H	4.71341	4.84506	0.98450
H	4.26436	4.20875	-0.60036
C	3.04185	3.53038	1.01029
C	2.06947	4.35869	1.60853
H	2.14656	5.41634	1.79650
C	1.00236	3.55335	1.92864
C	-0.27776	3.91122	2.60019
H	-1.12776	3.79182	1.92978
H	-0.22132	4.94715	2.93340
H	-0.47000	3.27367	3.46392
C	0.63248	1.09499	1.56242
C	-0.63249	-1.09490	1.56247
C	0.27779	-3.91107	2.60037
H	0.22138	-4.94700	2.93359
H	0.47001	-3.27351	3.46410
H	1.12779	-3.79165	1.92997
C	-1.00233	-3.55325	1.92881
C	-2.06941	-4.35862	1.60870
H	-2.14647	-5.41628	1.79667
C	-3.04179	-3.53037	1.01038
C	-4.35951	-3.95765	0.45827
H	-5.09578	-3.16330	0.54828
H	-4.71336	-4.84504	0.98458
H	-4.26405	-4.20905	-0.60033
C	4.91432	1.59642	-2.53489
C	5.89959	0.64535	-2.80800
H	6.60040	0.84000	-3.60768
C	6.00793	-0.55330	-2.10003
C	6.00777	0.55328	2.10019
C	5.89946	-0.64543	2.80806
H	6.60025	-0.84011	3.60775
C	4.91425	-1.59654	2.53484
N	2.61096	2.27433	0.97168
N	1.36255	2.29598	1.53133
N	1.37211	-0.01407	1.48706
N	0.67682	-1.19560	1.57976
N	-0.67682	1.19569	1.57970
N	-1.37211	0.01416	1.48706
N	-1.36254	-2.29590	1.53145
N	-2.61097	-2.27428	0.97184
O	4.03056	1.52945	-1.64180
O	5.27008	-0.93641	-1.15501
O	5.26994	0.93644	1.15517
O	4.03052	-1.52954	1.64172
H	6.81699	-1.23544	-2.40095
H	4.90858	2.49772	-3.16621
H	6.81679	1.23543	2.40120
H	4.90853	-2.49788	3.16608
H	-4.90859	2.49783	3.16611
H	-6.81701	-1.23534	2.40098
H	-6.81680	1.23535	-2.40126
H	-4.90854	-2.49798	-3.16601

4 low-spin state at the B3LYP-D3/def2-TZVP level

Y	4.41085	14.39622	10.13262
C	1.69695	11.44843	10.12760
H	1.43031	12.50138	10.10462
H	0.85153	10.86144	10.48754
H	1.91911	11.13546	9.10555
C	2.88185	11.22055	10.99906
C	3.19582	10.04822	11.71926
H	2.60365	9.15159	11.78539
C	4.40340	10.26968	12.33948
C	5.18835	9.37022	13.22499
H	6.11543	9.05706	12.74827
H	4.58552	8.49257	13.45558
H	5.46890	9.86740	14.15320
C	5.94798	12.24146	12.25012
C	8.09558	13.53552	12.56710
C	8.52939	16.59551	13.03891
H	9.02607	17.53442	13.28098
H	7.85560	16.32548	13.85166
H	7.90971	16.73199	12.15450
C	9.56382	15.55134	12.81741
C	10.93059	15.68073	12.73251
H	11.48767	16.59763	12.82156
C	11.45430	14.38714	12.52284
C	12.88188	14.01873	12.31868
H	13.07466	13.00850	12.66885
H	13.52707	14.72165	12.84639
H	13.12998	14.05930	11.25628
C	2.97583	13.47690	7.29854
C	2.63488	14.75746	6.85944
H	2.08828	14.85556	5.93228
C	2.99600	15.91894	7.54486
C	1.50768	15.36465	11.41746
C	2.01274	16.44236	12.14737
H	1.31932	17.05949	12.70085
C	3.37456	16.74017	12.22236
N	3.83550	12.12808	11.17336
N	4.76075	11.54313	11.99361
N	5.89370	13.56000	12.00539
N	7.04014	14.25293	12.28316
N	6.98325	11.53567	12.62340
N	8.17566	12.20211	12.69727
N	9.31642	14.21434	12.67534
N	10.46784	13.49862	12.49340
O	3.60506	13.18157	8.34613
O	3.63707	15.98593	8.62471
O	2.17013	14.54593	10.73017
O	4.31245	16.13172	11.64718
Y	10.26245	11.01706	11.89499
C	9.06562	7.19429	11.89990
H	10.11131	7.48829	11.92144
H	8.97798	6.16818	11.54181
H	8.68454	7.23280	12.92223
C	8.27655	8.10637	11.02767
C	7.10466	7.79233	10.30682
H	6.62404	6.83130	10.24044
C	6.69303	8.94899	9.68659

C	5.52159	9.17905	8.80107
H	4.78722	9.82608	9.27735
H	5.06233	8.21820	8.57152
H	5.81194	9.66956	7.87232
C	7.62836	11.27258	9.77717
C	7.67522	13.77967	9.46166
C	10.10797	15.68526	8.98872
H	10.67243	16.58436	8.74408
H	10.21075	14.96465	8.17781
H	10.53652	15.21928	9.87419
C	8.68655	16.05919	9.21027
C	8.11498	17.30751	9.29431
H	8.63015	18.24849	9.20406
C	6.73301	17.11415	9.50495
C	5.70009	18.16633	9.70850
H	4.72969	17.82958	9.35443
H	5.98843	19.07764	9.18393
H	5.60782	18.39881	10.77117
C	10.18303	9.31855	14.73155
C	11.46249	9.66407	15.17035
H	11.81999	9.24208	16.09887
C	12.28923	10.55436	14.48246
C	12.55225	8.98715	10.60923
C	13.23339	9.96356	9.87984
H	14.11469	9.67171	9.32653
C	12.81046	11.29187	9.80516
N	8.58591	9.38600	10.85355
N	7.61716	9.89506	10.03292
N	8.79713	11.88488	10.02311
N	8.82410	13.22437	9.74607
N	6.49961	11.81635	9.40373
N	6.48050	13.18227	9.33047
N	7.65263	15.17640	9.35375
N	6.45708	15.81555	9.53574
O	9.61337	9.71309	13.68252
O	12.02779	11.14022	13.40082
O	11.51175	9.15132	11.29616
O	11.81443	11.79963	10.38030
H	13.26725	10.77180	14.93620
H	9.61083	8.63205	15.37326
H	12.96317	7.96753	10.57406
H	13.40883	11.96462	9.17283
H	2.66538	12.63764	6.65840
H	2.69562	16.87450	7.09058
H	0.41920	15.21080	11.45242
H	3.65786	17.59456	12.85501

4 high-spin state at the B3LYP-D3/def2-TZVP level

Y	-3.44843	-0.00000	0.00001
C	-4.28074	3.93329	-0.17940
H	-5.02357	3.15897	-0.35029
H	-4.61481	4.87061	-0.62513
H	-4.19139	4.08090	0.89867
C	-2.96475	3.53817	-0.75140
C	-1.95164	4.39547	-1.23329

H	-1.99055	5.46919	-1.30105
C	-0.89970	3.59665	-1.61650
C	0.41156	3.97704	-2.20429
H	1.23059	3.74637	-1.52623
H	0.40432	5.04575	-2.41507
H	0.60846	3.43136	-3.12706
C	-0.60773	1.10838	-1.49271
C	0.60772	-1.10834	-1.49274
C	-0.41161	-3.97698	-2.20432
H	-0.40438	-5.04569	-2.41511
H	-0.60852	-3.43131	-3.12709
H	-1.23062	-3.74631	-1.52624
C	0.89967	-3.59661	-1.61655
C	1.95160	-4.39544	-1.23338
H	1.99050	-5.46916	-1.30114
C	2.96474	-3.53816	-0.75151
C	4.28074	-3.93331	-0.17955
H	5.02355	-3.15894	-0.35033
H	4.61485	-4.87056	-0.62540
H	4.19138	-4.08107	0.89850
C	-4.94819	1.49431	2.53576
C	-5.95881	0.54805	2.71467
H	-6.70499	0.72884	3.47529
C	-6.03095	-0.63722	1.98049
C	-6.03075	0.63720	-1.98071
C	-5.95860	-0.54811	-2.71483
H	-6.70473	-0.72891	-3.47550
C	-4.94805	-1.49441	-2.53577
N	-2.56997	2.27418	-0.84167
N	-1.30937	2.31562	-1.37206
N	-1.36861	0.01448	-1.45882
N	-0.70288	-1.18405	-1.53580
N	0.70287	1.18409	-1.53578
N	1.36860	-0.01444	-1.45883
N	1.30936	-2.31558	-1.37212
N	2.56998	-2.27416	-0.84177
O	-4.00737	1.44417	1.70345
O	-5.24470	-1.00767	1.07144
O	-5.24457	1.00768	-1.07161
O	-4.00730	-1.44427	-1.70339
Y	3.44843	-0.00000	-0.00001
C	4.28074	3.93330	0.17939
H	5.02357	3.15897	0.35029
H	4.61481	4.87061	0.62512
H	4.19138	4.08090	-0.89868
C	2.96475	3.53817	0.75140
C	1.95163	4.39547	1.23329
H	1.99055	5.46919	1.30105
C	0.89970	3.59665	1.61650
C	-0.41156	3.97704	2.20429
H	-1.23059	3.74636	1.52623
H	-0.40432	5.04575	2.41508
H	-0.60846	3.43136	3.12707
C	0.60773	1.10838	1.49271
C	-0.60772	-1.10834	1.49274
C	0.41161	-3.97699	2.20431

H	0.40438	-5.04570	2.41510
H	0.60853	-3.43131	3.12708
H	1.23062	-3.74631	1.52624
C	-0.89967	-3.59661	1.61655
C	-1.95160	-4.39544	1.23338
H	-1.99050	-5.46916	1.30113
C	-2.96474	-3.53816	0.75151
C	-4.28074	-3.93331	0.17955
H	-5.02355	-3.15894	0.35033
H	-4.61485	-4.87055	0.62540
H	-4.19138	-4.08107	-0.89850
C	4.94819	1.49432	-2.53576
C	5.95881	0.54806	-2.71467
H	6.70499	0.72884	-3.47529
C	6.03095	-0.63722	-1.98049
C	6.03075	0.63720	1.98071
C	5.95860	-0.54811	2.71482
H	6.70473	-0.72891	3.47549
C	4.94805	-1.49441	2.53577
N	2.56997	2.27418	0.84167
N	1.30937	2.31562	1.37206
N	1.36861	0.01448	1.45882
N	0.70288	-1.18405	1.53580
N	-0.70287	1.18409	1.53578
N	-1.36860	-0.01444	1.45883
N	-1.30936	-2.31558	1.37212
N	-2.56998	-2.27416	0.84177
O	4.00737	1.44417	-1.70345
O	5.24470	-1.00767	-1.07144
O	5.24457	1.00768	1.07161
O	4.00730	-1.44427	1.70339
H	6.85580	-1.32174	-2.22662
H	4.97443	2.37443	-3.19533
H	6.85557	1.32174	2.22695
H	4.97428	-2.37455	3.19531
H	-4.97443	2.37443	3.19533
H	-6.85580	-1.32174	2.22662
H	-6.85556	1.32174	-2.22695
H	-4.97427	-2.37455	-3.19531

4 low-spin state at the CAM-B3LYP/def2-TZVP level

Y	4.41480734	14.39369208	10.13327388
C	1.63546083	11.48508505	10.28842854
H	1.39610387	12.54155467	10.21351826
H	0.78292561	10.94444741	10.69818546
H	1.82381559	11.10959109	9.28196755
C	2.83107206	11.27118785	11.14653412
C	3.10903864	10.14000867	11.93478586
H	2.48231991	9.27562562	12.07200728
C	4.32936901	10.35630256	12.51554789
C	5.08693624	9.48851882	13.45343915
H	5.99377284	9.10320814	12.99179122
H	4.45017349	8.65776647	13.75218262
H	5.39772812	10.03539863	14.34220647
C	5.93406455	12.26290893	12.29838211

C	8.08511996	13.52643381	12.61993699
C	8.51491380	16.54298538	13.30271905
H	9.01016349	17.45633568	13.62735892
H	7.82730379	16.21574185	14.08096315
H	7.91169603	16.75056410	12.42125310
C	9.54914274	15.51483955	13.02014210
C	10.91042877	15.64993675	12.97747745
H	11.46650426	16.55543359	13.14958462
C	11.43339237	14.37713079	12.68656458
C	12.86624899	14.02666665	12.49767053
H	13.05543505	12.99786924	12.78878057
H	13.49271818	14.69526702	13.08721013
H	13.14464147	14.13748711	11.44901135
C	2.96787303	13.40227152	7.32606308
C	2.65919772	14.66333239	6.82535737
H	2.13604592	14.73642590	5.88359342
C	3.01917327	15.83378954	7.48610337
C	1.56258361	15.40579474	11.50043495
C	2.08625355	16.48219715	12.20984208
H	1.41682074	17.09777650	12.79197066
C	3.44534865	16.78073678	12.21135183
N	3.81675293	12.14413192	11.24473576
N	4.72859318	11.58062049	12.08017482
N	5.89418438	13.57009490	12.04577322
N	7.04502683	14.24944434	12.31629249
N	6.96330784	11.54608104	12.64987837
N	8.15605109	12.20133979	12.73517523
N	9.30511133	14.20051566	12.77307681
N	10.45250228	13.50112850	12.56955619
O	3.56250943	13.14775690	8.39858323
O	3.63550456	15.91752422	8.57366682
O	2.20426615	14.59559093	10.79227736
O	4.34618134	16.17180606	11.58976171
Y	10.25890342	11.01940960	11.89440873
C	9.12966436	7.15919349	11.73807829
H	10.16452084	7.47956105	11.81199784
H	9.08673977	6.15058885	11.32835026
H	8.71125608	7.13484494	12.74493559
C	8.34628750	8.08812801	10.88078590
C	7.22644758	7.76394117	10.09401575
H	6.79030287	6.78930029	9.95757851
C	6.80371910	8.92909470	9.51354562
C	5.67198947	9.15177079	8.57750684
H	4.88643124	9.74567488	9.04023668
H	5.26933049	8.18513239	8.28028158
H	5.98907978	9.69338878	7.68774790
C	7.65420526	11.27158351	9.72949666
C	7.67301899	13.76626408	9.40854489
C	10.06943023	15.64653377	8.72237483
H	10.61231381	16.53174386	8.39596042
H	10.12861474	14.88661376	7.94482168
H	10.55215392	15.22881977	9.60352713
C	8.66231951	16.02834870	9.00670505
C	8.09846496	17.27474856	9.04947580
H	8.60413848	18.20910820	8.87618549
C	6.73507142	17.09108707	9.34204065

C	5.71501009	18.15651291	9.53164724
H	4.73031664	17.80762084	9.23548430
H	5.98342726	19.03567201	8.94681790
H	5.66784172	18.44835945	10.58142351
C	10.12375525	9.27016690	14.70152602
C	11.36992232	9.63383983	15.20261206
H	11.69453520	9.21774279	16.14465191
C	12.20376453	10.53045204	14.54162538
C	12.56107300	9.05689116	10.52389025
C	13.23068448	10.04922111	9.81463747
H	14.09797482	9.77784346	9.23144726
C	12.80956543	11.37546709	9.81483814
N	8.61024095	9.37800644	10.78200328
N	7.66573847	9.88646762	9.94750716
N	8.80604744	11.89064337	9.98283688
N	8.81911933	13.22705305	9.71254415
N	6.51897940	11.80459423	9.37758723
N	6.49007744	13.16513529	9.29269894
N	7.64658807	15.15985178	9.25547646
N	6.46728598	15.80358929	9.45996362
O	9.60638633	9.65733393	13.62862884
O	11.96826891	11.10555145	13.45375152
O	11.53919004	9.20686507	11.23305661
O	11.83235392	11.85036870	10.43788503
H	13.16380684	10.76376201	15.02320584
H	9.52996144	8.57253062	15.30930155
H	12.96381753	8.03678480	10.45162914
H	13.39222223	12.08022218	9.20450473
H	2.66053910	12.53923947	6.71828216
H	2.74105773	16.78182112	7.00451086
H	0.47771283	15.24445199	11.57158066
H	3.76339969	17.63796423	12.82183081

4 high-spin state at the CAM-B3LYP/def2-TZVP level

Y	-3.46062562	0.00000424	-0.00000537
C	-4.33140721	3.92395268	-0.36327966
H	-5.06496865	3.13196715	-0.48084375
H	-4.68014060	4.82453843	-0.86760573
H	-4.24073365	4.14409065	0.70103009
C	-3.01364931	3.51172093	-0.91565117
C	-2.03314751	4.35355880	-1.47175336
H	-2.10057365	5.41760385	-1.62020026
C	-0.97488493	3.55396856	-1.80905282
C	0.31479110	3.92493221	-2.44607661
H	1.14904282	3.78357400	-1.76212509
H	0.26667775	4.96891328	-2.75035463
H	0.52053481	3.30953885	-3.32054458
C	-0.62455936	1.09220371	-1.52831197
C	0.62456183	-1.09214689	-1.52833850
C	-0.31483212	-3.92485678	-2.44612100
H	-0.26673853	-4.96884033	-2.75039393
H	-0.52058622	-3.30946471	-3.32058715
H	-1.14906802	-3.78348298	-1.76215357
C	0.97486261	-3.55390820	-1.80912593

C	2.03311507	-4.35351557	-1.47184082
H	2.10051752	-5.41756290	-1.62028248
C	3.01365265	-3.51169096	-0.91578071
C	4.33141529	-3.92395697	-0.36344669
H	5.06493937	-3.13191155	-0.48082444
H	4.68021441	-4.82442516	-0.86793907
H	4.24071180	-4.14432156	0.70081456
C	-4.91786291	1.57015259	2.52011035
C	-5.90872553	0.62665013	2.77341970
H	-6.62378714	0.81998264	3.55907388
C	-5.99757042	-0.56669725	2.06344316
C	-5.99738421	0.56665485	-2.06367607
C	-5.90855482	-0.62676187	-2.77353553
H	-6.62358505	-0.82013445	-3.55920852
C	-4.91774502	-1.57028670	-2.52009441
N	-2.59184177	2.26097022	-0.92019629
N	-1.34715264	2.29242036	-1.46572074
N	-1.36405195	-0.00798476	-1.47244923
N	-0.67804363	-1.18652064	-1.55236340
N	0.67804574	1.18657796	-1.55233952
N	1.36405487	0.00803991	-1.47245171
N	1.34715361	-2.29236627	-1.46579211
N	2.59186454	-2.26093261	-0.92031084
O	-4.02242991	1.49928539	1.64731139
O	-5.24224048	-0.94212019	1.13696599
O	-5.24208385	0.94213589	-1.13719693
O	-4.02235262	-1.49938724	-1.64725858
Y	3.46062983	0.00000460	0.00000574
C	4.33137431	3.92397147	0.36324656
H	5.06494907	3.13199598	0.48079235
H	4.68010781	4.82456245	0.86756321
H	4.24067110	4.14410797	-0.70106111
C	3.01363608	3.51172241	0.91565212
C	2.03313851	4.35354999	1.47177763
H	2.10055766	5.41759544	1.62022480
C	0.97488427	3.55395216	1.80908327
C	-0.31478997	3.92490363	2.44611770
H	-1.14904521	3.78354375	1.76217075
H	-0.26668176	4.96888324	2.75040131
H	-0.52052360	3.30950373	3.32058337
C	0.62456389	1.09219101	1.52832129
C	-0.62455716	-1.09215959	1.52833026
C	0.31483621	-3.92488511	2.44607701
H	0.26673809	-4.96886994	2.75034508
H	0.52060154	-3.30949906	3.32054483
H	1.14906754	-3.78351320	1.76210367
C	-0.97486138	-3.55392488	1.80909448
C	-2.03312341	-4.35352456	1.47181927
H	-2.10053308	-5.41757120	1.62026226
C	-3.01366375	-3.51169071	0.91577825
C	-4.33144446	-3.92394063	0.36347539
H	-5.06495598	-3.13188558	0.48086925
H	-4.68024403	-4.82440355	0.86797687
H	-4.24076802	-4.14430719	-0.70078763
C	4.91786757	1.57017404	-2.52009809
C	5.90873024	0.62667397	-2.77341545

H	6.62379111	0.82001262	-3.55906871
C	5.99757572	-0.56667857	-2.06344815
C	5.99739008	0.56663711	2.06368123
C	5.90856027	-0.62678465	2.77353165
H	6.62358991	-0.82016328	3.55920357
C	4.91775030	-1.57030708	2.52008285
N	2.59184378	2.26096571	0.92021151
N	1.34715528	2.29240897	1.46573846
N	1.36405732	-0.00799669	1.47244972
N	0.67804871	-1.18653330	1.55235338
N	-0.67804081	1.18656522	1.55235052
N	-1.36404952	0.00802785	1.47245211
N	-1.34715042	-2.29237788	1.46577519
N	-2.59186204	-2.26093776	0.92029654
O	4.02243449	1.49929953	-1.64729959
O	5.24224593	-0.94210939	-1.13697384
O	5.24208964	0.94212589	1.13720506
O	4.02235764	-1.49940035	1.64724766
H	6.80777355	-1.25360614	-2.34569237
H	4.91819314	2.47045057	-3.15104806
H	6.80754404	1.25357254	2.34603162
H	4.91808619	-2.47063679	3.15095748
H	-4.91819001	2.47042457	3.15106685
H	-6.80776847	-1.25362695	2.34568143
H	-6.80753838	1.25359236	-2.34602077
H	-4.91808234	-2.47061193	-3.15097547

4 low-spin state at the CAM-B3LYP-D3/def2-TZVP level

Y	4.43303612	14.38332539	10.13908874
C	1.72046462	11.44107475	10.14513782
H	1.46079262	12.49468491	10.10959833
H	0.87188650	10.86521523	10.51232910
H	1.94133231	11.11369851	9.12870676
C	2.90140464	11.21785879	11.01888698
C	3.20603484	10.05465936	11.75066424
H	2.61055260	9.16111585	11.82463851
C	4.40653535	10.28100403	12.36904606
C	5.18354695	9.39111300	13.26779065
H	6.11349459	9.07485620	12.80113828
H	4.57891754	8.51698960	13.50190311
H	5.45564567	9.89684929	14.19252249
C	5.94883759	12.24501893	12.27526845
C	8.08323450	13.53825531	12.58933276
C	8.51292140	16.58603670	13.08249786
H	9.00911407	17.52289729	13.32860476
H	7.84806389	16.30751653	13.89818098
H	7.88631616	16.72678610	12.20492333
C	9.54670016	15.54777744	12.84424199
C	10.90653546	15.68222704	12.75707142
H	11.46296539	16.59834145	12.85508785
C	11.42752835	14.39417845	12.53155894
C	12.85291214	14.02991019	12.32301833
H	13.04465528	13.01528261	12.65850475
H	13.49687222	14.72354789	12.86219640
H	13.10119216	14.08712065	11.26274043
C	3.00250359	13.45941256	7.31364832

C	2.67441260	14.73254385	6.85797194
H	2.13801847	14.82803479	5.92582521
C	3.03640958	15.88854410	7.54274471
C	1.54863833	15.34926983	11.44449557
C	2.04956461	16.42498203	12.17128977
H	1.36057686	17.03687899	12.73397828
C	3.40728262	16.72492430	12.22400424
N	3.85305120	12.11696872	11.18601725
N	4.76682692	11.54254745	12.01198811
N	5.88906776	13.55345487	12.03807596
N	7.03101523	14.24954790	12.30095783
N	6.98325301	11.54398407	12.64240675
N	8.16555215	12.21681648	12.72660838
N	9.30235738	14.21930770	12.68851645
N	10.44658364	13.51195261	12.49460104
O	3.61531552	13.17584335	8.36778967
O	3.66610298	15.95060225	8.62352669
O	2.21051937	14.54162776	10.75306331
O	4.33139926	16.12138563	11.63328765
Y	10.24016588	11.03017852	11.88870775
C	9.04771639	7.21074483	11.88261993
H	10.09024939	7.51192003	11.91760733
H	8.97237848	6.18770884	11.51623930
H	8.65412240	7.23952244	12.89915339
C	8.26436880	8.12184798	11.00848008
C	7.10486789	7.80423823	10.27636171
H	6.62859434	6.84186473	10.20229325
C	6.70094489	8.95714374	9.65790925
C	5.54187642	9.18516928	8.75903247
H	4.80344432	9.83323932	9.22517492
H	5.08654865	8.22458044	8.52575220
H	5.84406743	9.67269293	7.83385077
C	7.63075159	11.27482203	9.75240586
C	7.68353052	13.76999997	9.43921754
C	10.10788681	15.66606406	8.94545135
H	10.67075768	16.56386100	8.69721748
H	10.19903744	14.94927025	8.13132094
H	10.54355945	15.19590489	9.82394586
C	8.69183993	16.04223987	9.18362218
C	8.12814265	17.28707855	9.27017568
H	8.64303529	18.22708414	9.17138024
C	6.75227990	17.09412968	9.49621750
C	5.72400584	18.14641388	9.70428142
H	4.75006315	17.80611480	9.36595285
H	6.00432807	19.05175667	9.16736548
H	5.64695689	18.38808706	10.76481507
C	10.15521045	9.33114738	14.71535808
C	11.42174566	9.68404272	15.17090794
H	11.77230061	9.26850120	16.10373985
C	12.24247724	10.57400809	14.48485334
C	12.51803724	9.01536641	10.58137525
C	13.19896739	9.98714195	9.85452913
H	14.07301564	9.69645648	9.29125413
C	12.78008476	11.31303439	9.80265166
N	8.56739194	9.39551332	10.84143322
N	7.61337167	9.89981749	10.01518533

N	8.79360569	11.87731943	9.99036051
N	8.82555349	13.21440640	9.72786838
N	6.50650336	11.82020681	9.38516875
N	6.49802483	13.18054530	9.30142190
N	7.66372151	15.16633262	9.34016900
N	6.47897313	15.80345292	9.53404796
O	9.60359005	9.71860567	13.66047710
O	11.98180257	11.14887911	13.40317562
O	11.48803177	9.18470953	11.27336160
O	11.79576300	11.81142040	10.39418123
H	13.21624974	10.80246963	14.93996091
H	9.57613178	8.64305804	15.34748973
H	12.91905776	7.99310069	10.54002184
H	13.37184484	11.99456145	9.17517180
H	2.69523491	12.61362052	6.68228906
H	2.74741663	16.84594703	7.08731323
H	0.46277095	15.18563991	11.48533435
H	3.70130940	17.57829939	12.85145151

4 high-spin state at the CAM-B3LYP-D3/def2-TZVP level

Y	-3.43673224	0.00000118	-0.00000012
C	-4.27424783	3.91979835	-0.20627856
H	-5.01290972	3.13953265	-0.36283320
H	-4.61433288	4.84650884	-0.66681157
H	-4.18179692	4.08579689	0.86753229
C	-2.96028024	3.52249975	-0.77494359
C	-1.95667713	4.37703255	-1.27013959
H	-2.00043949	5.44941386	-1.35129466
C	-0.90988478	3.57873132	-1.64619592
C	0.39600861	3.95686318	-2.24212996
H	1.21628551	3.74358230	-1.56109422
H	0.38061984	5.02057013	-2.47162820
H	0.59482775	3.39682820	-3.15431139
C	-0.60822273	1.10117604	-1.49833592
C	0.60822076	-1.10113815	-1.49835860
C	-0.39604187	-3.95681186	-2.24216336
H	-0.38066459	-5.02051910	-2.47166020
H	-0.59486939	-3.39677584	-3.15434175
H	-1.21630692	-3.74352359	-1.56111736
C	0.90986392	-3.57869157	-1.64624928
C	1.95665342	-4.37700409	-1.27021349
H	2.00040251	-5.44938555	-1.35137311
C	2.96028001	-3.52248406	-0.77504260
C	4.27425572	-3.91980923	-0.20641579
H	5.01289561	-3.13950247	-0.36286426
H	4.61437366	-4.84645313	-0.66705994
H	4.18179636	-4.08594884	0.86737309
C	-4.91854875	1.50566263	2.53074447
C	-5.92063620	0.56203285	2.73441429
H	-6.65573749	0.74335574	3.50414814
C	-5.99452030	-0.62019069	2.00429591
C	-5.99437806	0.62016367	-2.00447258
C	-5.92048761	-0.56210064	-2.73452256
H	-6.65555397	-0.74344348	-3.50428517
C	-4.91843710	-1.50575004	-2.53075290

N	-2.56143786	2.26715002	-0.85157697
N	-1.31198807	2.30620085	-1.38587453
N	-1.36179434	0.01098989	-1.46248211
N	-0.69509207	-1.17835661	-1.53788398
N	0.69509040	1.17839541	-1.53786089
N	1.36179369	-0.01095311	-1.46248302
N	1.31198468	-2.30616614	-1.38592975
N	2.56144875	-2.26712827	-0.85165994
O	-3.99789523	1.44975596	1.68438694
O	-5.21856425	-0.98443901	1.09112878
O	-5.21845833	0.98444368	-1.09128611
O	-3.99782633	-1.44983066	-1.68435174
Y	3.43673374	0.00000076	-0.00000037
C	4.27424639	3.91980391	0.20628637
H	5.01291120	3.13954040	0.36283962
H	4.61432811	4.84651494	0.66682089
H	4.18179418	4.08580393	-0.86752440
C	2.96028039	3.52249962	0.77495065
C	1.95667422	4.37702946	1.27014593
H	2.00043354	5.44941085	1.35130067
C	0.90988308	3.57872652	1.64620016
C	-0.39601342	3.95685336	2.24213021
H	-1.21628693	3.74357074	1.56109136
H	-0.38062878	5.02055989	2.47162954
H	-0.59483330	3.39681674	3.15431022
C	0.60822396	1.10117273	1.49833732
C	-0.60821984	-1.10114119	1.49835607
C	0.39603816	-3.95682250	2.24215588
H	0.38065663	-5.02053006	2.47165202
H	0.59486866	-3.39678804	3.15433487
H	1.21630437	-3.74353685	1.56110996
C	-0.90986634	-3.57869622	1.64624239
C	-1.95665952	-4.37700610	1.27020922
H	-2.00041292	-5.44938730	1.35137098
C	-2.96028425	-3.52248228	0.77504150
C	-4.27426583	-3.91980017	0.20642279
H	-5.01290012	-3.13948913	0.36287506
H	-4.61438661	-4.84644151	0.66706981
H	-4.18181436	-4.08594118	-0.86736627
C	4.91855086	1.50566650	-2.53074388
C	5.92063811	0.56203717	-2.73441546
H	6.65573897	0.74336088	-3.50414947
C	5.99452242	-0.62018682	-2.00429828
C	5.99438065	0.62015870	2.00447317
C	5.92049025	-0.56210627	2.73452171
H	6.65555640	-0.74345005	3.50428424
C	4.91843994	-1.50575530	2.53075042
N	2.56143959	2.26714789	0.85158073
N	1.31198907	2.30619779	1.38587797
N	1.36179664	0.01098682	1.46248216
N	0.69509356	-1.17835986	1.53788002
N	-0.69508856	1.17839242	1.53786362
N	-1.36179141	-0.01095571	1.46248195
N	-1.31198449	-2.30616868	1.38592571
N	-2.56144819	-2.26712921	0.85165659
O	3.99789690	1.44975910	-1.68438610

O	5.21856615	-0.98443700	-1.09113158
O	5.21846047	0.98444069	1.09128740
O	3.99782839	-1.44983503	1.68434937
H	6.81210074	-1.30934098	-2.25743350
H	4.93315813	2.39135110	-3.18161735
H	6.81192812	1.30932004	2.25768801
H	4.93304179	-2.39147146	3.18158140
H	-4.93315705	2.39134607	3.18161925
H	-6.81209915	-1.30934451	2.25743006
H	-6.81192595	1.30932476	-2.25768651
H	-4.93303986	-2.39146501	-3.18158524

4 low-spin state at the PBE1PBE/def2-TZVP level

Y	4.41301200	14.39463016	10.13304808
C	1.61410831	11.50436150	10.33624817
H	1.39309273	12.56551481	10.24100066
H	0.75721007	10.98876373	10.77323179
H	1.77521940	11.10105705	9.33313354
C	2.81889710	11.28565995	11.17558367
C	3.10381239	10.15436302	11.96132134
H	2.47454285	9.29183591	12.11219369
C	4.33832179	10.36605715	12.52269527
C	5.10752047	9.50188446	13.44960357
H	6.00612145	9.10719766	12.97368267
H	4.47099307	8.67520630	13.76653248
H	5.44055644	10.05359354	14.33012535
C	5.94122644	12.26317474	12.27191240
C	8.09057974	13.51913968	12.59372403
C	8.49857249	16.52840681	13.29144614
H	8.98587192	17.44221781	13.63277933
H	7.79321758	16.19392514	14.05379291
H	7.91028022	16.74188919	12.39805868
C	9.53858454	15.50652675	13.02369500
C	10.90426306	15.64236296	13.00529683
H	11.45694695	16.54954363	13.19039842
C	11.43216907	14.37016597	12.72032313
C	12.86505184	14.01969823	12.55334823
H	13.04558685	12.98020335	12.81934309
H	13.48239599	14.67012856	13.17541080
H	13.16884165	14.16055966	11.51278573
C	2.98136979	13.37808473	7.33214227
C	2.66802635	14.63778700	6.82441855
H	2.14837361	14.70365480	5.87781253
C	3.01818884	15.81612100	7.48131189
C	1.57333279	15.41683095	11.50731187
C	2.10828902	16.48928611	12.21883788
H	1.44356718	17.10741165	12.80748540
C	3.47110559	16.78171719	12.21668350
N	3.81414240	12.15667247	11.25756423
N	4.73272174	11.58863620	12.07464502
N	5.90482650	13.57399176	12.00894793
N	7.05032506	14.24701981	12.29186339
N	6.96964771	11.54203521	12.62603523
N	8.16250885	12.18780688	12.69948762
N	9.30407853	14.19094719	12.76789362

N	10.44938945	13.49171809	12.58489979
O	3.57257519	13.12787184	8.40807836
O	3.62797256	15.91187007	8.57198943
O	2.20460269	14.60431071	10.79185767
O	4.36902808	16.17204859	11.59071206
Y	10.26080290	11.01829013	11.89495527
C	9.15791395	7.15023844	11.68992787
H	10.18717482	7.48992276	11.78562989
H	9.14049159	6.15091276	11.25159517
H	8.72805396	7.08643543	12.69292143
C	8.36548796	8.08485092	10.85186383
C	7.24171599	7.76670813	10.06809544
H	6.80830013	6.79081130	9.91818831
C	6.80776101	8.94187639	9.50724539
C	5.67275714	9.17647469	8.58297430
H	4.88358250	9.75851299	9.06068663
H	5.27324463	8.21207545	8.26780205
H	5.98225884	9.73989050	7.70129082
C	7.65116392	11.27802191	9.75649529
C	7.66428191	13.76746986	9.43547599
C	10.06517739	15.62484793	8.73350078
H	10.61249759	16.50337038	8.39049846
H	10.12652010	14.84622759	7.97153603
H	10.54577559	15.22255601	9.62622666
C	8.66073203	16.01501587	9.00350940
C	8.09538933	17.26562200	9.02188323
H	8.60420812	18.19779863	8.83521193
C	6.73008848	17.08669622	9.30878006
C	5.71011108	18.15228467	9.47611749
H	4.72062923	17.79072532	9.20374499
H	5.96825840	19.01491323	8.85944010
H	5.67523427	18.48053359	10.51817270
C	10.09628460	9.26860334	14.69518717
C	11.34337403	9.62787701	15.20366046
H	11.66000221	9.21094842	16.15042016
C	12.18861456	10.52062120	14.54706046
C	12.56494357	9.07245336	10.51510739
C	13.22429963	10.07273436	9.80284365
H	14.09056443	9.80689794	9.21178452
C	12.79608956	11.39915804	9.80789914
N	8.62304260	9.38204036	10.76921999
N	7.67095943	9.89416678	9.95347977
N	8.80437296	11.90193252	10.02029612
N	8.81468684	13.23056938	9.73770383
N	6.51265669	11.80816115	9.40190139
N	6.47549067	13.16407275	9.32893690
N	7.63913979	15.15429855	9.26138959
N	6.46104259	15.79639317	9.44545352
O	9.58437647	9.65518166	13.61895611
O	11.96666868	11.09638547	13.45627411
O	11.54737710	9.21208694	11.23315397
O	11.82062015	11.87088887	10.43695468
H	13.14769387	10.74811148	15.03963859
H	9.49640467	8.57346340	15.30509882
H	12.97669432	8.05353823	10.43446268
H	13.37462090	12.10685885	9.19185258

H	2.67977997	12.51111269	6.72184495
H	2.73514851	16.76043283	6.98897749
H	0.48493596	15.26385115	11.58614536
H	3.79308687	17.63744024	12.83241462

4 high-spin state at the PBE1PBE/def2-TZVP level

Y	-3.45009204	0.00000749	0.00000487
C	-4.32977559	3.92623210	-0.40370493
H	-5.05601115	3.12123314	-0.49668123
H	-4.68962189	4.80895473	-0.93513482
H	-4.24285840	4.18202520	0.65551373
C	-3.00939013	3.51356515	-0.94224158
C	-2.02401326	4.35234600	-1.49474344
H	-2.08905522	5.41714220	-1.65188045
C	-0.95963935	3.54816354	-1.81760558
C	0.33362010	3.90928122	-2.44594789
H	1.16486337	3.77103459	-1.75355964
H	0.29092578	4.95240542	-2.76052566
H	0.54656316	3.28391990	-3.31450773
C	-0.62096168	1.09157760	-1.52158133
C	0.62094185	-1.09155354	-1.52158136
C	-0.33369263	-3.90926128	-2.44588301
H	-0.29101961	-4.95239375	-2.76043650
H	-0.54666453	-3.28391861	-3.31444884
H	-1.16490833	-3.77098956	-1.75346669
C	0.95959514	-3.54814151	-1.81759966
C	2.02396711	-4.35233105	-1.49475366
H	2.08898663	-5.41713230	-1.65186577
C	3.00938512	-3.51354914	-0.94232592
C	4.32978569	-3.92623438	-0.40384129
H	5.05597494	-3.12117542	-0.49664157
H	4.68969836	-4.80883340	-0.93543365
H	4.24285495	-4.18224913	0.65532359
C	-4.89166078	1.57808400	2.51643977
C	-5.88632535	0.63572595	2.77167845
H	-6.59940233	0.83153298	3.56135905
C	-5.98265694	-0.55962025	2.06146479
C	-5.98247892	0.55959066	-2.06166025
C	-5.88618406	-0.63583734	-2.77173989
H	-6.59924125	-0.83168828	-3.56142763
C	-4.89157728	-1.57822366	-2.51637157
N	-2.58557284	2.25853434	-0.93575432
N	-1.33971848	2.28990359	-1.46679906
N	-1.36584323	-0.00800089	-1.46201230
N	-0.68578307	-1.18590027	-1.54563290
N	0.68576276	1.18592445	-1.54564787
N	1.36582404	0.00802481	-1.46202499
N	1.33969948	-2.28987983	-1.46682356
N	2.58558259	-2.25851224	-0.93583955
O	-3.99708228	1.50757438	1.64207654
O	-5.23357807	-0.94000260	1.13145524
O	-5.23341469	0.94003649	-1.13166390
O	-3.99702567	-1.50767885	-1.64198544
Y	3.45008453	0.00000719	-0.00000536
C	4.32983770	3.92620309	0.40378340

H	5.05605225	3.12118904	0.49679895
H	4.68967467	4.80891816	0.93523226
H	4.24298110	4.18199670	-0.65543995
C	3.00941455	3.51356362	0.94224792
C	2.02402094	4.35236256	1.49469285
H	2.08906941	5.41715935	1.65182304
C	0.95963511	3.54819146	1.81754532
C	-0.33363393	3.90932471	2.44585887
H	-1.16486464	3.77107558	1.75345616
H	-0.29093884	4.95245227	2.76042507
H	-0.54659755	3.28397510	3.31442214
C	0.62095433	1.09160063	1.52156346
C	-0.62094951	-1.09153012	1.52159876
C	0.33368080	-3.90921870	2.44596408
H	0.29100857	-4.95234750	2.76053014
H	0.54663613	-3.28386393	3.31452524
H	1.16490654	-3.77095089	1.75355890
C	-0.95959947	-3.54811347	1.81765686
C	-2.02396264	-4.35231294	1.49480778
H	-2.08897734	-5.41711299	1.65192983
C	-3.00936444	-3.51354836	0.94232514
C	-4.32973147	-3.92625885	0.40377691
H	-5.05593892	-3.12121257	0.49653945
H	-4.68965333	-4.80886273	0.93535489
H	-4.24274649	-4.18227641	-0.65538296
C	4.89165443	1.57803992	-2.51646605
C	5.88631721	0.63567586	-2.77168903
H	6.59939360	0.83146832	-3.56137371
C	5.98264900	-0.55965806	-2.06145419
C	5.98247173	0.55962817	2.06164740
C	5.88617719	-0.63578764	2.77174822
H	6.59923416	-0.83162394	3.56143971
C	4.89157218	-1.57818012	2.51639604
N	2.58557057	2.25854223	0.93572772
N	1.33971397	2.28992402	1.46676672
N	1.36583657	-0.00797867	1.46201464
N	0.68577574	-1.18587658	1.54565359
N	-0.68576973	1.18594847	1.54562645
N	-1.36583071	0.00804761	1.46202196
N	-1.33970471	-2.28985872	1.46685569
N	-2.58558579	-2.25850309	0.93586662
O	3.99707640	1.50754803	-1.64210044
O	5.23357073	-0.94002369	-1.13143745
O	5.23340777	0.94005716	1.13164414
O	3.99702056	-1.50765306	1.64200802
H	6.79709274	-1.24322720	-2.35040297
H	4.88997546	2.47851205	-3.15209920
H	6.79686832	1.24320881	2.35070129
H	4.88991841	-2.47871224	3.15194479
H	-4.88998074	2.47856706	3.15205728
H	-6.79710126	-1.24318383	2.35042530
H	-6.79687588	1.24316572	-2.35072633
H	-4.88992216	-2.47876675	-3.15190461

4 low-spin state at the PBE1PBE-D3/def2-TZVP level

Y	4.42528984	14.38766158	10.13720254
C	1.69664833	11.46498129	10.18508716
H	1.45417718	12.52446881	10.13576869
H	0.84355327	10.90916081	10.57734159
H	1.89180080	11.11519899	9.16823190
C	2.88751359	11.23492524	11.03870674
C	3.19880939	10.06942944	11.76373709
H	2.60019267	9.17676076	11.84809260
C	4.41422148	10.29024055	12.36358718
C	5.20359481	9.40035826	13.24597976
H	6.12116697	9.07156641	12.75697749
H	4.59610995	8.53156346	13.50050545
H	5.50672572	9.90952303	14.16172141
C	5.95644854	12.24584508	12.24280422
C	8.09101102	13.52861354	12.55793287
C	8.50518430	16.57030156	13.05716360
H	8.99539605	17.50669076	13.32457915
H	7.81516404	16.28434455	13.85202551
H	7.90062162	16.71956151	12.16195186
C	9.54287066	15.53638701	12.83823091
C	10.90806854	15.67056646	12.77475970
H	11.46304148	16.58845393	12.88338026
C	11.43184045	14.38222566	12.55833054
C	12.85726404	14.01651978	12.37332425
H	13.03831960	12.99117314	12.68893318
H	13.49351613	14.69558299	12.94310977
H	13.13111586	14.09906545	11.31850598
C	3.00359175	13.43937341	7.32089926
C	2.66779557	14.71128178	6.86038186
H	2.13023334	14.79980207	5.92582928
C	3.02498601	15.87503616	7.53905677
C	1.55235265	15.36704595	11.44472936
C	2.06370059	16.44199037	12.16969759
H	1.37851122	17.05968129	12.73465394
C	3.42561948	16.73348940	12.22232035
N	3.84934186	12.13273704	11.19322909
N	4.77041024	11.55177281	11.99849816
N	5.90120582	13.55892561	11.99759740
N	7.03945587	14.24620017	12.27238470
N	6.98889415	11.53927883	12.61304551
N	8.17241092	12.20042992	12.68706656
N	9.30535469	14.20625480	12.67710559
N	10.44690289	13.49782707	12.50578451
O	3.61897279	13.15989839	8.37522418
O	3.65381803	15.94861106	8.62010683
O	2.20508851	14.55325178	10.75106038
O	4.34797435	16.12504076	11.63281128
Y	10.24818699	11.02540560	11.89060358
C	9.08174916	7.20174395	11.84179142
H	10.12073360	7.52099367	11.89022077
H	9.02607664	6.18493574	11.44992614
H	8.68203470	7.19649049	12.85895513
C	8.28701748	8.11820216	10.98842442
C	7.12196217	7.80526134	10.26342412
H	6.64804759	6.84059407	10.17898590
C	6.70548306	8.96837044	9.66382455

C	5.53976209	9.20693233	8.78186832
H	4.79639558	9.83720768	9.27105798
H	5.09093724	8.24636349	8.52791457
H	5.82865281	9.72374683	7.86580821
C	7.62804522	11.28179716	9.78513944
C	7.67167853	13.77191427	9.47101755
C	10.09849873	15.65118259	8.97090510
H	10.66411121	16.54343010	8.70142851
H	10.19547105	14.90907696	8.17746181
H	10.53058032	15.20406491	9.86679562
C	8.68435181	16.03312998	9.19002125
C	8.11783311	17.28251529	9.25291609
H	8.63501349	18.22210787	9.14337486
C	6.74034668	17.09194058	9.47006355
C	5.71092823	18.14364914	9.65458633
H	4.73357913	17.78978582	9.33308104
H	5.98428728	19.03620981	9.08965406
H	5.64055194	18.41768146	10.71022044
C	10.13604804	9.32284675	14.70887698
C	11.40485162	9.66930307	15.17015841
H	11.74915619	9.25030454	16.10615824
C	12.23534663	10.55812457	14.48987931
C	12.53140558	9.02756918	10.57929759
C	13.20525328	10.00783601	9.85295747
H	14.08150000	9.72325787	9.28603279
C	12.77705564	11.33321129	9.80205851
N	8.58369171	9.40008478	10.83403378
N	7.62000342	9.90751205	10.02893526
N	8.79261210	11.89058273	10.03125110
N	8.81880241	13.22007077	9.75693974
N	6.50003290	11.82268558	9.41467224
N	6.48085594	13.17826603	9.34105336
N	7.65132897	15.16242401	9.35213042
N	6.46704060	15.79673989	9.52357268
O	9.58757535	9.71328008	13.65287621
O	11.98602709	11.13677238	13.40704237
O	11.50177879	9.18605253	11.27515800
O	11.79034449	11.82758497	10.39404608
H	13.20868023	10.78048157	14.95551359
H	9.55193891	8.63601750	15.34274195
H	12.94207348	8.00645516	10.53107663
H	13.36644945	12.01757331	9.17043471
H	2.69937321	12.58994846	6.68794750
H	2.73041522	16.82909464	7.07360304
H	0.46264038	15.21236527	11.49204992
H	3.72276837	17.58697594	12.85315826

4 high-spin state at the PBE1PBE-D3/def2-TZVP level

Y	-3.43114394	0.00000867	-0.00001023
C	-4.27722217	3.91976496	-0.24208350
H	-5.00866556	3.12639981	-0.38160442
H	-4.62573644	4.83301344	-0.72694226
H	-4.19166867	4.11545184	0.82982632
C	-2.95900801	3.52321210	-0.79409009
C	-1.94979898	4.37600840	-1.28099326

H	-1.99140404	5.44977312	-1.36826239
C	-0.89556338	3.57350613	-1.64165461
C	0.41550074	3.94363716	-2.22309749
H	1.22874105	3.73796483	-1.52678557
H	0.40352683	5.00638634	-2.46570294
H	0.62905351	3.37057070	-3.12645209
C	-0.60494985	1.10026385	-1.48510090
C	0.60496626	-1.10023161	-1.48511898
C	-0.41548010	-3.94359193	-2.22318581
H	-0.40350294	-5.00633723	-2.46580963
H	-0.62902108	-3.37050852	-3.12653260
H	-1.22873101	-3.73793199	-1.52688207
C	0.89557561	-3.57347152	-1.64171642
C	1.94980024	-4.37598370	-1.28104615
H	1.99140053	-5.44974783	-1.36832584
C	2.95900732	-3.52319726	-0.79412100
C	4.27720867	-3.91976952	-0.24209773
H	5.00864329	-3.12638154	-0.38152545
H	4.62575704	-4.83297259	-0.72701811
H	4.19161788	-4.11555064	0.82979182
C	-4.90383787	1.51719961	2.52099165
C	-5.91233622	0.57664099	2.72271021
H	-6.64982843	0.76318991	3.49178499
C	-5.98930039	-0.61042207	1.99648689
C	-5.98927060	0.61037411	-1.99655283
C	-5.91232103	-0.57672964	-2.72271013
H	-6.64982806	-0.76332091	-3.49176050
C	-4.90381126	-1.51727190	-2.52096896
N	-2.55741552	2.26318998	-0.86190170
N	-1.30542477	2.30318745	-1.37785835
N	-1.36366848	0.01052714	-1.44885811
N	-0.70257572	-1.17810597	-1.52547428
N	0.70259130	1.17813825	-1.52545415
N	1.36368357	-0.01049569	-1.44885536
N	1.30543937	-2.30315748	-1.37789677
N	2.55742996	-2.26317162	-0.86193893
O	-3.97863240	1.45813506	1.67910356
O	-5.21433283	-0.98293601	1.08525407
O	-5.21428290	0.98294116	-1.08535822
O	-3.97858822	-1.45816356	-1.67910397
Y	3.43114692	0.00000863	0.00001016
C	4.27719286	3.91977423	0.24203919
H	5.00864553	3.12641554	0.38154287
H	4.62571196	4.83302636	0.72688731
H	4.19161178	4.11545900	-0.82986848
C	2.95899580	3.52321266	0.79408059
C	1.94979442	4.37600352	1.28100923
H	1.99139625	5.44976825	1.36828039
C	0.89556728	3.57349569	1.64168282
C	-0.41548934	3.94362036	2.22314731
H	-1.22873986	3.73794846	1.52684645
H	-0.40351531	5.00636868	2.46575771
H	-0.62902748	3.37054859	3.12650240
C	0.60495480	1.10025479	1.48510748
C	-0.60496133	-1.10024063	1.48511214
C	0.41549187	-3.94360912	2.22313395

H	0.40351494	-5.00635542	2.46575227
H	0.62904812	-3.37053153	3.12648041
H	1.22873210	-3.73794840	1.52681871
C	-0.89557173	-3.57348201	1.64168727
C	-1.94980521	-4.37598842	1.28102983
H	-1.99140888	-5.44975248	1.36830750
C	-2.95902053	-3.52319623	0.79413191
C	-4.27724022	-3.91975928	0.24214604
H	-5.00866476	-3.12636420	0.38159161
H	-4.62578363	-4.83295802	0.72707844
H	-4.19167895	-4.11554348	-0.82974562
C	4.90383998	1.51721510	-2.52098182
C	5.91233891	0.57665830	-2.72270656
H	6.64983113	0.76321252	-3.49177995
C	5.98930298	-0.61040970	-1.99649152
C	5.98927319	0.61036161	1.99655727
C	5.91232383	-0.57674719	2.72270612
H	6.64983092	-0.76334381	3.49175505
C	4.90381355	-1.51728773	2.52095869
N	2.55741616	2.26318835	0.86190942
N	1.30542808	2.30317954	1.37787115
N	1.36367207	0.01051837	1.44885510
N	0.70258008	-1.17811462	1.52546526
N	-0.70258691	1.17812963	1.52546292
N	-1.36367998	-0.01050441	1.44885812
N	-1.30543616	-2.30316529	1.37788376
N	-2.55742955	-2.26317297	0.86193136
O	3.97863532	1.45814336	-1.67909441
O	5.21433559	-0.98292929	-1.08526120
O	5.21428557	0.98293434	1.08536522
O	3.97859124	-1.45817216	1.67909445
H	6.81210703	-1.29577064	-2.25494404
H	4.91923363	2.40443908	-3.17454123
H	6.81208089	1.29570895	2.25503376
H	4.91921470	-2.40454066	3.17447888
H	-4.91923164	2.40441977	3.17455672
H	-6.81210428	-1.29578517	2.25493444
H	-6.81207819	1.29572359	-2.25502432
H	-4.91921246	-2.40452097	-3.17449488

4 low-spin state at the LC-ωPBE/def2-TZVP level

Y	4.42243	14.38938	10.13616
C	1.65736	11.46233	10.28064
H	1.44924	12.52078	10.15306
H	0.79246	10.97161	10.72665
H	1.82569	11.02509	9.29568
C	2.85344	11.25618	11.13772
C	3.13272	10.12896	11.92908
H	2.50820	9.26141	12.06953
C	4.35053	10.35349	12.50574
C	5.11308	9.49743	13.44852
H	6.02205	9.11663	12.98637
H	4.48105	8.66477	13.75310
H	5.41935	10.05491	14.33262
C	5.94538	12.26018	12.28372

C	8.08191	13.52572	12.60113
C	8.49418	16.53184	13.29161
H	8.98291	17.44743	13.62086
H	7.81157	16.19216	14.06934
H	7.88948	16.73678	12.41003
C	9.53543	15.51431	13.00250
C	10.89321	15.65798	12.96029
H	11.44639	16.56682	13.13462
C	11.41855	14.38853	12.66472
C	12.85165	14.04537	12.47455
H	13.03539	13.00143	12.71194
H	13.47190	14.67842	13.10883
H	13.14074	14.21675	11.43690
C	2.98867	13.40642	7.31971
C	2.67515	14.66613	6.82088
H	2.15326	14.74216	5.87737
C	3.03247	15.83092	7.49055
C	1.57235	15.39615	11.50438
C	2.08887	16.46989	12.22075
H	1.41690	17.08364	12.80396
C	3.44808	16.76400	12.22554
N	3.83571	12.12857	11.23330
N	4.74253	11.57342	12.06451
N	5.89757	13.56400	12.03773
N	7.04176	14.24509	12.29817
N	6.97465	11.54706	12.63478
N	8.15730	12.20596	12.72506
N	9.30034	14.20359	12.75075
N	10.44162	13.51302	12.54579
O	3.58087	13.15085	8.39151
O	3.64603	15.90874	8.57851
O	2.21775	14.59077	10.79657
O	4.34835	16.15743	11.60396
Y	10.25073	11.02432	11.89185
C	9.10058	7.16562	11.74400
H	10.12172	7.51401	11.86977
H	9.10661	6.17130	11.29780
H	8.63955	7.09291	12.72980
C	8.32301	8.09896	10.88848
C	7.20627	7.77768	10.09822
H	6.76697	6.80316	9.95782
C	6.79121	8.94490	9.52261
C	5.66722	9.17761	8.58153
H	4.88364	9.77420	9.04512
H	5.26168	8.21401	8.27723
H	5.99550	9.72197	7.69716
C	7.64553	11.27921	9.74448
C	7.67317	13.76228	9.42712
C	10.06985	15.62181	8.73418
H	10.61831	16.50263	8.40416
H	10.11618	14.86056	7.95664
H	10.55033	15.20079	9.61549
C	8.66830	16.01512	9.02423
C	8.11388	17.26287	9.06617
H	8.62427	18.19626	8.89101
C	6.75205	17.08329	9.36280

C	5.73866	18.15308	9.55322
H	4.74249	17.79060	9.31618
H	5.97688	19.00666	8.91885
H	5.74300	18.48916	10.59086
C	10.11474	9.29018	14.70785
C	11.36137	9.64998	15.20835
H	11.68741	9.23638	16.15227
C	12.19138	10.54261	14.53968
C	12.54826	9.06018	10.52324
C	13.21845	10.04425	9.80537
H	14.08530	9.76927	9.22114
C	12.79305	11.36825	9.80066
N	8.58729	9.38589	10.79332
N	7.65226	9.89410	9.96331
N	8.79844	11.88985	9.99086
N	8.81621	13.22126	9.73028
N	6.51335	11.81398	9.39327
N	6.49259	13.16763	9.30321
N	7.65089	15.15636	9.27712
N	6.48228	15.79953	9.48244
O	9.59829	9.67462	13.63537
O	11.95274	11.11261	13.45140
O	11.52896	9.21640	11.23232
O	11.81822	11.84445	10.42335
H	13.15508	10.77927	15.01531
H	9.51624	8.59625	15.31777
H	12.94825	8.03700	10.45955
H	13.37106	12.07333	9.18381
H	2.68758	12.54147	6.70901
H	2.75434	16.78405	7.01607
H	0.48634	15.23051	11.56822
H	3.76916	17.61800	12.84145

4 high-spin state at the LC-ωPBE/def2-TZVP level

Y	-3.45355	0.00000	-0.00001
C	-4.31176	3.93083	-0.36224
H	-5.03089	3.11856	-0.41761
H	-4.68819	4.79012	-0.91699
H	-4.20395	4.22224	0.68330
C	-2.99595	3.51169	-0.91058
C	-2.01560	4.34895	-1.47084
H	-2.08018	5.41397	-1.62568
C	-0.96251	3.54392	-1.80053
C	0.32773	3.90192	-2.44109
H	1.15998	3.76030	-1.75405
H	0.28484	4.94374	-2.75456
H	0.52688	3.27608	-3.31001
C	-0.61855	1.08875	-1.50768
C	0.61855	-1.08872	-1.50769
C	-0.32775	-3.90187	-2.44114
H	-0.28487	-4.94369	-2.75460
H	-0.52690	-3.27604	-3.31006
H	-1.15999	-3.76024	-1.75409
C	0.96250	-3.54388	-1.80058
C	2.01558	-4.34892	-1.47090

H	2.08015	-5.41394	-1.62575
C	2.99594	-3.51168	-0.91063
C	4.31173	-3.93084	-0.36229
H	5.03086	-3.11856	-0.41756
H	4.68820	-4.79007	-0.91711
H	4.20390	-4.22236	0.68322
C	-4.90326	1.56432	2.52790
C	-5.89817	0.62629	2.78109
H	-6.61363	0.81928	3.56800
C	-5.98597	-0.56245	2.06551
C	-5.98590	0.56245	-2.06561
C	-5.89812	-0.62632	-2.78114
H	-6.61357	-0.81932	-3.56805
C	-4.90323	-1.56437	-2.52790
N	-2.57545	2.26373	-0.90787
N	-1.33893	2.29043	-1.44873
N	-1.36011	-0.00604	-1.45673
N	-0.68160	-1.18078	-1.53107
N	0.68160	1.18081	-1.53105
N	1.36011	0.00607	-1.45671
N	1.33893	-2.29040	-1.44877
N	2.57545	-2.26371	-0.90793
O	-4.00983	1.49215	1.65535
O	-5.23059	-0.93468	1.13971
O	-5.23053	0.93470	-1.13981
O	-4.00981	-1.49218	-1.65535
Y	3.45356	-0.00001	-0.00000
C	4.31178	3.93081	0.36230
H	5.03092	3.11854	0.41767
H	4.68821	4.79009	0.91707
H	4.20399	4.22224	-0.68324
C	2.99597	3.51167	0.91062
C	2.01561	4.34893	1.47088
H	2.08020	5.41394	1.62573
C	0.96252	3.54390	1.80056
C	-0.32772	3.90189	2.44112
H	-1.15996	3.76028	1.75407
H	-0.28483	4.94371	2.75460
H	-0.52688	3.27605	3.31003
C	0.61856	1.08873	1.50768
C	-0.61855	-1.08873	1.50767
C	0.32776	-3.90190	2.44105
H	0.28488	-4.94373	2.75451
H	0.52694	-3.27608	3.30997
H	1.15998	-3.76028	1.75398
C	-0.96250	-3.54390	1.80053
C	-2.01561	-4.34893	1.47088
H	-2.08020	-5.41394	1.62574
C	-2.99599	-3.51166	0.91068
C	-4.31184	-3.93079	0.36244
H	-5.03093	-3.11848	0.41776
H	-4.68829	-4.79000	0.91730
H	-4.20409	-4.22232	-0.68308
C	4.90326	1.56434	-2.52790
C	5.89817	0.62631	-2.78110
H	6.61363	0.81931	-3.56801

C	5.98597	-0.56243	-2.06554
C	5.98591	0.56242	2.06560
C	5.89813	-0.62636	2.78112
H	6.61358	-0.81937	3.56803
C	4.90324	-1.56440	2.52787
N	2.57546	2.26371	0.90789
N	1.33894	2.29041	1.44874
N	1.36012	-0.00605	1.45672
N	0.68160	-1.18080	1.53105
N	-0.68160	1.18080	1.53105
N	-1.36011	0.00606	1.45671
N	-1.33893	-2.29041	1.44874
N	-2.57546	-2.26370	0.90791
O	4.00984	1.49216	-1.65535
O	5.23059	-0.93468	-1.13973
O	5.23053	0.93468	1.13981
O	4.00982	-1.49221	1.65532
H	6.79761	-1.25206	-2.34218
H	4.89677	2.46472	-3.16109
H	6.79753	1.25205	2.34228
H	4.89676	-2.46480	3.16103
H	-4.89677	2.46469	3.16110
H	-6.79761	-1.25208	2.34214
H	-6.79752	1.25208	-2.34228
H	-4.89675	-2.46476	-3.16107

4 low-spin state at the LC-ωPBE-D3/def2-TZVP level

Y	-3.45504	-0.00174	0.00153
C	-4.28315	3.90790	-0.19308
H	-5.01082	3.10976	-0.30874
H	-4.64198	4.80698	-0.69312
H	-4.18018	4.12548	0.87059
C	-2.96854	3.50696	-0.75377
C	-1.96385	4.35979	-1.24575
H	-2.00600	5.43361	-1.33044
C	-0.91858	3.55850	-1.61104
C	0.39052	3.92873	-2.20124
H	1.20399	3.71790	-1.51036
H	0.37828	4.99080	-2.43981
H	0.59190	3.35823	-3.10661
C	-0.61311	1.09016	-1.44199
C	0.61172	-1.09322	-1.44271
C	-0.39303	-3.93177	-2.20072
H	-0.38117	-4.99390	-2.43906
H	-0.59537	-3.36144	-3.10597
H	-1.20573	-3.72070	-1.50899
C	0.91677	-3.56157	-1.61207
C	1.96238	-4.36297	-1.24798
H	2.00429	-5.43680	-1.33261
C	2.96778	-3.51023	-0.75730
C	4.28303	-3.91136	-0.19825
H	5.01041	-3.11296	-0.31383
H	4.64157	-4.80989	-0.69951
H	4.18112	-4.13002	0.86530
C	-4.93660	1.50554	2.52972

C	-5.95648	0.57901	2.71715
H	-6.70343	0.77028	3.47453
C	-6.02517	-0.60351	1.98914
C	-6.02501	0.60028	-1.98610
C	-5.95697	-0.58265	-2.71351
H	-6.70403	-0.77387	-3.47079
C	-4.93762	-1.50969	-2.52564
N	-2.56817	2.25456	-0.82539
N	-1.32461	2.29198	-1.34894
N	-1.36073	-0.00527	-1.40101
N	-0.68507	-1.17839	-1.48445
N	0.68364	1.17533	-1.48493
N	1.35937	0.00219	-1.40225
N	1.32328	-2.29508	-1.35058
N	2.56750	-2.25777	-0.82855
O	-4.00300	1.43635	1.70091
O	-5.23658	-0.97696	1.09271
O	-5.23622	0.97380	-1.08988
O	-4.00392	-1.44062	-1.69693
Y	3.45504	-0.00174	-0.00153
C	4.28315	3.90790	0.19308
H	5.01082	3.10976	0.30874
H	4.64198	4.80698	0.69312
H	4.18018	4.12548	-0.87059
C	2.96854	3.50696	0.75377
C	1.96385	4.35979	1.24575
H	2.00600	5.43361	1.33044
C	0.91858	3.55850	1.61104
C	-0.39052	3.92873	2.20124
H	-1.20399	3.71790	1.51036
H	-0.37828	4.99080	2.43981
H	-0.59191	3.35823	3.10661
C	0.61311	1.09016	1.44199
C	-0.61172	-1.09322	1.44271
C	0.39303	-3.93177	2.20072
H	0.38117	-4.99390	2.43906
H	0.59537	-3.36144	3.10597
H	1.20573	-3.72070	1.50899
C	-0.91677	-3.56157	1.61207
C	-1.96238	-4.36296	1.24798
H	-2.00429	-5.43680	1.33261
C	-2.96778	-3.51023	0.75730
C	-4.28303	-3.91136	0.19826
H	-5.01041	-3.11296	0.31383
H	-4.64157	-4.80989	0.69951
H	-4.18112	-4.13002	-0.86530
C	4.93660	1.50554	-2.52972
C	5.95648	0.57901	-2.71715
H	6.70343	0.77028	-3.47453
C	6.02517	-0.60351	-1.98914
C	6.02501	0.60028	1.98610
C	5.95697	-0.58265	2.71351
H	6.70403	-0.77387	3.47079
C	4.93762	-1.50969	2.52564
N	2.56817	2.25456	0.82539
N	1.32461	2.29198	1.34894

N	1.36073	-0.00527	1.40100
N	0.68507	-1.17839	1.48445
N	-0.68364	1.17533	1.48493
N	-1.35937	0.00219	1.40225
N	-1.32328	-2.29508	1.35058
N	-2.56750	-2.25777	0.82855
O	4.00300	1.43635	-1.70091
O	5.23658	-0.97696	-1.09271
O	5.23622	0.97380	1.08988
O	4.00392	-1.44062	1.69693
H	6.85239	-1.28806	-2.22886
H	4.94643	2.39231	-3.18158
H	6.85190	1.28511	2.22617
H	4.94801	-2.39681	3.17701
H	-4.94643	2.39231	3.18158
H	-6.85239	-1.28806	2.22886
H	-6.85190	1.28511	-2.22617
H	-4.94801	-2.39681	-3.17701

4 high-spin state at the LC-ωPBE-D3/def2-TZVP level

Y	-3.42874	-0.00013	0.00014
C	-4.25073	3.92420	-0.18530
H	-4.97944	3.12718	-0.30281
H	-4.60925	4.82582	-0.68098
H	-4.14557	4.13721	0.87911
C	-2.93815	3.52293	-0.75049
C	-1.93111	4.37514	-1.24020
H	-1.96921	5.44961	-1.31839
C	-0.88997	3.57188	-1.61237
C	0.41860	3.93784	-2.20650
H	1.23505	3.70539	-1.52639
H	0.41657	5.00383	-2.42706
H	0.60551	3.38090	-3.12348
C	-0.60043	1.09891	-1.47079
C	0.60010	-1.09878	-1.47087
C	-0.41926	-3.93766	-2.20648
H	-0.41744	-5.00371	-2.42672
H	-0.60604	-3.38096	-3.12365
H	-1.23567	-3.70481	-1.52647
C	0.88941	-3.57177	-1.61252
C	1.93050	-4.37513	-1.24049
H	1.96842	-5.44962	-1.31857
C	2.93778	-3.52302	-0.75109
C	4.25044	-3.92438	-0.18615
H	4.97908	-3.12728	-0.30350
H	4.60898	-4.82582	-0.68215
H	4.14541	-4.13773	0.87821
C	-4.92752	1.50687	2.51527
C	-5.94512	0.57713	2.69912
H	-6.69748	0.76798	3.45125
C	-6.00437	-0.60838	1.97523
C	-6.00325	0.60877	-1.97623
C	-5.94386	-0.57669	-2.70018
H	-6.69574	-0.76721	-3.45286
C	-4.92687	-1.50694	-2.51550

N	-2.54284	2.26976	-0.82876
N	-1.30008	2.30561	-1.35523
N	-1.35769	0.01533	-1.44382
N	-0.70081	-1.17162	-1.51137
N	0.70049	1.17176	-1.51117
N	1.35736	-0.01519	-1.44367
N	1.29971	-2.30551	-1.35553
N	2.54263	-2.26981	-0.82938
O	-3.98835	1.43852	1.69276
O	-5.20906	-0.98191	1.08469
O	-5.20854	0.98198	-1.08502
O	-3.98833	-1.43901	-1.69224
Y	3.42874	-0.00013	-0.00014
C	4.25072	3.92420	0.18529
H	4.97943	3.12718	0.30279
H	4.60924	4.82582	0.68097
H	4.14554	4.13721	-0.87912
C	2.93815	3.52293	0.75050
C	1.93112	4.37513	1.24022
H	1.96921	5.44961	1.31841
C	0.88998	3.57186	1.61240
C	-0.41858	3.93783	2.20654
H	-1.23504	3.70538	1.52644
H	-0.41655	5.00382	2.42710
H	-0.60549	3.38088	3.12351
C	0.60044	1.09890	1.47080
C	-0.60010	-1.09879	1.47086
C	0.41929	-3.93768	2.20640
H	0.41746	-5.00373	2.42664
H	0.60609	-3.38098	3.12356
H	1.23568	-3.70483	1.52636
C	-0.88940	-3.57178	1.61248
C	-1.93052	-4.37514	1.24048
H	-1.96844	-5.44962	1.31858
C	-2.93780	-3.52302	0.75112
C	-4.25049	-3.92436	0.18624
H	-4.97912	-3.12725	0.30362
H	-4.60902	-4.82579	0.68227
H	-4.14552	-4.13772	-0.87812
C	4.92753	1.50689	-2.51527
C	5.94512	0.57714	-2.69912
H	6.69748	0.76800	-3.45125
C	6.00437	-0.60837	-1.97524
C	6.00325	0.60876	1.97623
C	5.94386	-0.57671	2.70017
H	6.69575	-0.76724	3.45285
C	4.92687	-1.50696	2.51549
N	2.54285	2.26976	0.82877
N	1.30008	2.30560	1.35525
N	1.35770	0.01532	1.44382
N	0.70082	-1.17163	1.51135
N	-0.70048	1.17175	1.51118
N	-1.35736	-0.01520	1.44366
N	-1.29971	-2.30552	1.35551
N	-2.54263	-2.26981	0.82938
O	3.98835	1.43853	-1.69276

O	5.20907	-0.98190	-1.08470
O	5.20854	0.98197	1.08503
O	3.98833	-1.43903	1.69223
H	6.82979	-1.29575	-2.21293
H	4.94463	2.39558	-3.16429
H	6.82826	1.29642	2.21451
H	4.94391	-2.39569	3.16447
H	-4.94463	2.39556	3.16430
H	-6.82979	-1.29576	2.21291
H	-6.82826	1.29644	-2.21450
H	-4.94391	-2.39566	-3.16449

4 low-spin state at the M06/def2-TZVP level

Y	4.42972168	14.38451065	10.14218374
C	1.73823011	11.40303019	10.12802947
H	1.43415973	12.44874381	10.11969763
H	0.90706007	10.78087999	10.46248648
H	1.98134877	11.11816979	9.10070153
C	2.91500829	11.19537987	11.00229326
C	3.23649849	10.02535262	11.71120519
H	2.65309942	9.11994469	11.77114890
C	4.43202500	10.26025229	12.33627084
C	5.20939728	9.36700205	13.22292758
H	6.14839250	9.05645004	12.75875780
H	4.60967357	8.48349173	13.44348660
H	5.47835647	9.85889003	14.15859842
C	5.95237625	12.24389194	12.26139379
C	8.08349887	13.53396183	12.57715745
C	8.50512069	16.59813163	13.01626646
H	9.00221868	17.53903190	13.25422461
H	7.82725262	16.33605898	13.82944187
H	7.88169988	16.73750702	12.12962305
C	9.53491528	15.55811222	12.80050745
C	10.89404285	15.69872462	12.70960628
H	11.44555069	16.62256983	12.78750303
C	11.42126532	14.41038752	12.51698328
C	12.84485076	14.06140915	12.30673809
H	13.06369344	13.05980081	12.67408547
H	13.48746652	14.78594398	12.80868583
H	13.08082550	14.08450472	11.23922951
C	2.82484293	13.47929676	7.42412883
C	2.41737807	14.75408322	7.04064752
H	1.76011977	14.85260407	6.18699249
C	2.87559193	15.91169962	7.66569772
C	1.51895544	15.43938353	11.27183239
C	2.00936917	16.58549154	11.89376721
H	1.30295347	17.28028137	12.32818712
C	3.37017384	16.83777658	12.04485155
N	3.84867760	12.11447000	11.18655473
N	4.77093863	11.53799727	12.00484284
N	5.89045029	13.55582198	12.02089442
N	7.02902409	14.24756439	12.29449848
N	6.98625149	11.54180846	12.63450524
N	8.16966951	12.20827815	12.71084154
N	9.29900425	14.22102620	12.68221787

N	10.44828087	13.51385452	12.50491068
O	3.58054334	13.18397686	8.37466236
O	3.64239917	15.98065126	8.65015097
O	2.18802945	14.53258645	10.73150585
O	4.31737287	16.14432922	11.61596985
Y	10.24138178	11.02872995	11.89133596
C	9.00166569	7.20986862	11.90989458
H	10.05198569	7.49358838	11.95507097
H	8.91399647	6.18295376	11.55230093
H	8.59997851	7.24672327	12.92632829
C	8.23658181	8.12346985	11.03085158
C	7.06569851	7.81514351	10.31704978
H	6.57461673	6.85664339	10.25524289
C	6.67205789	8.96750889	9.69080788
C	5.51355147	9.19372629	8.79921010
H	4.77788855	9.86027113	9.25518118
H	5.04337571	8.23369742	8.58449648
H	5.81119282	9.66309841	7.86049633
C	7.62666471	11.27794232	9.77099951
C	7.67804903	13.76908941	9.45767974
C	10.11882602	15.66490554	9.00662424
H	10.68569884	16.56504302	8.76721890
H	10.22715421	14.94704135	8.19266814
H	10.55254075	15.19304940	9.89167182
C	8.70439344	16.03811864	9.22688353
C	8.14664522	17.28552377	9.31667914
H	8.67044593	18.22500855	9.23472594
C	6.76795201	17.09793187	9.51473452
C	5.75454191	18.15657625	9.72696413
H	4.77290887	17.83943953	9.37809265
H	6.05099066	19.06983818	9.20918774
H	5.67314286	18.38604179	10.79301583
C	10.26831415	9.18139551	14.60353864
C	11.57991557	9.45936078	14.97842384
H	11.99793956	8.93403822	15.82680980
C	12.35246493	10.43600957	14.35367729
C	12.60446136	9.03619837	10.74737709
C	13.34938661	10.03442399	10.12340414
H	14.30167964	9.77002233	9.68326372
C	12.88852566	11.34016092	9.97826474
N	8.56431694	9.39193270	10.84764856
N	7.60649009	9.90126374	10.02613634
N	8.79312461	11.88061377	10.01395954
N	8.82308996	13.21300149	9.74165880
N	6.50162535	11.82244073	9.39846036
N	6.48687025	13.18058668	9.32298244
N	7.66515097	15.16521865	9.35169162
N	6.47861276	15.80706175	9.53086744
O	9.62956948	9.69469141	13.65981182
O	12.02537619	11.14066141	13.37475706
O	11.48796102	9.16249499	11.29459040
O	11.81695015	11.81404528	10.41294792
H	13.35475135	10.61074231	14.78316659
H	9.73589987	8.43230839	15.21739690
H	13.04727154	8.02455419	10.74194646
H	13.54090231	12.02428460	9.40560156

H	2.44337518	12.64252317	6.81103699
H	2.53140381	16.86705215	7.23167659
H	0.42128375	15.31827443	11.27275226
H	3.63523865	17.74580389	12.61642590

4 high-spin state at the M06/def2-TZVP level

Y	-3.42586367	-0.00000474	0.00000463
C	-4.21883771	3.95016804	-0.15147215
H	-4.98098529	3.19127579	-0.32328368
H	-4.54184400	4.89983791	-0.58008757
H	-4.11846174	4.08546521	0.92899446
C	-2.92078428	3.54175042	-0.73501371
C	-1.90711700	4.39281296	-1.20933801
H	-1.93555878	5.46959393	-1.26812298
C	-0.87410774	3.58791161	-1.60910179
C	0.42203098	3.96567393	-2.21369508
H	1.25983392	3.72026462	-1.55824291
H	0.41928935	5.03835339	-2.40865587
H	0.59973426	3.43431690	-3.14996451
C	-0.60253941	1.10206260	-1.50065526
C	0.60253000	-1.10205170	-1.50066289
C	-0.42206774	-3.96565091	-2.21368895
H	-0.41933532	-5.03832942	-2.40865527
H	-0.59978217	-3.43428802	-3.14995310
H	-1.25986027	-3.72024011	-1.55822320
C	0.87408277	-3.58789915	-1.60911444
C	1.90709653	-4.39280720	-1.20937667
H	1.93553363	-5.46958785	-1.26817123
C	2.92076577	-3.54175273	-0.73504162
C	4.21881601	-3.95018182	-0.15150063
H	4.98096259	-3.19128276	-0.32328450
H	4.54182814	-4.89983930	-0.58013907
H	4.11843156	-4.08550982	0.92896119
C	-5.05497298	1.55596387	2.38068026
C	-6.10770914	0.65000725	2.47646321
H	-6.93645771	0.88693404	3.13030010
C	-6.10381218	-0.58214114	1.82653090
C	-6.10377672	0.58214378	-1.82656362
C	-6.10768126	-0.65001355	-2.47647908
H	-6.93642469	-0.88693780	-3.13032345
C	-5.05495971	-1.55598491	-2.38067001
N	-2.54755645	2.27785797	-0.84433021
N	-1.29734415	2.31266638	-1.38196462
N	-1.36437792	0.01579951	-1.46676187
N	-0.70452137	-1.17600245	-1.54620407
N	0.70451202	1.17601222	-1.54620282
N	1.36436924	-0.01578968	-1.46676729
N	1.29733102	-2.31265742	-1.38198134
N	2.54754917	-2.27785707	-0.84436020
O	-4.02304367	1.44055344	1.68557981
O	-5.22826766	-1.01940549	1.04891315
O	-5.22823715	1.01940777	-1.04893994
O	-4.02303687	-1.44057995	-1.68555934
Y	3.42586507	-0.00000471	-0.00000467
C	4.21884774	3.95016983	0.15149606

H	4.98099197	3.19127563	0.32331214
H	4.54185138	4.89983682	0.58011974
H	4.11848329	4.08547266	-0.92897069
C	2.92078730	3.54175176	0.73502205
C	1.90711688	4.39281422	1.20934020
H	1.93555898	5.46959504	1.26812832
C	0.87410264	3.58791271	1.60909062
C	-0.42204295	3.96567390	2.21366949
H	-1.25983872	3.72026435	1.55820755
H	-0.41930432	5.03835328	2.40863118
H	-0.59975643	3.43431606	3.14993678
C	0.60253840	1.10206403	1.50065010
C	-0.60253122	-1.10205031	1.50066942
C	0.42205047	-3.96565070	2.21372700
H	0.41931449	-5.03832959	2.40869090
H	0.59974829	-3.43428981	3.14999517
H	1.25985429	-3.72023871	1.55827700
C	-0.87408950	-3.58789792	1.60913008
C	-1.90709493	-4.39280621	1.20937120
H	-1.93553082	-5.46958716	1.26816046
C	-2.92076052	-3.54175182	0.73502862
C	-4.21880100	-3.95018088	0.15146619
H	-4.98095273	-3.19128533	0.32324451
H	-4.54181594	-4.89984276	0.58009282
H	-4.11840088	-4.08550051	-0.92899544
C	5.05497367	1.55596234	-2.38068153
C	6.10770930	0.65000503	-2.47646502
H	6.93645771	0.88693135	-3.13030222
C	6.10381249	-0.58214292	-1.82653178
C	6.10377778	0.58214538	1.82656358
C	6.10768210	-0.65001132	2.47648030
H	6.93642548	-0.88693513	3.13032481
C	5.05496077	-1.55598310	2.38067118
N	2.54755650	2.27785967	0.84432991
N	1.29734259	2.31266766	1.38195979
N	1.36437689	0.01580147	1.46676337
N	0.70452022	-1.17599998	1.54621227
N	-0.70451302	1.17601466	1.54619617
N	-1.36437029	-0.01578766	1.46676658
N	-1.29733291	-2.31265615	1.38198713
N	-2.54754882	-2.27785556	0.84435981
O	4.02304474	1.44055219	-1.68558078
O	5.22826796	-1.01940642	-1.04891376
O	5.22823807	1.01940850	1.04893974
O	4.02303820	-1.44057837	1.68556038
H	6.96188341	-1.24475380	-2.03644389
H	5.14139216	2.46861252	-2.99794341
H	6.96183805	1.24476392	2.03649497
H	5.14138487	-2.46864012	2.99792220
H	-5.14139093	2.46861420	2.99794220
H	-6.96188325	-1.24475183	2.03644322
H	-6.96183694	1.24476226	-2.03649562
H	-5.14138331	-2.46864219	-2.99792091

4 low-spin state at the ωB97XD/def2-TZVP level

Y	4.43165836	14.38528420	10.14088250
C	1.74895118	11.41528969	10.11082782
H	1.49837025	12.47208508	10.06156994
H	0.89349796	10.85115023	10.48299024
H	1.97239430	11.07085806	9.09944606
C	2.92652893	11.19238261	10.99239791
C	3.23857252	10.02332768	11.71056684
H	2.65375176	9.12093240	11.76905738
C	4.43398733	10.25687148	12.33903330
C	5.21613818	9.36278334	13.23246923
H	6.15769766	9.07178125	12.76899489
H	4.62262855	8.47382536	13.44194928
H	5.46707119	9.85719518	14.17044226
C	5.95439152	12.24058548	12.27784046
C	8.07948993	13.54297472	12.58828960
C	8.50355935	16.60260529	13.03020562
H	9.00086621	17.54648843	13.24962553
H	7.85056172	16.33775727	13.86123812
H	7.86586203	16.72123688	12.15533079
C	9.53928067	15.56166729	12.79966188
C	10.89913444	15.69953304	12.69875635
H	11.45360747	16.61945133	12.77659473
C	11.41987406	14.40933932	12.48894800
C	12.84519028	14.04249598	12.27104805
H	13.03677007	13.02496841	12.60289536
H	13.49376135	14.73358760	12.80976345
H	13.08558175	14.10429812	11.20814231
C	2.96958386	13.47800684	7.32719944
C	2.62024919	14.75616860	6.89425376
H	2.05505826	14.85705852	5.97888798
C	3.00577393	15.91133449	7.57270810
C	1.52558544	15.35516624	11.39636579
C	2.01651369	16.44678656	12.11106792
H	1.31687297	17.07393775	12.64466962
C	3.37689535	16.73813341	12.19802894
N	3.86750236	12.10191241	11.17624191
N	4.78013355	11.52723153	12.00006225
N	5.88341255	13.55029938	12.04610475
N	7.02176383	14.25249780	12.30798065
N	6.99039606	11.54366698	12.65427387
N	8.16927168	12.22233151	12.73625422
N	9.29869489	14.23008376	12.66797221
N	10.44040259	13.52236227	12.47420242
O	3.61882305	13.18539712	8.35697138
O	3.66747548	15.97066029	8.63455967
O	2.19704126	14.52938546	10.73608778
O	4.31464127	16.11709395	11.64785288
Y	10.24181787	11.02856934	11.89015102
C	9.01032520	7.22116110	11.91468458
H	10.05462052	7.52175055	11.95074896
H	8.93440123	6.19594707	11.55195850
H	8.61163343	7.25641156	12.93012995
C	8.22945839	8.13071461	11.03356768
C	7.06144641	7.81774384	10.31423964
H	6.57215082	6.86028910	10.25412500
C	6.66681634	8.97062214	9.68685731

C	5.50244314	9.20233574	8.79246245
H	4.78105576	9.87486975	9.25428269
H	5.02732403	8.24465986	8.58394397
H	5.80704248	9.66491375	7.85408694
C	7.62463986	11.27889082	9.75202776
C	7.69002193	13.77078511	9.44331036
C	10.12538681	15.66763757	8.98705733
H	10.69195054	16.56955368	8.75915450
H	10.21869203	14.96523156	8.15938390
H	10.55268648	15.18063035	9.86243086
C	8.70704679	16.04421333	9.22340234
C	8.14639910	17.29102140	9.32246262
H	8.66505874	18.23114727	9.23946631
C	6.76963045	17.09695712	9.53818125
C	5.73925779	18.14779318	9.75647645
H	4.76311536	17.80625530	9.42060844
H	6.01553372	19.05659811	9.22159260
H	5.66922769	18.38332605	10.81994761
C	10.18849527	9.30854802	14.70374344
C	11.47001091	9.64560799	15.13648062
H	11.84012711	9.20701218	16.05200859
C	12.27770854	10.55659308	14.45741095
C	12.53640430	8.99939901	10.63455576
C	13.23704455	9.97161235	9.92231425
H	14.13106607	9.68045029	9.38990574
C	12.80812067	11.29506840	9.83556225
N	8.54723341	9.40051172	10.85144795
N	7.59402722	9.90487003	10.02751082
N	8.79407210	11.87238406	9.98535249
N	8.83318550	13.20957634	9.72430993
N	6.50314679	11.82786591	9.37581396
N	6.50147163	13.18815143	9.29498869
N	7.67513052	15.17017672	9.36249266
N	6.49180091	15.80512142	9.55822263
O	9.61007480	9.72393231	13.67390905
O	11.99813377	11.15860661	13.39524389
O	11.48425631	9.16659119	11.29320813
O	11.80007416	11.79534754	10.38445284
H	13.25881898	10.77664557	14.90342958
H	9.62203410	8.60856733	15.33630128
H	12.94364069	7.97789118	10.60979836
H	13.41501215	11.97094946	9.21439087
H	2.64678394	12.63713340	6.69498503
H	2.70579503	16.87088985	7.12640339
H	0.43738451	15.19652885	11.42040054
H	3.65814553	17.60092135	12.82048241

4 high-spin state at the ωB97XD/def2-TZVP level

Y	-3.43795574	0.00001088	-0.00000431
C	-4.24504252	3.93056235	-0.16183627
H	-4.98291656	3.14564131	-0.30920861
H	-4.59191699	4.85413507	-0.62571480
H	-4.14234443	4.10355620	0.91102994
C	-2.93225394	3.53400563	-0.73870325
C	-1.92278719	4.38897731	-1.21966016

H	-1.95694236	5.46344457	-1.28386686
C	-0.88155135	3.58640438	-1.60659753
C	0.42917121	3.96289899	-2.19797035
H	1.24885306	3.71075315	-1.52718505
H	0.42999843	5.03476046	-2.39108549
H	0.61144097	3.42980421	-3.13091254
C	-0.60050548	1.10343856	-1.49474197
C	0.60051694	-1.10341730	-1.49475877
C	-0.42912684	-3.96286562	-2.19809729
H	-0.42994092	-5.03472177	-2.39124231
H	-0.61136220	-3.42974381	-3.13103065
H	-1.24883823	-3.71074325	-1.52733933
C	0.88156796	-3.58638109	-1.60665593
C	1.92277439	-4.38896277	-1.21965772
H	1.95692261	-5.46343055	-1.28385776
C	2.93222764	-3.53399878	-0.73866027
C	4.24497791	-3.93056837	-0.16171475
H	4.98287712	-3.14566815	-0.30907148
H	4.59185290	-4.85416522	-0.62554405
H	4.14222091	-4.10352237	0.91115225
C	-4.95772250	1.50373628	2.50826356
C	-5.97424588	0.56575855	2.68125157
H	-6.73384765	0.75584051	3.42584112
C	-6.02710397	-0.62705914	1.96176883
C	-6.02712746	0.62701222	-1.96175958
C	-5.97427699	-0.56582662	-2.68120632
H	-6.73390210	-0.75594441	-3.42576290
C	-4.95772788	-1.50377919	-2.50822948
N	-2.54343113	2.27501987	-0.83317146
N	-1.29545202	2.31388599	-1.36587510
N	-1.36350405	0.01847105	-1.46780338
N	-0.70455734	-1.17510512	-1.54282147
N	0.70456786	1.17512736	-1.54281365
N	1.36351480	-0.01844974	-1.46781279
N	1.29546254	-2.31386635	-1.36590016
N	2.54343019	-2.27500834	-0.83316795
O	-4.00604256	1.43856812	1.69732529
O	-5.22543882	-1.00367264	1.07606604
O	-5.22543276	1.00366631	-1.07610017
O	-4.00602034	-1.43857117	-1.69732747
Y	3.43795512	0.00000984	0.00000278
C	4.24503184	3.93055936	0.16181229
H	4.98290845	3.14563912	0.30917529
H	4.59191176	4.85413321	0.62568444
H	4.14231912	4.10355132	-0.91105275
C	2.93225139	3.53400225	0.73869771
C	1.92279013	4.38897304	1.21966683
H	1.95694594	5.46344024	1.28387442
C	0.88156070	3.58639898	1.60661969
C	-0.42915077	3.96289466	2.19801670
H	-1.24884529	3.71075373	1.52724555
H	-0.42997175	5.03475558	2.39113541
H	-0.61140586	3.42979738	3.13096037
C	0.60050874	1.10343292	1.49474471
C	-0.60051307	-1.10342228	1.49474407
C	0.42918058	-3.96287374	2.19796197

H	0.43000394	-5.03472880	2.39111181
H	0.61147666	-3.42974837	3.13088148
H	1.24884939	-3.71075588	1.52714841
C	-0.88155083	-3.58638721	1.60660342
C	-1.92278771	-4.38896339	1.21967565
H	-1.95694215	-5.46343023	1.28388953
C	-2.93225513	-3.53399602	0.73871200
C	-4.24504161	-3.93056069	0.16184586
H	-4.98292344	-3.14564882	0.30922912
H	-4.59190286	-4.85414377	0.62571301
H	-4.14234529	-4.10353725	-0.91102333
C	4.95772141	1.50374146	-2.50826221
C	5.97424556	0.56576514	-2.68125250
H	6.73384701	0.75584924	-3.42584189
C	6.02710444	-0.62705385	-1.96177228
C	6.02712630	0.62700355	1.96176075
C	5.97427578	-0.56583845	2.68120223
H	6.73390051	-0.75595915	3.42575842
C	4.95772709	-1.50379079	2.50822104
N	2.54343266	2.27501630	0.83317461
N	1.29545578	2.31388091	1.36588337
N	1.36350673	0.01846500	1.46779826
N	0.70456081	-1.17511175	1.54280562
N	-0.70456471	1.17512138	1.54281696
N	-1.36351210	-0.01845529	1.46780988
N	-1.29545875	-2.31387075	1.36588451
N	-2.54343415	-2.27500877	0.83317160
O	4.00604212	1.43857065	-1.69732370
O	5.22543969	-1.00366961	-1.07607021
O	5.22543202	1.00366117	1.07610254
O	4.00601980	-1.43857938	1.69731928
H	6.85269974	-1.31332842	-2.20104968
H	4.99012305	2.39239915	-3.15641254
H	6.85274028	1.31325824	2.20102990
H	4.99013400	-2.39246600	3.15634735
H	-4.99012506	2.39239277	3.15641561
H	-6.85269879	-1.31333481	2.20104450
H	-6.85274123	1.31326822	-2.20102580
H	-4.99013518	-2.39245251	-3.15635862