Supporting Information

Stabilizing an exotic dianionic tetrazine bridge in a Ln_2 metallocene

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1. Experimental Section

General Procedures and Materials: All operations were performed in a Mbraun glovebox under a N_2 atmosphere with rigorous exclusion of oxygen and water using both Schlenk and glovebox techniques, unless otherwise noted. Solvents were dried using a J. C. Meyer solvent system, degassed by free-pump-thaw method and stored over activated 4 Å molecular sieves prior to use. The water content of the solvents used was monitored using a Karl Fischer titration. The 1,2,4,5-tetrazine (tz) ligand was prepared according to the literature.[1] [Cp*$_2$Ln][(μ-Ph$_2$)BPh$_2$] and [Cp*$_2$Ln(C$_3$H$_5$)] (Ln = Gd^{III}, Y^{III}) starting materials were prepared according to the literature.[2] All reagents were purchased from TCI, Alfa Aesar, or Strem Chemicals and used without further purification. HCp* (99+%) was purchased from Alfa Aesar and was degassed/dried as previously described prior to use. Elemental Analysis was performed by Midwest Microlab. All sample manipulations took place inside the glovebox.

Synthesis of [(Cp*$_2$Y)$_2$(tz$^{\bullet-}$)(THF)$_2$][BPh$_4$] (1-Y): Complex **1-Y** was prepared by slightly modifying a previously published procedure.[3] In 5 mL THF, one equivalent of tz (0.125 mmol, 10 mg) was combined with one equivalent of KC$_8$ (0.125 mmol, 17 mg). After 5 h, the dark grey colour mixture was added dropwise to a solution of two equivalents of [(Cp*$_2$Y)[(μ-Ph$_2$)(BPh$_2$)] (0.25 mmol, 169 mg) in THF (5 mL). The colour of the resulting solution became dark red (almost black) upon stirring. The reaction solution was left to stir overnight and then was filtered. Upon slow diffusion with Et$_2$O, dark red crystals of **1-Y** were isolated after one week in 59% yield. Elemental Analysis: Calcd: C, 70.30 %; H, 7.81 %; N, 4.43%, Found: C, 70.58%; H, 8.13%; N, 4.19%.

Synthesis of [(Cp*$_2$Gd)$_2$(tz^{2-})(THF)$_2$]·2THF (2-Gd): To a solution of tz (0.125 mmol, 10 mg) in THF (5 mL), one equivalent of KC$_8$ (0.125 mmol, 17 mg) was added and the resulting mixture was left to stir for 5 h. In a separate vial one equivalent of KC$_8$ (0.125 mmol, 17 mg) was combined with two equivalents of [(Cp*$_2$Gd)(C$_3$H$_5$)] (0.25 mmol, 117 mg) and was left to stir for 5 minutes resulting in a very dark green mixture. The dark grey colour mixture of the tz and KC$_8$ was slowly added to the dark green mixture of the metal and KC$_8$ and the resulting dark green-yellow mixture was left to stir for 10 additional minutes. Upon filtration, a dark red-brown (almost black) solution was isolated. Upon slow diffusion with Et$_2$O at low temperature, violet crystals of **2-Gd** were isolated after 8 days in 30% yield. Prior to any analysis the sample was purified by washing with trifluorotoluene. Elemental Analysis: Calcd: C, 56.83%; H, 7.73%; N, 4.57%, Found: C, 56.59%; H, 7.36%; N, 4.74%.

Synthesis of [(Cp*$_2$Y)$_2$(tz^{2-})(THF)$_2$]·THF (2-Y): This complex was prepared in a similar manner as **2-Gd** by simply replacing [Cp*$_2$Gd][(μ-Ph$_2$)BPh$_2$] with [Cp*$_2$Y][(μ-Ph$_2$)BPh$_2$] (0.25 mmol, 100 mg) in **2-Y.** Yield = 31%. Elemental Analysis: Calcd: C, 63.96%; H, 8.70%; N, 5.14%, Found: C, 64.13%; H, 8.29%; N, 4.87%.

Infrared Spectroscopy: Fourier transform infrared (FTIR) spectra were recorded on a Nicolet Nexus 550 FT-IR spectrometer in the transmission window of 400-4000 cm^{-1}. All samples comprised suspensions of crushed polycrystalline solid in a thin layer of Parabar 10312 oil, which were prepared inside the glovebox. All spectra were corrected for the presence of the oil.

Diffuse reflectance and UV-Vis absorption spectroscopy: Diffuse reflectance (DR) and UV-visible absorption spectra were recorded on an Agilent Cary 5000 UV-Vis-NIR spectrophotometer. The DR spectra for **1-Y** and **2-Y** were collected on crushed polycrystalline solids using air-tight sample holders, in the 200-800 nm range. Samples were prepared inside the glovebox and after ensuring an airtight seal, they were transferred out of the glovebox and mounted onto the spectrometer's sample holder. The UV-vis spectrum of **1-Y** was collected in dichloromethane (DCM; degassed by freeze-pump-thaw method, dried by J. C. Meyer solvent system and stored over molecular sieves for several days prior to use) at ambient temperature in the range of 250-800 nm using an airtight cuvette. The sample was prepared inside the glovebox.

EPR spectroscopy: The X-band EPR spectrum of **1-Y** was recorded at ambient temperature using a Bruker EMX-200 spectrometer. The sample was prepared inside the glovebox where polycrystalline sample of **1-Y** was dissolved in THF solution (the solvent was degassed by freeze-pump-thaw method, dried by J. C. Meyer solvent system and stored over molecular sieves for several days prior to use). The sample was sealed with a septum, Teflon tape and a layer of Parafilm to minimize incursion of air and moisture. After ensuring an airtight seal, the sample was transferred out of the glovebox and mounted onto the spectrometer's sample holder.

Electrochemical analysis: Cyclic voltammetry (CV) was performed inside the glovebox using a Princeton Applied Research Versastat 3 potentiostat employing a glass cell, platinum auxiliary wires for the counter and pseudo-reference electrodes and a glassy carbon electrode as a working electrode. The measurements were carried out in DCM solutions (dried by J. C. Meyer solvent system and stored over molecular sieves for several days prior to use) containing 0.1 M tetrabutylammonium hexafluorophosphate (Sigma Aldrich) as supporting electrolyte with a scan rate of 100 mV/s. The experiments were referenced to the Fc/Fc^+ redox couple of ferrocene (Sigma Aldrich) at +0.48 V *vs.* SCE.

Single crystal X-ray diffraction: Suitable crystals of **1-Y**, **2-Gd** and **2-Y** for single-crystal X-ray diffraction (SCXRD) analysis were covered, inside the glovebox, in parabar oil and then mounted on a MiTeGen MicroLoop. Full data (Table S1) were collected on a Bruker KAPPA APEX-II CCD single-crystal diffractometer (graphite monochromated Mo-Kα radiation, λ = 0.71073 Å), at 213 K (**1-Y**) and 200 K (**2-Gd** and **2-Y**) temperatures. Absorption corrections were applied by using multi-scan of the SADABS[4] program. All structures were solved using direct methods with SHELXT[5] and refined by the full-matrix least-squares methods on F^2 with SHELXL-2018/3[6] in anisotropic approximation for all non-hydrogen atoms. All carbon-bound hydrogen atoms were generated geometrically and included in the refinement in the riding model approximation. The temperature factors of all H atoms were set to multiple of the equivalent isotropic temperature factors of the parent site (aromatic and methylene at 1.2 times; methyl at 1.5 times the factor). The crystal structure of **1-Y** contains an area of highly disordered solvent molecules (two diethyl ether) resulting in a smeared-out electron density. Attempts to model the disordered area with chemically and crystallographically reasonable geometry were unsuccessful. Therefore, the SQUEEZE[7] function of PLATON[8] was employed to remove the contribution of the electron density associated with those molecules from the intensity data. In structures **2-Gd** and **2-Y**, there is a positional disorder on the two crystallographically unique Cp* ligands and after careful refinement, the ratio was found to be 0.514(5):0.486(5) and 0.481(9):0.519(9) for **2-Gd**, 0.499(5):0.501(5) and 0.485(9):0.515(9) for **2-Y**. The disordered components were left to refine with free variables and soft restraints were used to handle the disordered groups (SIMU, SADI, ISOR, DFIX etc). All geometric/crystallographic calculations were carried out using PLATON[8] and WINGX[9]

packages while the molecular/packing graphics were prepared with DIAMOND[10] and MERCURY.[11]

Magnetic measurements: Magnetic susceptibility measurements were obtained using a Quantum Design SQUID magnetometer MPMS-XL7 for **1-Y** and MPMS3 for **2-Gd** operating between 1.8 and 300 K. Direct current (dc) measurements were performed on 56.9 mg for **1-Y** and 17.3 mg for **2-Gd** of crushed polycrystalline samples, which were sealed in a polyethylene membrane. All samples were prepared inside the glovebox and after ensuring an airtight seal, they were transferred outside the glovebox and mounted onto the SQUID's sample holder. Diamagnetic corrections were applied for the polyethylene membrane and the silicon grease that was used to restrain **2-Gd**. The samples were subjected to dc fields of 70 to -70 kOe.

Thermogravimetric analysis (TGA): The analysis was performed using a TA Instruments Discovery TGA 55, which was housed in a "chemical-free", nitrogen-filled (99.998%) MBraun Labmaster 130 glovebox. Analyte was placed in a platinum pan and was heated to 800 $^{\circ}$C with a ramp rate of 10 $^{\circ}$C min^{-1}, using nitrogen (99.999% purity, 60 sccm) as the purge gas.

2. Single-crystal X-ray data and molecular features

Table S1. Crystallographic data and refinement details for **1-Y**, **2-Gd** and **2-Y**.

Compound reference	1-Y	2-Gd	2-Y
Chemical formula	$C_{74}H_{98}BY_2N_4O_2$	$C_{50}H_{78}Gd_2N_4O_2 \cdot 2(C_4H_8O)$	$C_{50}H_{78}Y_2N_4O_2 \cdot 2(C_4H_8O)$
Formula mass	1264.19	1225.87	1089.19
Crystal system	Monoclinic	Monoclinic	Monoclinic
a/Å	15.2944(4)	14.3222(4)	14.2304(8)
b/Å	20.2938(6)	13.3614(3)	13.3587(8)
c/Å	25.5590(9)	14.9998(4)	15.0126(10)
α/°	90	90	90
β/°	96.449(2)	94.976(1)	95.235(4)
γ/°	90	90	90
Unit cell volume/Å^3	7882.8(4)	2859.61(13)	2842.0(3)
Temperature/K	213(2)	200(2)	200(2)
Space group	$I2/a$	$P2_1/n$	$P2_1/n$
No. of formula units/unit cell, Z	4	2	2
Radiation type	Mo Kα	Mo Kα	Mo Kα
Absorption coefficient, μ/mm^{-1}	1.505	2.345	2.078
No. of reflections measured	56747	64834	45212
No. of independent reflections	8623	6637	6636
Data / parameters / restraints	8623 / 385 / 6	6637 / 342 / 270	6636 / 509 / 480
R_{int}	0.0356	0.0643	0.0763
Final R_1 values (all data)	0.0465	0.0563	0.0718
Final $wR_2(F^2)$ values (all data)	0.0954	0.1233	0.1470
Final R_1 values ($I > 2\sigma(I)$)	0.0337	0.0460	0.0471
Final $wR_2(F^2)$ values ($I > 2\sigma(I)$)	0.0875	0.1112	0.1282
Goodness of fit on F^2	1.037	1.075	1.045
Largest diff. peak and hole (eÅ^{-3})	0.845 / -0.507	2.737 / -1.923	0.878 / -1.000
CCDC number	2358823	2358824	2358825

Table S2. Selected bond distances (Å) and angles (º) for **1-Y**, **2-Gd** and **2-Y**.

	Distance/angle		Distance/angle
1-Y			
Y-Y′	7.051(5)	Y−O	2.364(1)
Y−N1	2.437(2)	Y−N2′	2.462(2)
Y−Cp$_{cent}$*A	2.386(4)	Y−Cp$_{cent}$*B	2.390(5)
Y−tz$_{cent}$	3.525(4)	N1−N2′	1.395(2)
C1−N1	1.322(3)	C1−N2	1.317(3)
N1-C1-N2	126.83(2)	C1-N2-N1′	116.55(2)
N2′-N1-C1	116.61(2)	N2-Y-O	81.14(5)
O−Y−Cp$_{cent}$*A	101.96(4)	O−Y−Cp$_{cent}$*B	102.88(4)
N1−Y−Cp$_{cent}$*A	101.87(4)	N1−Y−Cp$_{cent}$*B	99.93(4)
N2′−Y−Cp$_{cent}$*A	111.16(4)	N2′−Y−Cp$_{cent}$*B	107.81(4)
Cp$_{cent}$*A−Y−Cp$_{cent}$*B	136.28(2)	N1−Y−N2′	33.08(6)
2-Gd			
Gd−Gd′	6.792(4)	Gd−O	2.475(3)
Gd−N1	2.354(4)	Gd−N2′	2.363(4)
Gd−Cp$_{cent}$*A	2.535(3)	Gd−Cp$_{cent}$*B	2.426(3)
Gd−tz$_{cent}$	3.396(3)	N1−N2′	1.481(6)
C1−N1	1.308(6)	C1−N2	1.317(7)
N1-C1-N2	129.64(5)	C1-N2-N1′	114.41(4)
N2′-N1-C1	115.96(4)	N2-Gd-O	81.02(1)
O−Gd−Cp$_{cent}$*A	102.63(9)	O−Gd−Cp$_{cent}$*B	102.97(1)
N1−Gd−Cp$_{cent}$*A	103.38(1)	N1−Gd−Cp$_{cent}$*B	101.79(1)
N2′−Gd−Cp$_{cent}$*A	117.29(1)	N2′−Gd−Cp$_{cent}$*B	108.74(1)
Cp$_{cent}$*A−Gd−Cp$_{cent}$*B	129.91(1)	N1−Gd−N2′	36.60(1)
2-Y			
Y-Y′	6.732(5)	Y−O	2.439(2)
Y−N1	2.326(3)	Y−N2′	2.320(3)
Y−Cp$_{cent}$*A	2.390(3)	Y−Cp$_{cent}$*B	2.413(3)
Y−tz$_{cent}$	3.366(3)	N1−N2′	1.481(4)
C1−N1	1.304(4)	C1−N2	1.322(5)
N1-C1-N2	129.76(3)	C1-N2-N1′	113.75(3)
N2′-N1-C1	116.48(3)	N2-Y-O	81.05(9)
O−Y−Cp$_{cent}$*A	103.04(6)	O−Y−Cp$_{cent}$*B	99.35(6)
N1−Y−Cp$_{cent}$*A	101.64(7)	N1−Y−Cp$_{cent}$*B	98.01(7)
N2′−Y−Cp$_{cent}$*A	109.35(7)	N2′−Y−Cp$_{cent}$*B	108.51(7)
Cp$_{cent}$*A−Y−Cp$_{cent}$*B	138.35(1)	N1−Y−N2′	37.17(9)

Cp$_{cent}$*A: C6-C10; Cp$_{cent}$*B: C16-C20
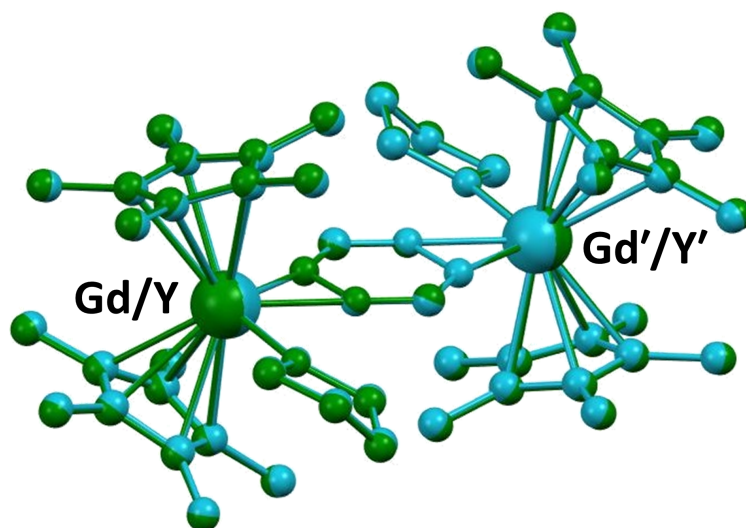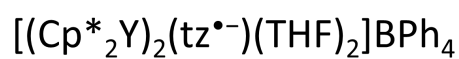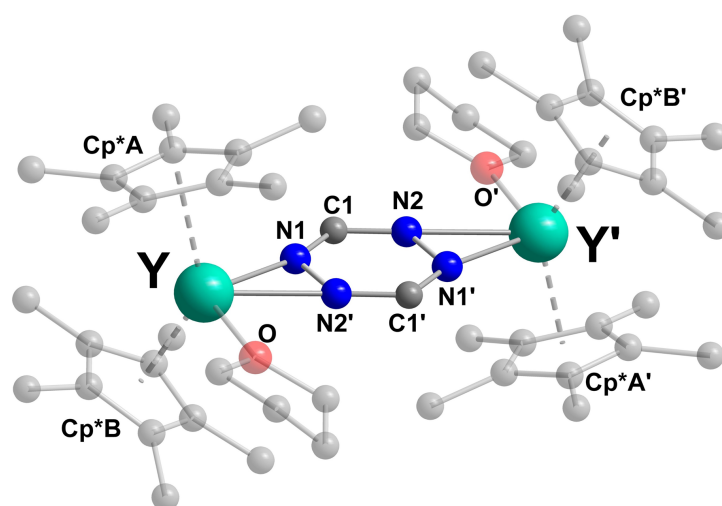
$[(Cp^*_2Y)_2(tz^{\bullet-})(THF)_2]BPh_4$

Figure S1: Molecular structures of **1-Y** (top), as well as structural overlay (bottom) of **1-Gd**[3] (green) and **1-Y** (blue), highlighting that both complexes are isostructural. For clarity reasons BPh_4^- moieties, and H-atoms have been omitted, while partial labeling and transparency have been employed.

$[(Cp*_2Gd)_2(tz^{2-})(THF)_2] \cdot 2THF$

$[(Cp*_2Y)_2(tz^{2-})(THF)_2] \cdot 2THF$
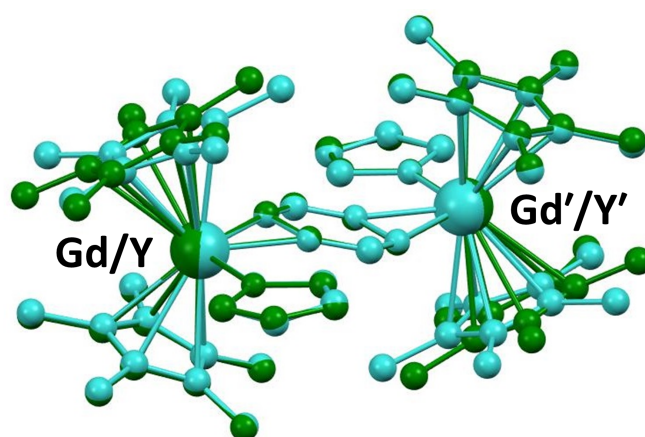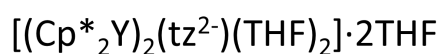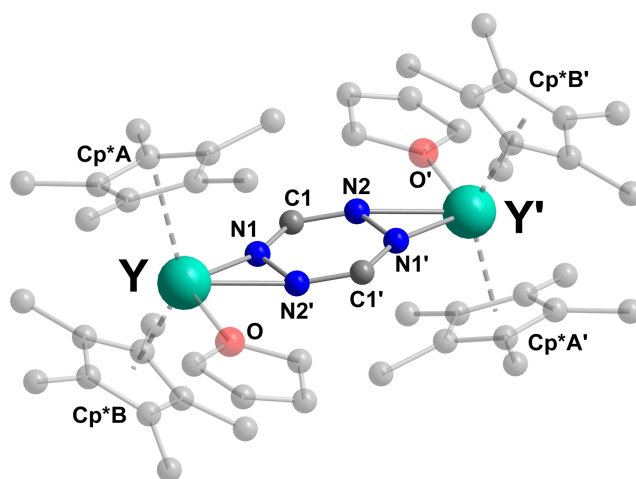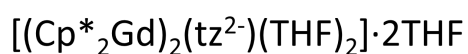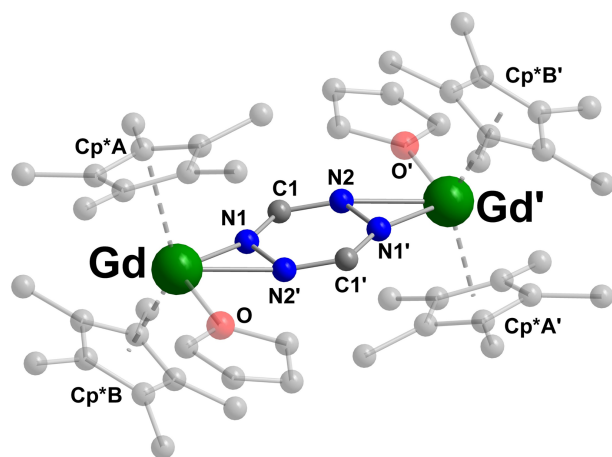
Figure S2: Molecular structures of **2-Gd** (top) and **2-Y** (middle), as well as structural overlay (bottom) of **2-Y** (green) and **2-Y** (blue), highlighting that both complexes are isostructural. For clarity reasons disorder conformers, THF lattice solvents and H-atoms have been omitted, while partial labeling and transparency have been employed.

3. Cyclic voltammetry and UV-Vis absorption spectroscopy
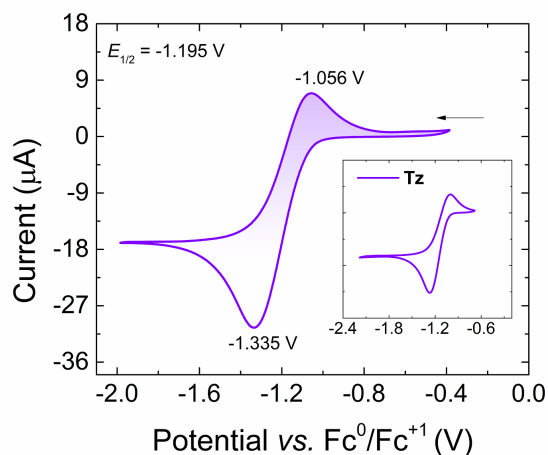
Figure S3: Cyclic voltammograms of tz measured in DCM at room temperature with [Bu$_4$N][PF$_6$] (0.1 M) as supporting electrolyte, using a scan rate of 0.1 V/s. Inset: Cyclic voltammogram of tz extended to more negative potential (-2.2 V).
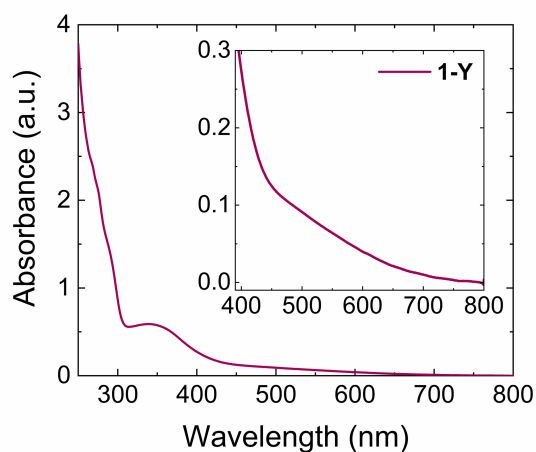
Figure S4: UV-Vis absorption spectrum of **1-Y** in DCM at room temperature. Inset: Zoomed-in area of the visible range of the spectrum highlighting the broad absorption band of the tz$^{\bullet-}$ between 450 and 700 nm.

4. IR Spectroscopy
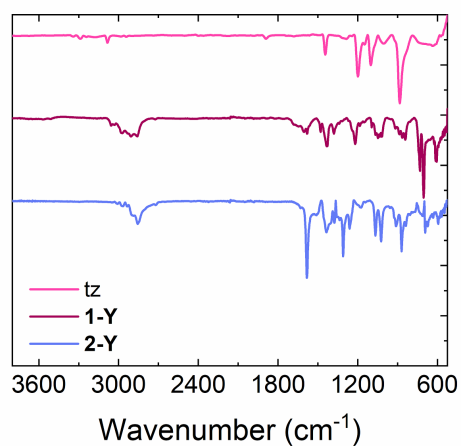
Figure S5: Comparison of the solid-state infrared (IR) spectra of the free tz ligand (pink), with complexes **1-Y** (purple) and **2-Y** (violet), in which the tz ligand is its radical and dianionic state, respectively.
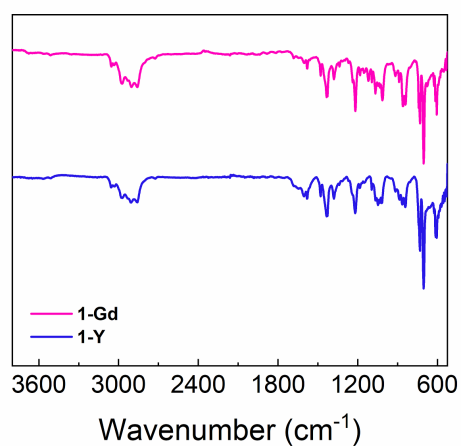
Figure S6: Solid-state infrared (IR) spectra of complexes **1-Gd**[3] (magenta) and **1-Y** (blue).
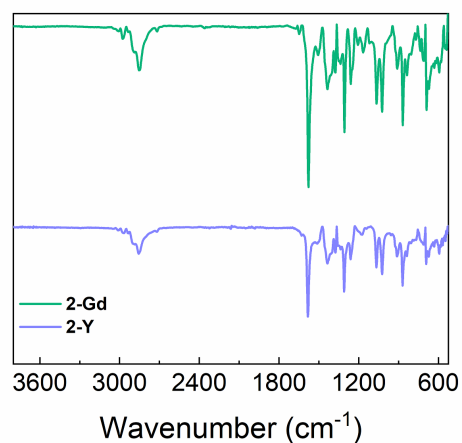
Figure S7: Solid-state infrared (IR) spectra of complexes **2-Gd** (green) and **2-Y** (violet).
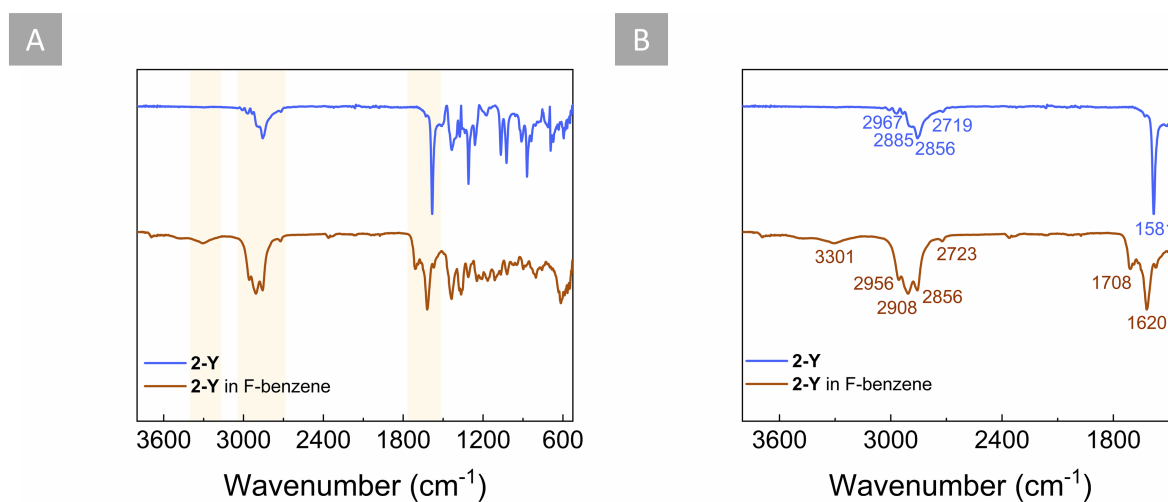
Figure S8: (A) Solid-state infrared (IR) spectra of complex **2-Y** (blue) and the obtained orange powder after dissolution of **2-Y** in F-benzene (orange). The major bands discussed in the main manuscript are highlighted with light-orange lines. (B) Zoomed-in area (3800-1450 cm^{-1}) of the IR spectra for **2-Y** (blue) and the obtained orange powder after dissolution of **2-Y** in F-benzene (orange), with the respective wavenumbers.

5. Thermogravimetric analysis
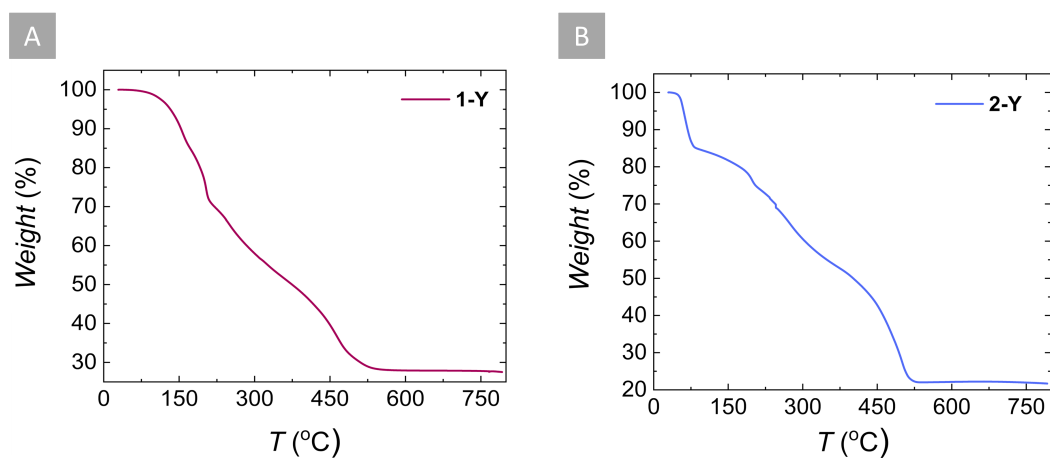
Figure S9: TGA curves of complexes **1-Y** (A) and **2-Y** (B).

6. Additional dc magnetic and EPR data
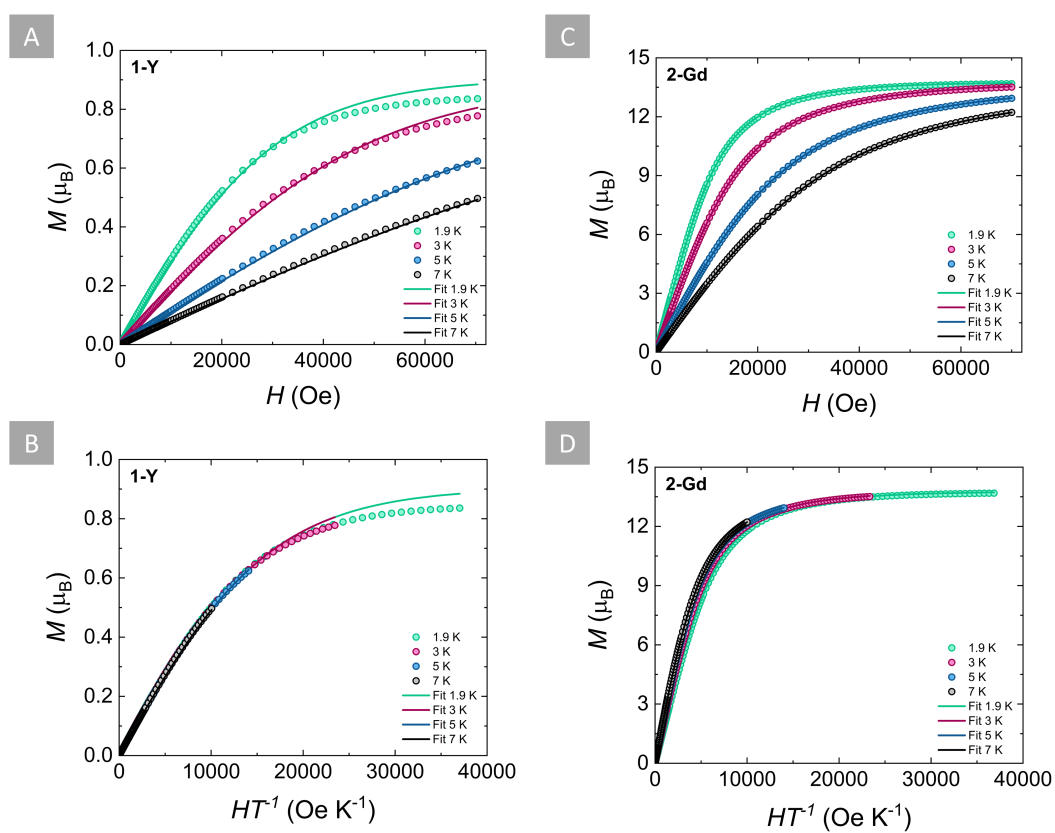
Figure S10: Field dependence of the magnetization (top) and the reduced magnetization (bottom) for **1-Y** and **2-Gd** at the indicated temperatures.

Table S3. Simulated isotropic hyperfine coupling constants for the selected nitrogen, hydrogen and yttrium atoms in **1-Y**.

Nucleus	mT	MHz
^{14}N	0.584	16.367
^{14}N	0.584	16.367
^{14}N	0.584	16.367
^{14}N	0.584	16.367
^{89}Y	0.105	2.943
^{89}Y	0.105	2.943
^{1}H	0.021	0.589
^{1}H	0.021	0.589

7. Computational details and discussion

All calculations were carried out using density functional theory (DFT) as implemented in the *Amsterdam Density Functional* (ADF) code[12] of the *Amsterdam Modelling Suite* (AMS) package version 2023.101.[13] Geometry optimizations utilized the pure GGA exchange-correlation (XC) functional PBE,[14] while single-point calculations utilized either the hybrid XC PBE0[14,15] or the range-separated hybrid XC CAM-B3LYP.[16] Dispersion effects were estimated with the empirical DFT-D3 correction[17] with the Becke–Johnson damping function.[18] Scalar relativistic effects were introduced using the zeroth-order regular approximation (ZORA) as implemented in ADF.[19] All calculations used the default ADF Slater-type orbital (STO) basis sets designed for ZORA calculations.[20] Valence triple-ζ basis sets with two sets of polarization functions (TZ2P) were used for all atoms. In the geometry optimizations the $1s$ orbitals of C, N and O atoms and all orbitals of Y up to $4p$ were treated as frozen cores, while in the single-point calculations all orbitals were optimized. The "NumericalQuality" keyword in ADF was set to "Good" in the geometry optimizations and to "VeryGood" in the single-point calculations.

The calculations were carried out on three systems: the hypothetical **[Y$_2$]$^{2+}$**, **[Y$_2$]$^+$** and **[Y$_2$]**, where the tetrazine ligand is diamagnetic neutral, a radical monoanion or a diamagnetic dianion, respectively. Two types of geometries were considered: crystal-structure geometries were only the positions of the hydrogen atoms were optimized and fully optimized structures with no constraints on the symmetry. Frequency calculations were carried out on the freely optimized structure to ensure that the stationary structures correspond to minima on the potential energy surface and to produce IR frequencies and absorption intensities. The initial structures of **[Y$_2$]$^+$** and **[Y$_2$]** were extracted from their respective crystal structures, while the initial structure of **[Y$_2$]$^{2+}$** was extracted from the crystal structure of **[Y$_2$]$^+$**.

Atomic charges were calculated using the quantum theory of atoms in molecules (QTAIM)[21] as it is implemented in ADF.[22] The fully optimized geometries and the PBE0 functional were used in the charge calculations. Nuclear-independent chemical shifts (NICS)[23] were calculated on both the optimized and crystal-structure geometries using the PBE0 functional. The shifts were calculated at the centroid of the tetrazine rings that also corresponds to the molecule inversion center. The calculations utilized the gauge-including atomic orbitals (GIAOs) as implemented in ADF.[24] The shifts were also calculated for the free ligands as well as some other systems used as a reference. The geometries of these systems were fully optimized at the same level as the complexes. The sign convention was chosen to correspond to that used in ref. [23]; namely, negative sign indicates aromaticity and positive sign anti-

aromacity. Time-dependent density functional theory (TD-DFT) calculations[25] were carried out on the crystal-structure geometries using the CAM-B3LYP functional and the Tamm–Dancoff approximation.[26] The 50 lowest singlet-singlet excitations were solved in the calculations.
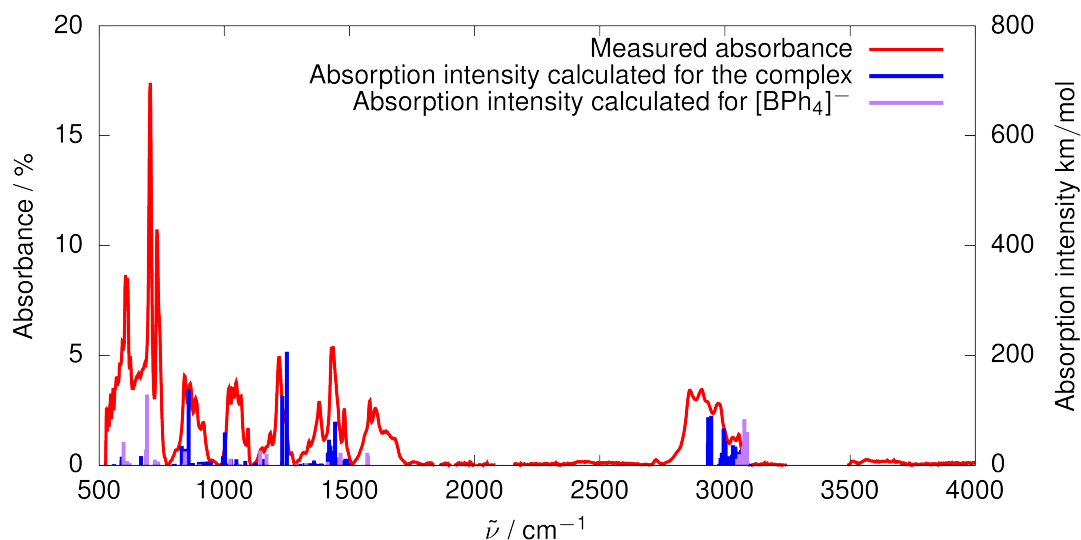
Figure S11: Calculated IR frequencies and absorption intensities along with the measured IR absorbance of **[Y₂]⁺**.
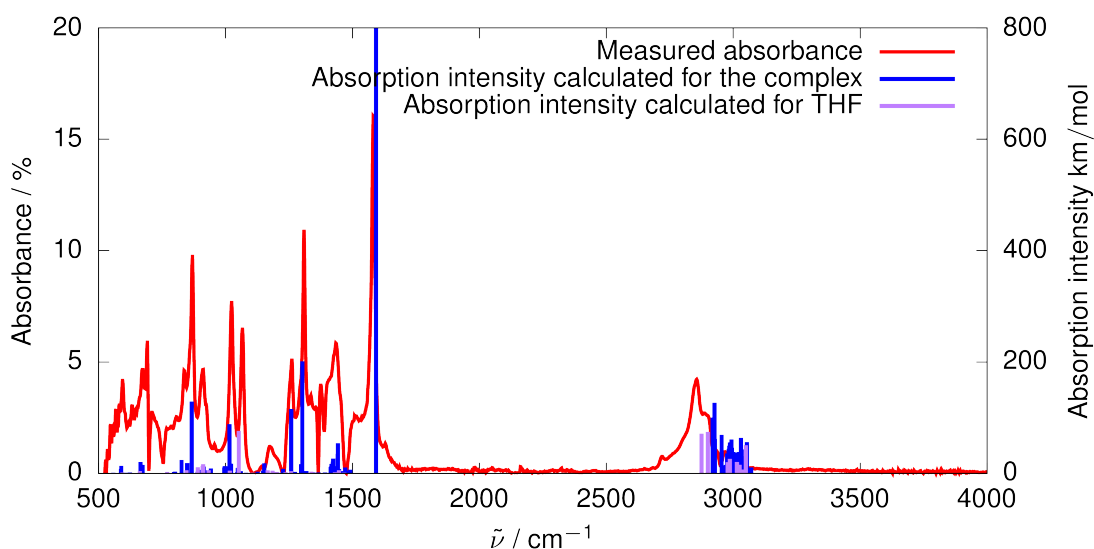
Figure S12: Calculated IR frequencies and absorption intensities along with the measured IR absorbance of **[Y₂]**.
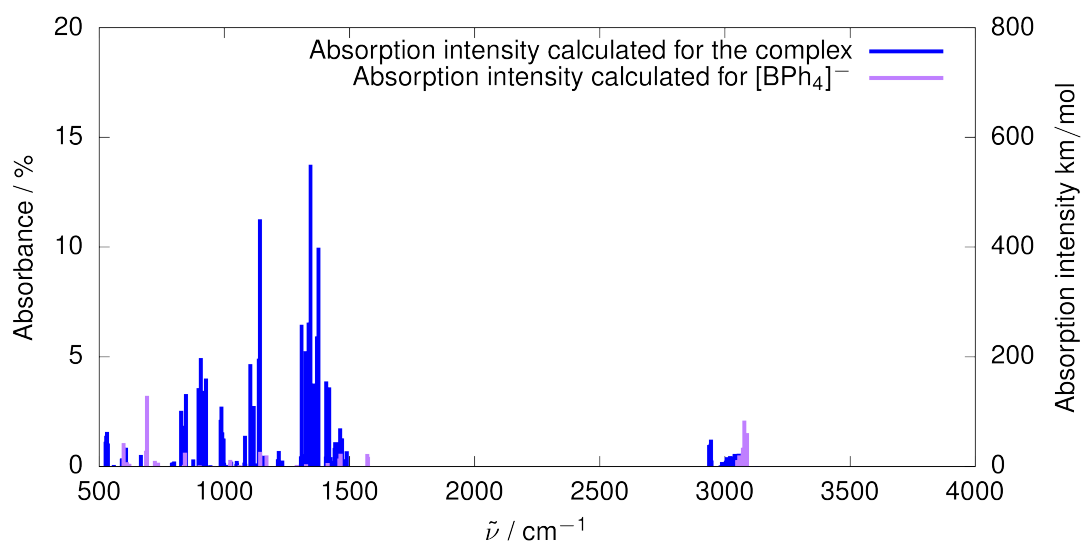
Figure S13: Calculated IR frequencies and absorption intensities of **[Y₂]²⁺**.

Table S4. Selected optimized bond distances (in Å, using the crystal-structure labels) in **[Y₂]²⁺**, **[Y₂]⁺** and **[Y₂]**, and their comparison to the respective crystal-structure parameters. For **[Y₂]²⁺** only the optimized bond distances are provided.

Structure	Source	N1–Y	N2–Y	N1–N2	N1–C1	N2–C2
[Y₂]²⁺	DFT	2.391	2.459	1.368	1.332	1.333
[Y₂]⁺	DFT	2.398	2.474	1.390	1.327	1.330
	XRD	2.437	2.462	1.395	1.317	1.322
[Y₂]	DFT	2.322	2.347	1.476	1.313	1.327
	XRD	2.326	2.320	1.481	1.304	1.322

Table S5. QTAIM charges calculated for the Y(III) ions and the atoms in the tetrazine bridge in $[Y_2]^{2+}$, $[Y_2]^+$ and $[Y_2]$ using the crystal-structure labels of the atoms.

	$[Y_2]^{2+}$	$[Y_2]^+$	$[Y_2]$
Y	1.97	1.98	2.01
Y	1.97	1.98	2.01
H	0.11	0.07	0.02
H	0.11	0.07	0.02
C1/C2	1.00	1.01	1.07
C1/C2	1.00	1.01	1.07
N1/N2	–0.68	–0.74	–0.92
N1/N2	–0.67	–0.74	–0.91
N1/N2	–0.68	–0.74	–0.92
N1/N2	–0.67	–0.74	–0.91
Total bridge charge	–0.47	–0.78	–1.49

Table S6. Final bond energies (defined with respect to default ADF atomic fragments) of the optimized structures.

Structure	E(PBE) / Hartree	E(PBE0) / Hartree
$[Y_2]^{2+}$	–29.05762379	–35.09185103
$[Y_2]^+$	–29.35685799	–35.41815800
$[Y_2]$	–29.52004967	–35.57954371

Table S7. NICS values (in ppm) calculated at the centroid of a given ring in crystal structure and optimized geometries of the complexes as well as the free ligands.

	DFT geometry	XRD geometry	Free ligand
$[Y_2]$	25.75	22.08	9.02
$[Y_2]^+$	24.94	38.98	14.53
$[Y_2]^{2+}$	16.37	-	–1.35
Benzene	-	-	–7.88
Pyridine	-	-	–6.58
Pyrazine	-	-	–4.95

Optimized Cartesian coordinates
$[Y_2]^{2+}$

```
Y       0.146943    0.037807   -3.501597
C      -0.135041    1.295613   -0.037759
H      -0.247299    2.378456   -0.075026
C       0.752148   -2.933541   -5.278524
H       1.448491   -2.265984   -5.793744
H      -0.179361   -3.006737   -5.853803
C       1.314851   -4.301872   -4.942302
H       1.184982   -5.011741   -5.767018
H       2.385603   -4.236616   -4.706744
C       0.504682   -4.680648   -3.696493
H       0.983627   -5.461215   -3.094353
H      -0.496289   -5.033282   -3.980249
C       0.415556   -3.359007   -2.949076
H      -0.507687   -3.236732   -2.368207
H       1.285208   -3.194441   -2.293897
C       2.174482    0.590568   -5.198698
C       2.786705   -0.088309   -4.104016
C       2.666515    0.739450   -2.942835
C       2.012065    1.944799   -3.323627
C       1.717429    1.860210   -4.720601
C       2.236991    0.213303   -6.649303
H       2.622015   -0.802438   -6.799484
H       2.916901    0.888719   -7.190775
H       1.262406    0.281616   -7.152227
C       3.588182   -1.350530   -4.155161
H       4.658539   -1.125725   -4.030015
H       3.486470   -1.870690   -5.114005
H       3.320223   -2.056817   -3.356107
C       3.301918    0.463013   -1.618370
H       3.408369   -0.612852   -1.427962
H       2.724619    0.900402   -0.792507
H       4.310378    0.902286   -1.563302
C       1.830113    3.165466   -2.475061
H       2.577349    3.932955   -2.729788
H       1.957261    2.940055   -1.408603
H       0.843362    3.631100   -2.613002
C       1.332642    3.011580   -5.590714
H       0.754589    3.770694   -5.052954
H       0.765991    2.701996   -6.476660
H       2.244401    3.509017   -5.961253
C      -1.844732    0.611106   -5.217828
C      -2.236827   -0.626954   -4.619292
C      -2.520402   -0.395921   -3.235483
C      -2.362769    0.993183   -2.990216
C      -1.931199    1.620095   -4.214177
C      -1.636662    0.825586   -6.685711
H      -1.087603   -0.000613   -7.157480
H      -1.089804    1.751464   -6.894024
H      -2.604219    0.899822   -7.205912
C      -2.536429   -1.893117   -5.349509
H      -3.619186   -1.962696   -5.544762
H      -2.265613   -2.787984   -4.773369
H      -2.040581   -1.937952   -6.326436
C      -3.110643   -1.405644   -2.300145
H      -2.901415   -1.167077   -1.250574
H      -2.737750   -2.419859   -2.497246
H      -4.206302   -1.447727   -2.405116
C      -2.845435    1.739982   -1.788832
H      -2.256315    2.647657   -1.598745
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H       -2.840693    1.122540   -0.882162
H       -3.885781    2.068699   -1.943368
C       -1.894237    3.098568   -4.425056
H       -2.917559    3.506758   -4.399117
H       -1.467330    3.366114   -5.396281
H       -1.327477    3.627915   -3.645369
N        0.018699    0.652651   -1.194480
N       -0.170618    0.706857    1.157746
O        0.435588   -2.317816   -3.979773
C        0.135041   -1.295613    0.037759
H        0.247299   -2.378456    0.075026
N       -0.018699   -0.652651    1.194480
N        0.170618   -0.706857   -1.157746
Y       -0.146943   -0.037807    3.501597
C       -0.752148    2.933541    5.278524
H       -1.448491    2.265984    5.793744
H        0.179361    3.006737    5.853803
C       -1.314851    4.301872    4.942302
H       -1.184982    5.011741    5.767018
H       -2.385603    4.236616    4.706744
C       -0.504682    4.680648    3.696493
H       -0.983627    5.461215    3.094353
H        0.496289    5.033282    3.980249
C       -0.415556    3.359007    2.949076
H        0.507687    3.236732    2.368207
H       -1.285208    3.194441    2.293897
C       -2.174482   -0.590568    5.198698
C       -2.786705    0.088309    4.104016
C       -2.666515   -0.739450    2.942835
C       -2.012065   -1.944799    3.323627
C       -1.717429   -1.860210    4.720601
C       -2.236991   -0.213303    6.649303
H       -2.622015    0.802438    6.799484
H       -2.916901   -0.888719    7.190775
H       -1.262406   -0.281616    7.152227
C       -3.588182    1.350530    4.155161
H       -4.658539    1.125725    4.030015
H       -3.486470    1.870690    5.114005
H       -3.320223    2.056817    3.356107
C       -3.301918   -0.463013    1.618370
H       -3.408369    0.612852    1.427962
H       -2.724619   -0.900402    0.792507
H       -4.310378   -0.902286    1.563302
C       -1.830113   -3.165466    2.475061
H       -2.577349   -3.932955    2.729788
H       -1.957261   -2.940055    1.408603
H       -0.843362   -3.631100    2.613002
C       -1.332642   -3.011580    5.590714
H       -0.754589   -3.770694    5.052954
H       -0.765991   -2.701996    6.476660
H       -2.244401   -3.509017    5.961253
C        1.844732   -0.611106    5.217828
C        2.236827    0.626954    4.619292
C        2.520402    0.395921    3.235483
C        2.362769   -0.993183    2.990216
C        1.931199   -1.620095    4.214177
C        1.636662   -0.825586    6.685711
H        1.087603    0.000613    7.157480
H        1.089804   -1.751464    6.894024
H        2.604219   -0.899822    7.205912
C        2.536429    1.893117    5.349509
H        3.619186    1.962696    5.544762
H        2.265613    2.787984    4.773369
H        2.040581    1.937952    6.326436
C        3.110643    1.405644    2.300145
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H        2.737750    2.419859    2.497246
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H          4.206302      1.447727      2.405116
C          2.845435     -1.739982      1.788832
H          2.256315     -2.647657      1.598745
H          2.840693     -1.122540      0.882162
H          3.885781     -2.068699      1.943368
C          1.894237     -3.098568      4.425056
H          2.917559     -3.506758      4.399117
H          1.467330     -3.366114      5.396281
H          1.327477     -3.627915      3.645369
O         -0.435588      2.317816      3.979773
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$[Y_2]^+$

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Y          0.003967      0.166860     -3.511620
C         -0.288687      1.268388      0.007303
H         -0.533422      2.331333      0.006377
C          0.980345     -2.752884     -5.264795
H          1.740046     -2.087022     -5.681251
H          0.110286     -2.777905     -5.934474
C          1.485102     -4.148771     -4.939778
H          1.410415     -4.824525     -5.799401
H          2.534577     -4.113401     -4.616456
C          0.573917     -4.554983     -3.775274
H          0.990380     -5.363869     -3.163863
H         -0.407509     -4.876784     -4.149560
C          0.450481     -3.255332     -2.994217
H         -0.504182     -3.136287     -2.467976
H          1.276650     -3.129661     -2.277214
C         -2.602126     -0.482064     -3.282397
C         -2.546333      0.937198     -3.151266
C         -2.146641      1.484466     -4.403677
C         -1.959303      0.398774     -5.318671
C         -2.260857     -0.810437     -4.625167
C         -3.118656     -1.442319     -2.256482
H         -4.212747     -1.552537     -2.329997
H         -2.899779     -1.109792     -1.235496
H         -2.694270     -2.448350     -2.379260
C         -3.021733      1.738305     -1.979830
H         -2.430885      2.654248     -1.837199
H         -2.989135      1.162979     -1.046079
H         -4.067004      2.055637     -2.125210
C         -2.208880      2.942366     -4.743188
H         -3.257232      3.279443     -4.774759
H         -1.772317      3.156538     -5.723434
H         -1.697984      3.576084     -4.004105
C         -1.717096      0.513455     -6.793636
H         -1.128827     -0.327019     -7.187845
H         -1.185144      1.435698     -7.054492
H         -2.667596      0.523196     -7.350303
C         -2.424904     -2.164583     -5.241845
H         -2.013375     -2.970529     -4.618963
H         -1.956446     -2.226252     -6.231700
H         -3.493192     -2.391740     -5.385481
C          2.429363      1.125845     -2.899966
C          1.681318      2.238286     -3.392500
C          1.465979      2.036288     -4.784834
C          2.066674      0.791257     -5.152406
C          2.672567      0.237425     -3.985424
C          3.018386      0.986132     -1.533026
H          2.966928     -0.046263     -1.158001
H          2.510689      1.633730     -0.808548
H          4.081788      1.274138     -1.527169
C          1.322794      3.472829     -2.623104
H          2.076638      4.263701     -2.762969
H          1.264230      3.276899     -1.544397
H          0.358420      3.893867     -2.939448
C          1.016006      3.078207     -5.760529
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H        0.403288    3.853685   -5.289163
H        0.448045    2.658805   -6.599923
H        1.894388    3.582837   -6.195865
C        2.228411    0.333224   -6.572811
H        2.873726   -0.550828   -6.648064
H        2.702932    1.121284   -7.177111
H        1.275334    0.094341   -7.067802
C        3.556411   -0.969660   -3.893358
H        4.559796   -0.685978   -3.542007
H        3.687919   -1.460173   -4.865278
H        3.177292   -1.725824   -3.189407
N       -0.155207    0.681440   -1.175123
N       -0.152904    0.674028    1.189213
O        0.554232   -2.187953   -3.984339
C        0.288687   -1.268388   -0.007303
H        0.533422   -2.331333   -0.006377
N        0.155207   -0.681440    1.175123
N        0.152904   -0.674028   -1.189213
Y       -0.003967   -0.166860    3.511620
C       -0.980345    2.752884    5.264795
H       -1.740046    2.087022    5.681251
H       -0.110286    2.777905    5.934474
C       -1.485102    4.148771    4.939778
H       -1.410415    4.824525    5.799401
H       -2.534577    4.113401    4.616456
C       -0.573917    4.554983    3.775274
H       -0.990380    5.363869    3.163863
H        0.407509    4.876784    4.149560
C       -0.450481    3.255332    2.994217
H        0.504182    3.136287    2.467976
H       -1.276650    3.129661    2.277214
C        2.602126    0.482064    3.282397
C        2.546333   -0.937198    3.151266
C        2.146641   -1.484466    4.403677
C        1.959303   -0.398774    5.318671
C        2.260857    0.810437    4.625167
C        3.118656    1.442319    2.256482
H        4.212747    1.552537    2.329997
H        2.899779    1.109792    1.235496
H        2.694270    2.448350    2.379260
C        3.021733   -1.738305    1.979830
H        2.430885   -2.654248    1.837199
H        2.989135   -1.162979    1.046079
H        4.067004   -2.055637    2.125210
C        2.208880   -2.942366    4.743188
H        3.257232   -3.279443    4.774759
H        1.772317   -3.156538    5.723434
H        1.697984   -3.576084    4.004105
C        1.717096   -0.513455    6.793636
H        1.128827    0.327019    7.187845
H        1.185144   -1.435698    7.054492
H        2.667596   -0.523196    7.350303
C        2.424904    2.164583    5.241845
H        2.013375    2.970529    4.618963
H        1.956446    2.226252    6.231700
H        3.493192    2.391740    5.385481
C       -2.429363   -1.125845    2.899966
C       -1.681318   -2.238286    3.392500
C       -1.465979   -2.036288    4.784834
C       -2.066674   -0.791257    5.152406
C       -2.672567   -0.237425    3.985424
C       -3.018386   -0.986132    1.533026
H       -2.966928    0.046263    1.158001
H       -2.510689   -1.633730    0.808548
H       -4.081788   -1.274138    1.527169
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H      -0.403288   -3.853685    5.289163
H      -0.448045   -2.658805    6.599923
H      -1.894388   -3.582837    6.195865
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H      -2.873726    0.550828    6.648064
H      -2.702932   -1.121284    7.177111
H      -1.275334   -0.094341    7.067802
C      -3.556411    0.969660    3.893358
H      -4.559796    0.685978    3.542007
H      -3.687919    1.460173    4.865278
H      -3.177292    1.725824    3.189407
O      -0.554232    2.187953    3.984339
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[Y₂]

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Y      -0.041096    0.243874   -3.389154
C      -0.259349    1.280742    0.070679
H      -0.478119    2.354895    0.118763
C       0.745716   -2.754008   -5.218816
H       1.551778   -2.145040   -5.637054
H      -0.116767   -2.726477   -5.899903
C       1.155860   -4.182270   -4.888636
H       1.034698   -4.856141   -5.745291
H       2.206647   -4.214420   -4.566739
C       0.226795   -4.515593   -3.715926
H       0.588131   -5.347342   -3.099112
H      -0.778447   -4.768559   -4.082472
C       0.203892   -3.203481   -2.946345
H      -0.723060   -3.009748   -2.394941
H       1.052478   -3.122966   -2.249997
C       2.133029    0.684374   -5.023880
C       2.657691    0.119059   -3.823818
C       2.452634    1.051700   -2.770474
C       1.805098    2.200318   -3.313402
C       1.619510    1.979494   -4.706727
C       2.320480    0.186075   -6.428235
H       2.900906   -0.745741   -6.455964
H       2.880746    0.922299   -7.026998
H       1.374408    0.006541   -6.962135
C       3.416589   -1.163481   -3.665474
H       4.464417   -0.966303   -3.387672
H       3.436542   -1.752232   -4.591447
H       2.995888   -1.801680   -2.873615
C       2.950798    0.893110   -1.371165
H       2.775986   -0.121280   -0.986151
H       2.451375    1.590054   -0.689023
H       4.034278    1.087685   -1.306358
C       1.491961    3.462595   -2.569233
H       2.350552    4.154365   -2.562481
H       1.232204    3.254636   -1.522498
H       0.647083    4.003425   -3.018036
C       1.284738    3.024347   -5.725344
H       0.727164    3.862608   -5.292905
H       0.699263    2.628465   -6.565465
H       2.211498    3.441674   -6.156271
C      -1.915286    0.563861   -5.344068
C      -2.349090   -0.588768   -4.626689
C      -2.724665   -0.184182   -3.315304
C      -2.555853    1.226829   -3.227289
C      -2.057282    1.692855   -4.475812
C      -1.586045    0.605264   -6.806559
H      -1.069013   -0.305372   -7.142709
H      -0.939541    1.455018   -7.058789
H      -2.495917    0.700101   -7.422975
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C      -2.595438   -1.950348   -5.199496
H      -3.675589   -2.120495   -5.340031
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H      -2.127619   -2.071735   -6.185044
C      -3.332331   -1.064991   -2.269281
H      -3.079046   -0.723984   -1.260125
H      -2.990060   -2.105570   -2.359057
H      -4.432770   -1.082256   -2.346078
C      -2.973437    2.099892   -2.085428
H      -2.298294    2.958035   -1.957714
H      -2.984939    1.546552   -1.138773
H      -3.986239    2.505805   -2.249077
C      -1.972436    3.138605   -4.861622
H      -2.982415    3.573068   -4.946823
H      -1.478155    3.277880   -5.828804
H      -1.431293    3.746076   -4.121098
N      -0.253780    0.762018   -1.135889
N      -0.036245    0.681899    1.233368
O       0.350120   -2.159544   -3.952447
C       0.259349   -1.280742   -0.070679
H       0.478119   -2.354895   -0.118763
N       0.253780   -0.762018    1.135889
N       0.036245   -0.681899   -1.233368
Y       0.041096   -0.243874    3.389154
C      -0.745716    2.754008    5.218816
H      -1.551778    2.145040    5.637054
H       0.116767    2.726477    5.899903
C      -1.155860    4.182270    4.888636
H      -1.034698    4.856141    5.745291
H      -2.206647    4.214420    4.566739
C      -0.226795    4.515593    3.715926
H      -0.588131    5.347342    3.099112
H       0.778447    4.768559    4.082472
C      -0.203892    3.203481    2.946345
H       0.723060    3.009748    2.394941
H      -1.052478    3.122966    2.249997
C      -2.133029   -0.684374    5.023880
C      -2.657691   -0.119059    3.823818
C      -2.452634   -1.051700    2.770474
C      -1.805098   -2.200318    3.313402
C      -1.619510   -1.979494    4.706727
C      -2.320480   -0.186075    6.428235
H      -2.900906    0.745741    6.455964
H      -2.880746   -0.922299    7.026998
H      -1.374408   -0.006541    6.962135
C      -3.416589    1.163481    3.665474
H      -4.464417    0.966303    3.387672
H      -3.436542    1.752232    4.591447
H      -2.995888    1.801680    2.873615
C      -2.950798   -0.893110    1.371165
H      -2.775986    0.121280    0.986151
H      -2.451375   -1.590054    0.689023
H      -4.034278   -1.087685    1.306358
C      -1.491961   -3.462595    2.569233
H      -2.350552   -4.154365    2.562481
H      -1.232204   -3.254636    1.522498
H      -0.647083   -4.003425    3.018036
C      -1.284738   -3.024347    5.725344
H      -0.727164   -3.862608    5.292905
H      -0.699263   -2.628465    6.565465
H      -2.211498   -3.441674    6.156271
C       1.915286   -0.563861    5.344068
C       2.349090    0.588768    4.626689
C       2.724665    0.184182    3.315304
C       2.555853   -1.226829    3.227289
C       2.057282   -1.692855    4.475812
C       1.586045   -0.605264    6.806559
```

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H        1.069013     0.305372    7.142709
H        0.939541    -1.455018    7.058789
H        2.495917    -0.700101    7.422975
C        2.595438     1.950348    5.199496
H        3.675589     2.120495    5.340031
H        2.230990     2.759415    4.550123
H        2.127619     2.071735    6.185044
C        3.332331     1.064991    2.269281
H        3.079046     0.723984    1.260125
H        2.990060     2.105570    2.359057
H        4.432770     1.082256    2.346078
C        2.973437    -2.099892    2.085428
H        2.298294    -2.958035    1.957714
H        2.984939    -1.546552    1.138773
H        3.986239    -2.505805    2.249077
C        1.972436    -3.138605    4.861622
H        2.982415    -3.573068    4.946823
H        1.478155    -3.277880    5.828804
H        1.431293    -3.746076    4.121098
O       -0.350120     2.159544    3.952447
```

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