Investigation and Preparation of a TREN-Based Bifunctional Chelator for ^{89}Zr

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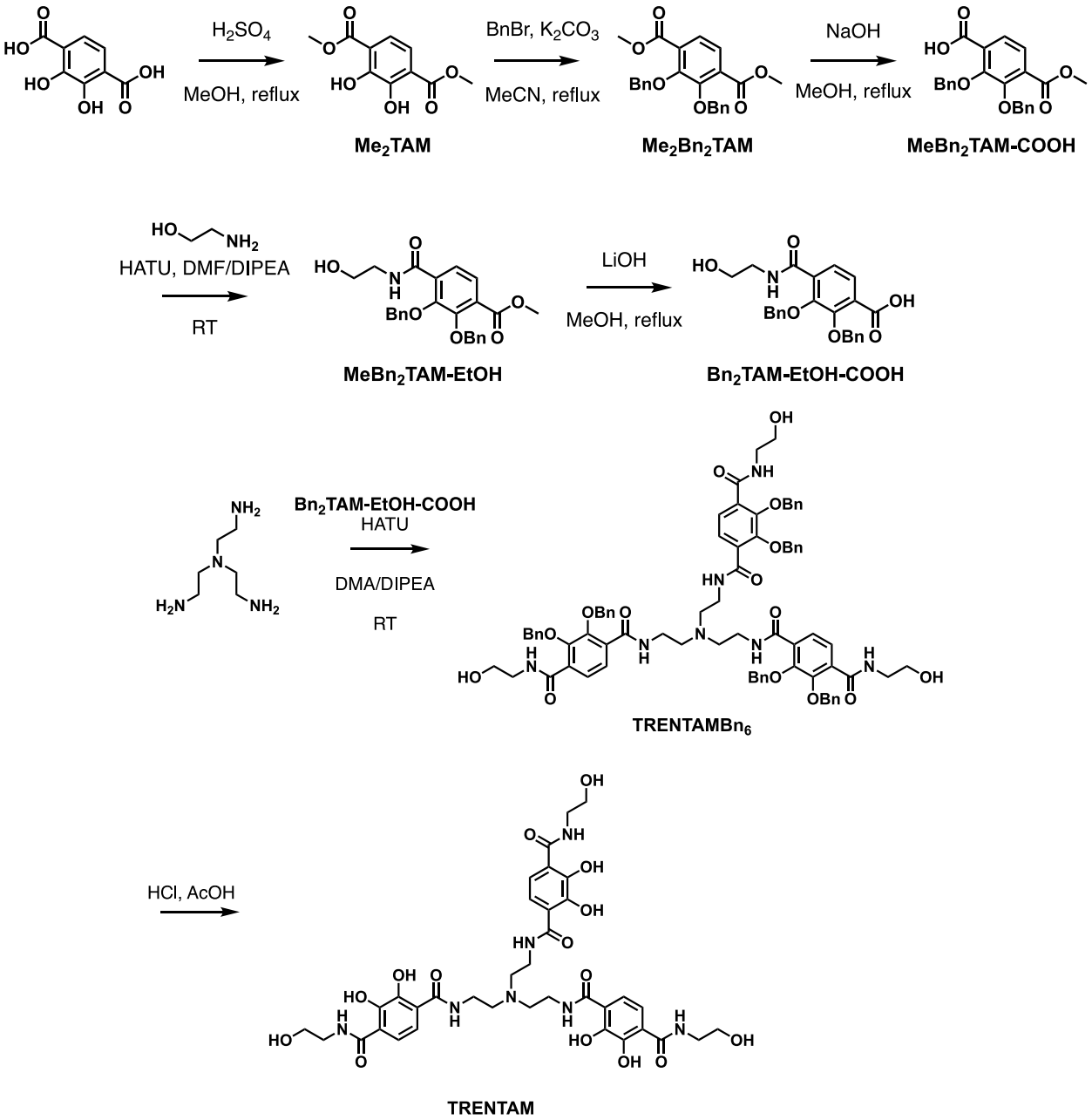
Materials. Materials were purchased from commercial vendors and used without further purification. Terephthalic acid, tris(2-aminoethyl)amine (TREN), TREN-Boc, benzyl bromide, ethanolamine, O-(7-azabenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate (HATU), sulfuric acid, acetic acid, hydrochloric acid, sodium hydroxide, lithium hydroxide, N,N-diisopropylethylamine (DIPEA), potassium carbonate, sodium sulfate, sodium chloride, thiazolyl blue tetrazolium bromide (MTT reagent), methanol, anhydrous N,N-dimethylformamide (DMF), anhydrous dimethylacetamide (DMA), anhydrous tetrahydrofuran (THF), anhydrous acetonitrile (MeCN) were purchased from Sigma-Aldrich, VWR, Oakwood, Ambeed, AK Scientific, or AA Blocks. All deuterated solvents were purchased from Cambridge Isotope Laboratories. Phosphate buffered saline (PBS, 10 mM, pH 7.2), Dulbecco's Modified Eagle's medium (DMEM), and trypsin/EDTA solution were purchased from ThermoFisher Scientific. Ultrapure water (over 18 MΩ·cm) was produced by a Milli-Q reference system (Millipore).

Instruments and Software. ^{1}H and ^{13}C NMR spectra were acquired on Bruker spectrometers. The following abbreviations were used to describe coupling constants: singlet (s), doublet (d), triplet (t), or multiplet (m). Spectra were visualized and analyzed using MestReNova (version 15.0.0) and referenced to deuterated solvent. High-resolution mass spectrometry (HRMS) data were collected on an Agilent 6250 Accurate - Mass Q-TOF LC/MS. Flash column chromatography was performed using reversed phase (RediSep® Rf Gold® Reversed-phase C18) and normal phase on a CombiFlash® Rf 200i (Teledyne Isco, Inc.). LC/MS was performed using a Shimadzu LCMS-2020 Single Quadrupole with a Kinetex 2.6 µm C18 100 Å (2.1 x 50 mm) column obtained from Phenomenex, Inc (Torrance, CA), and a gradient of 0-90% MeCN/H2O with 0.1% formic acid over 4.5 min at a flow rate of 0.2 mL/min. Ultraviolet-visible spectroscopy was performed on a Jasco V-770 operated by SpectraManager software. A Synergy Mx plate reader was used for cell viability assays. Chemical structures were drawn and cLogP values were calculated using ChemDraw (version 25.0.2.7). Data was analyzed using Microsoft Excel.

Statistical Analysis. Statistical analysis was performed using Graphpad Prism (version 10.3.1) and Microsoft Excel. The student's *t*-test was used as the statisitcal test. The *n* value is indicated in the corresponding figure captions.



Synthetic scheme 1. Synthesis of TRENTAM

Synthesis of Me_2TAM

Me_2TAM was prepared with the following modified procedure.[1] Terephthalic acid (2.04 g, 12.3 mmol) was dissolved in 50 mL MeOH containing a few drops of concentrated H_2SO_4. Further concentrated H_2SO_4 (6 mL) was added slowly with rapid stirring. The resulting mixture was heated to reflux for 2 days, then cooled to 0°C for 30 minutes. The grey microcrystalline precipitate was isolated via filtration and washed with 40 mL ice-cold MeOH (1.2 g, 43%). ^1H NMR (500 MHz, $CDCl_3$) δ 10.91 (s, 2H), 7.32 (s, 2H), 3.96 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.13, 151.56, 118.33, 115.90, 52.75. MS (ES+): m/z calcd for $C_{10}H_{10}O_6Na$ 249.0375, found 249.0363.

Synthesis of Me_2Bn_2TAM

Me_2Bn_2TAM was prepared with the following modified procedure.[2] Me_2TAM (2.3 g, 10 mmol) was suspended in 120 mL MeCN, and K_2CO_3 (5 g) was added. Benzyl bromide (3.6 mL) was added slowly to the resulting suspension with rapid stirring. The mixture was then heated to reflux with a drying tube for 2 days. The resulting yellow suspension was evaporated exhaustively to yield a yellow powder, which was suspended in 50 mL EtOAc and extracted 3x with saturated $NaHCO_3$ (50 mL), followed by brine (50 mL), then dried using Na_2SO_4. The resulting solution was evaporated to yield a crude yellow solid. This solid was dissolved in 10 mL DMF and added dropwise to water (20 mL), with rapid stirring, resulting in a yellow precipitate. The precipitate was isolated via filtration and recrystallized from boiling hexanes to yield the product as a fine, white powder (2.6 g, 64%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.53 (s, 2H), 7.43 – 7.36 (m, 4H), 7.36 – 7.29 (m, 6H), 5.10 (s, 4H), 3.87 (s, 6H). ^{13}C NMR (125 MHz, CD_3OD) δ 165.92, 152.29, 136.76, 130.38, 128.38, 128.21, 127.98, 127.89, 127.83, 125.09, 76.04, 51.54. MS (ES+): m/z calcd for $C_{24}H_{22}O_6$ 407.1495, found 407.1489.

Synthesis of $MeBn_2TAM$-COOH

Me_2Bn_2TAM-COOH was prepared with the following modified procedure.[3] Bn_2Me_2TAM (1 g, 2.5 mmol) was suspended in MeOH (20 mL) and heated to reflux until completely dissolved. NaOH (98 mg, 2.5 mmol) was added, followed by 0.5 mL of water. The resulting mixture was refluxed overnight, evaporated to dryness, and the resulting solid was suspended in water (100 mL). The white precipitate was removed via vacuum filtration and 0.1 M HCl was used to precipitate the filtrate. The precipitate was isolated via vacuum filtration to yield the product as a fine white powder (0.50 g, 52%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.61 – 7.51 (m, 2H), 7.43 (dq, *J* = 5.3, 3.1 Hz, 2H), 7.41 – 7.37 (m, 2H), 7.34 (tt, *J* = 3.7, 1.8 Hz, 7H), 5.12 (s, 2H), 5.10 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 167.23, 166.01, 152.28, 152.26, 136.88, 136.84, 136.83, 131.15, 130.85, 130.10, 128.41, 128.38, 127.96, 127.94, 127.92, 127.85, 127.81, 125.21, 125.19, 125.05, 76.03, 76.01, 51.51. MS (ES+): m/z calcd for $C_{23}H_{20}O_6$ 393.1338, found 393.1337.

Synthesis of $MeBn_2TAM$-EtOH

$MeBn_2TAM$-COOH (0.23 g, 0.58 mmol) was dissolved in dry DMF (0.5 mL), and DIPEA (0.12 mL, 0.7 mmol) was added, followed by HATU (0.24 g, 0.63 mmol). This mixture was stirred under N_2 at RT for 1 h, and ethanolamine (0.042 mL, 0.69 mmol) was added, causing the solution to turn bright yellow. The yellow solution was stirred at RT under N_2 overnight, diluted with EtOAc (100 mL), washed with equal volumes 1 M HCl (2x) and brine (1x), and dried using Na_2SO_4. The resulting solution was evaporated to dryness, taken up in minimal CH_2Cl_2, and purified using flash chromatography (silica gel, 0-10% MeOH/CH_2Cl_2) to yield the product as a yellow solid (0.23 g, 91%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (t, *J* = 5.7 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.32 – 7.29 (m, 2H), 7.26 (tdd, *J* = 8.5, 3.5, 1.9 Hz, 7H), 5.04 (d, *J* = 11.7 Hz, 4H), 3.79 (s, 3H), 3.54 (dd, *J* = 5.7, 4.6 Hz, 2H), 3.33 (q, *J* = 5.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.68, 165.23, 151.87, 151.55, 136.57, 135.77, 130.61, 129.77, 129.00, 128.80, 128.65, 128.55, 128.41, 126.15, 126.13, 62.04, 52.46, 42.78, 38.62, 29.71. MS (ES+): m/z calcd for $C_{25}H_{25}NO_6$ 436.1760, found 436.1764.

Synthesis of Bn_2TAM-EtOH-COOH

$MeBn_2TAM$-EtOH (0.25 g, 0.57 mmol) was suspended in 15 mL MeOH and heated to reflux. Once the material fully dissolved, water (1.5 mL) was added, followed by LiOH (0.15 g). The mixture was refluxed overnight, evaporated to dryness, and the resulting powder was dissolved in water (50 mL) and acidified to pH < 1 using 6 M HCl. The mixture was extracted 2x with CH_2Cl_2 (50 mL). The CH_2Cl_2 extract was washed with brine (50 mL), dried using Na_2SO_4, and evaporated to yield the product as a fine white powder (0.21 g, 88%). ^{1}H NMR (400 MHz, CD_3OD) δ 7.55 (t, *J* = 5.5 Hz, 2H), 7.49 – 7.38 (m, 2H), 7.32 (dp, *J* = 9.2, 3.3 Hz, 8H), 5.13 (d, *J* = 4.3 Hz, 4H), 3.61 (t, *J* = 5.8 Hz, 2H), 3.41 (t, *J* =

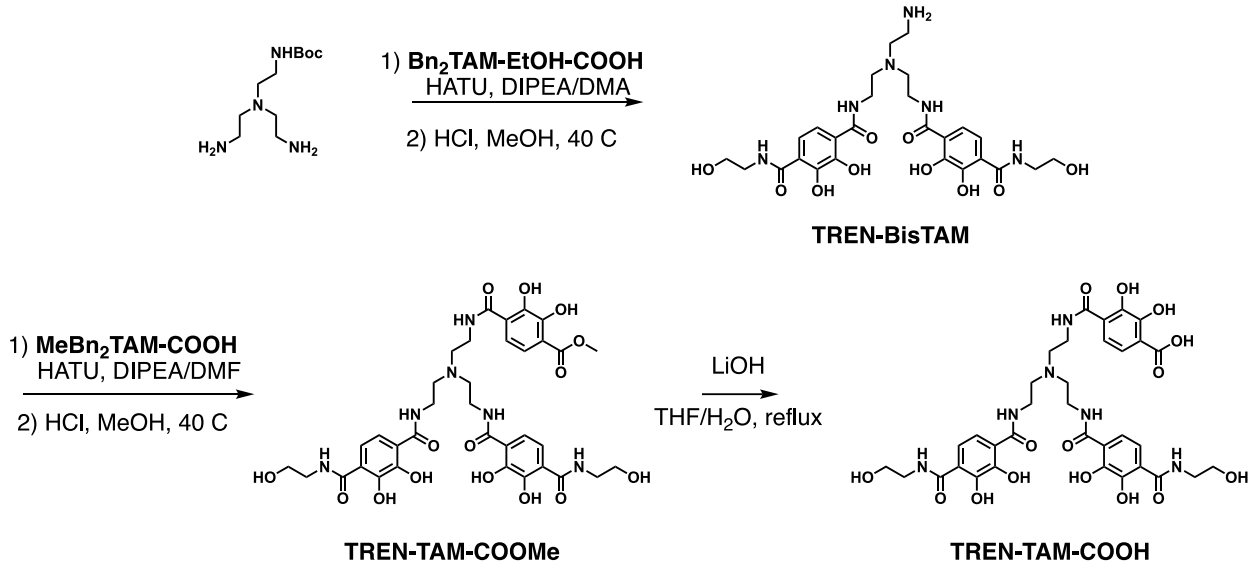
5.7 Hz, 2H). ^{13}C NMR (125 MHz, CD_3OD) δ 167.28, 166.27, 151.72, 150.84, 136.85, 136.17, 132.49, 130.24, 128.67, 128.51, 128.42, 128.27, 128.23, 128.15, 128.00, 127.93, 127.89, 127.82, 125.49, 124.39, 76.42, 76.06, 59.88, 41.93. MS (ES+): m/z calcd for $C_{24}H_{23}NO_6$ 422.1604, found 422.1607.

Synthesis of TRENTAMBn$_6$

TRENTAMBn$_6$ was prepared with the following modified procedure.[4] Bn_2TAM-EtOH-COOH (0.27 g, 0.64 mmol) was dissolved in dry DMA/DIPEA (1:1, 6 mL) and the mixture was sparged with N_2. HATU (0.24 g, 0.64 mmol) was added, and the mixture was stirred at RT for 20 min. TREN (0.029 mL, 0.19 mmol) was added, resulting in an immediate color change to bright yellow. The yellow solution was stirred at RT overnight, diluted with MeCN (70 mL), and evaporated exhaustively. The residue was dissolved in MeCN (70 mL) and evaporated again to yield a yellow oil. The mixture was dissolved in EtOAc (70 mL), washed with an equal volume of saturated Na_2CO_3 (2x), brine (1x), and dried using Na_2SO_4. The resulting solution was concentrated by evaporation and purified using flash chromatography (silica gel, 0-10% MeOH/CH_2Cl_2) to yield a yellow powder (0.22 g, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (t, *J* = 5.7 Hz, 1H), 7.62 (t, *J* = 5.3 Hz, 1H), 7.28 (s, 9H), 7.21 – 7.18 (m, 2H), 6.82 (d, *J* = 8.2 Hz, 1H), 4.97 (d, *J* = 12.2 Hz, 4H), 3.63 (q, *J* = 4.9 Hz, 2H), 3.40 (q, *J* = 5.2 Hz, 2H), 3.17 (q, *J* = 5.6 Hz, 2H), 2.31 (t, *J* = 5.7 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.72, 165.54, 150.52, 150.29, 136.31, 135.88, 132.20, 130.28, 128.90, 128.82, 128.75, 128.65, 128.48, 125.74, 124.94, 71.82, 65.79, 61.49, 52.67, 49.66, 42.83, 37.30, 32.18, 30.33, 27.73, 24.39. MS (ES+): m/z calcd for $C_{78}H_{81}N_7O_{15}$ 1356.5869, found 1356.5908.

Synthesis of TRENTAM

TRENTAM was prepared with the following modified procedure.[4] TRENTAMBn$_6$ (0.22 g, 0.16 mmol) was dissolved in glacial acetic acid (5 mL), and concentrated HCl (5 mL) was added dropwise with rapid stirring. The resulting solution was stirred at room temperature for 48 h. The mixture was diluted with methanol (50 mL) and evaporated exhaustively to yield a yellow oil. The oil was dissolved in methanol (5 mL), and water (5 mL) was added slowly with rapid stirring, followed by the addition of solid NH_4OAc (0.5 g). The mixture was stirred at room temperature for 3 h and concentrated to remove methanol, resulting in the formation of a white precipitate. The precipitate was isolated via filtration, washed with water, cold methanol, and ethyl ether to yield the product as a white solid (68 mg, 52%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.04 (d, *J* = 8.7 Hz, 3H), 6.97 (d, *J* = 8.7 Hz, 3H), 3.86 (t, *J* = 5.3 Hz, 6H), 3.71 (t, *J* = 5.7 Hz, 8H), 3.68 (t, *J* = 5.4 Hz, 6H), 3.50 (t, *J* = 5.7 Hz, 8H). ^{13}C NMR (125 MHz, CD_3OD) δ 170.06, 169.02, 148.80, 148.35, 118.04, 117.40, 117.05, 116.31, 60.04, 54.25, 41.77, 34.68. MS (ES+): m/z calcd for $C_{36}H_{45}N_7O_{15}$ 816.3007, found 816.3055.



Synthetic scheme 2. Synthesis of TRENTAM-COOH

Synthesis of TREN-BisTAM

Bn_2TAM-EtOH-COOH (1.0 g, 2.37 mmol) was dissolved in dry DMA/DIPEA (1:1, 10 mL) and the mixture was sparged with N_2. HATU (0.90 g, 2.37 mmol) was added, and the mixture was stirred at RT for 20 min. TREN-Boc (0.27 g, 1.08 mmol) was added, resulting in an immediate color change to bright yellow. The yellow solution was stirred at RT overnight, diluted with MeCN (200 mL), and evaporated exhaustively. The residue was dissolved in MeCN (200 mL) and evaporated again to yield a yellow oil. The mixture was dissolved in EtOAc (200 mL), washed with an equal volume of saturated Na_2CO_3 (2x), brine (1x), and dried using Na_2SO_4 to obtain a brown oil. MS (ES+): m/z calcd for $C_{59}H_{68}N_6O_{12}$ 1053.4973, found 1053.5007. Without further purification, 30% concentrated HCl in MeOH (13 mL) was added, and stirred at 40 °C for 3 h. The reaction mixture was precipitated using Et_2O (20 mL) and decanted, resulting in a white solid. The white solid was dissolved in water (5 mL) and washed with CH_2Cl_2 (3x). The aqueous layer was lyophilized to yield TREN-BisTAM as a white solid (418 mg, 65%). ^{1}H NMR (500 MHz, D_2O) δ 6.53 (q, *J* = 8.7 Hz, 4H), 3.76 – 3.65 (m, 5H), 3.61 (t, *J* = 5.6 Hz, 6H), 3.51 (t, *J* = 5.2 Hz, 6H), 3.30 (t, *J* = 5.7 Hz, 4H). ^{13}C NMR (125 MHz, D_2O) δ 169.42, 168.00, 147.09, 146.84, 115.97, 115.48, 115.18, 114.93, 58.96, 52.95, 48.01, 40.69, 34.08, 32.93.

Synthesis of TRENTAM-COOMe

$MeBn_2$TAM-COOH (72 mg, 0.18 mmol) was dissolved in dry DMA (1 mL), and DIPEA (0.35 mL 2.0 mmol) was added, followed by HATU (69 mg, 0.18 mmol). The reaction mixture was stirred under N_2 at RT for 0.5 h, and TREN-BisTAM (0.10 g, 0.17 mmol) was added, causing the solution to turn bright yellow. The yellow solution was stirred at RT under N_2 for 2 h and evaporated under N_2. The residue was dissolved in minimal water and loaded onto a reverse phase chromatography column (C18, 0-100% H_2O/MeCN) to remove major impurities, resulting in a clear oil (58 mg, approx. 35%). The residue was dissolved in MeOH (1 mL) and concentrated HCl (1 mL) was added. The reaction mixture was stirred at 40 °C for 3 h, and purified using reverse phase chromatography (C18, 0-100% H_2O/MeCN) to yield TRENTAM-COOMe as a colorless oil (40 mg, 85%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.11 (d, *J* = 1.3 Hz, 4H), 6.97 (d, *J* = 3.3 Hz, 2H), 3.95 (s, 3H), 3.74 (t, *J* = 5.7 Hz, 4H), 3.63 – 3.46 (m, 12H), 2.85 (d, *J* = 7.9 Hz, 4H). ^{13}C NMR (125 MHz, CD_3OD) δ 169.98, 168.77, 168.69, 150.37, 148.79, 148.60, 147.68, 119.83, 118.10, 117.86, 117.66, 116.83, 116.37, 116.34, 114.10, 65.50, 60.06, 52.76, 52.41, 51.77, 41.73, 37.35, 14.03.

Synthesis of TRENTAM-COOH

TRENTAM-COOMe (40 mg, 0.05 mmol) was dissolved in THF/H_2O (1:1, 2 mL), and LiOH was added (12 mg, 0.5 mmol). The reaction mixture was stirred under reflux for 1 h, and purified using reverse phase column chromatography (C18, 0-100% H_2O/MeCN) to yield TRENTAM-COOH as a white solid (30 mg, 76%). ^{1}H NMR (500 MHz, CD_3OD) δ 7.16 (d, *J* = 8.5 Hz, 1H), 7.10 (d, *J* = 8.7 Hz, 2H), 7.07 – 6.96 (m, 3H), 3.77 (t, *J* = 5.7 Hz, 6H), 3.71 (s, 5H), 3.55 (t, *J* = 5.7 Hz, 5H), 3.27 – 3.13 (m, 4H). ^{13}C NMR (125 MHz, CD_3OD) δ 173.01, 168.99, 150.64, 148.89, 148.22, 147.55, 119.20, 117.81, 117.71, 116.70, 116.32, 115.96, 60.03, 53.32, 41.78, 36.33. MS (ES+): m/z calcd for $C_{34}H_{40}N_6O_{15}$ 773.2585, found 773.2618.

Radio-HPLC Analysis

Radio-HPLC analysis (Agilent 1260 Infinity II, Agilent Technologies Inc., Santa Clara, CA, USA) was conducted on a TSK-gel Octadecyl-4PW column (5 µm, 4.6 mm ID × 15 cm, Tosoh Co. Tokyo, Japan) with gradient elution with 0.1% trifluoroacetic acid in water as mobile phase A. Mobile phase B contained 0.1% trifluoroacetic acid in acetonitrile. The elution sequence was 0-15 min of 5-100% B, 15-20 min of 100-5% B at a flow rate of 0.5 mL/min.

Computational Chemistry

Methods: Quantum chemistry calculations were performed with the GAMESS[5-7] package where density functional theory (DFT)[8] utilizing the B3LYP[9-11] and M11-L[12] functionals were used with the all-electron DGauss DZVP[13,14] basis sets (spherical harmonics). Water solvent effects were included using the polarizable continuum model (PCM).[15-18] Geometries were first optimized using the B3LYP functional and subsequent Hessians were computed to verify their natures as true minima and to compute non-electronic contributions to the Gibbs free energy at 298.15 K. All final geometries were optimized using the M11-L functional and these electronic energies were combined with B3LYP thermochemical quantities to produce total Gibbs free energies $G_{298.15}$. All optimized structures and energies are provided in the **Quantum Chemistry Data** section. Molecules were illustrated using MacMolPlt.[19] Holland[20] has performed an extensive study of Zr(IV) complexes, using the B3LYP/DZVP/PCM level of theory, that included determining the lowest-energy structures of $[Zr(DFO)(H_2O)_n]^+$ (n=0,1,2) systems where the model DFO ligand used had the terminal $–(CH_2)_5NH_3^+$ chain truncated to a methyl group. Here, we have also used the truncated DFO ligand and started $[Zr(DFO)(H_2O)_n]^+$ (n=0,1,2) geometry optimizations from the lowest-energy structures reported by Holland.[20] Initial $[Zr(TRENCAM)]^{2–}$ and $[Zr(TRENTAM)]^{2–}$ structures were built from the DFT-optimized geometry of $[Ti(TRENCAM)]^{2–}$ determined by Koller *et al*.[21] Following geometry optimizations of $Zr(TRENCAM)^{2–}$ and $Zr(TRENTAM)^{2–}$, seven-coordinate $[Zr(TRENCAM)(H_2O)]^{2–}$ and $[Zr(TRENTAM)(H_2O)]^{2–}$ complexes were constructed (by addition of a water molecule) and optimized. Attempts to optimize eight-coordinate $[Zr(TRENCAM)(H_2O)_2]^{2–}$ and $[Zr(TRENTAM)(H_2O)_2]^{2–}$ complexes (by addition of a water molecule to the seven-coordinate structures) at the B3LYP/DZVP/PCM level resulted in the second water becoming unbound to Zr, i.e., the additional water prefers to be in the second coordination sphere rather than the first/inner. As such, no further consideration was given to the eight-coordinate $[Zr(TRENCAM)(H_2O)_2]^{2–}$ and $[Zr(TRENTAM)(H_2O)_2]^{2–}$ complexes. With regards to the isolated $DFO^{3–}$, $TRENCAM^{6–}$, and $TRENTAM^{6–}$ ligands, we have followed the process of Holland[20] whereby starting structures were generated by removal of the metal atom from optimized $[Zr(DFO)]^+$, $[Zr(TRENCAM)]^{2–}$ and $[Zr(TRENTAM)]^{2–}$ complexes.

Results: We first gauged our methodology by comparing computed vs. experimental[22] gas-phase inner-sphere hydration reaction energies ($\Delta G_{298.15}$) of $[Zr(DFO)]^+$: $[Zr(DFO)]^+ + H_2O \rightarrow [Zr(DFO)(H_2O)]^+$ (Table S1). Here the computed M11-L value of –14.1 kcal/mol is in excellent agreement with the experimental value of –13.5 ± 0.9 kcal/mol, while the B3LYP value of –5.7 kcal/mol

is somewhat underestimated. All subsequent calculations described below included water solvent effects via the polarizable continuum model (PCM).

Table S1. Computed and experimental gas-phase inner-sphere hydration reaction energies (kcal/mol) for $[Zr(DFO)]^+ + H_2O \rightarrow [Zr(DFO)(H_2O)]^+$ at 298.15 K.

Method	**Δ*E***	**Δ*G***
B3LYP/DZVP	–17.2	–5.7
M11-L/DZVP	–25.6	–14.1[a]
Exp.[22]		–13.5 ± 0.9

a M11-L electronic energies were combined with B3LYP thermochemical quantities

Satisfied that the M11-L method could provide reliable results, we next turned our focus to determining the preferred coordination spheres for each type of Zr-DFO, ZR-TRENCAM, and Zr-TRENTAM complexes via computations of the reaction energies ($\Delta G_{298.15}$): $[Zr(X)] + nH_2O \rightarrow [Zr(X)(H_2O)_n]$ (n=1, 2; X = DFO, TRENCAM, TRENTAM) (Table S2 and Figure S1). Attempts to optimize eight-coordinate $[Zr(TRENCAM)(H_2O)_2]^{2-}$ and $[Zr(TRENTAM)(H_2O)_2]^{2-}$ complexes resulted in the dissociation of the second water molecule. As such, no further consideration was given to these systems. At the M11-L/DZVP/PCM level of theory seven-coordinate species are invariably preferred, however, in contrast with M11-L, B3LYP/DZVP/PCM predicts the six-coordinate $[Zr(TRENCAM)]^{2-}$ and $[Zr(TRENTAM)]^{2-}$ species to be the most stable of the Zr-TRENCAM and Zr-TRENTAM systems. Finally, we computed the relative coordination energies of DFO^{3-} vs. $TRENCAM^{6-}$ and $TRENTAM^{6-}$ to Zr(IV) (Table S3). Since the M11-L/DZVP/PCM level of theory predicts seven-coordinate species to be lowest in energy, we computed the reaction energies ($\Delta G_{298.15}$) for direct DFO^{3-} replacement by $TRENCAM^{6-}$ and $TRENTAM^{6-}$: 1) $[Zr(DFO)(H_2O)]^+ + TRENCAM^{6-} \rightarrow [Zr(TRENCAM)(H_2O)]^{2-} + DFO^{3-}$ and 2) $[Zr(DFO)(H_2O)]^+ + TRENTAM^{6-} \rightarrow [Zr(TRENTAM)(H_2O)]^{2-} + DFO^{3-}$. Both M11-L and B3LYP methods predict $[Zr(TRENCAM)(H_2O)]^{2-}$ to be more stable by 55.9 and 55.7 kcal/mol, respectively, and $[Zr(TRENTAM)(H_2O)]^{2-}$ to be more stable by 29.0 and 27.2 kcal/mol, respectively, where the M11-L/DZVP/PCM result should be considered the most reliable here. Since the B3LYP/DZVP/PCM method predicts that six-coordinate $[Zr(TRENCAM)]^{2-}$ and $[Zr(TRENTAM)]^{2-}$ are lowest in energy of the Zr-TRENCAM and Zr-TRENTAM systems, we also computed the replacement reaction energies for: 1) $[Zr(DFO)(H_2O)]^+ + TRENCAM^{6-} \rightarrow Zr(TRENCAM)^{2-} + H_2O + DFO^{3-}$ and 2) $[Zr(DFO)(H_2O)]^+ + TRENTAM^{6-} \rightarrow Zr(TRENTAM)^{2-} + H_2O + DFO^{3-}$, where B3LYP obtains –64.1 and –35.3 kcal/mol, respectively (Table S3). In conclusion, both M11-L/DZVP/PCM and B3LYP/DZVP/PCM levels of theory predict that $TRENCAM^{6-}$ complexation to Zr(IV) is preferred over DFO^{3-} by 55.9 and 64.1 kcal/mol, respectively, while $TRENTAM^{6-}$ complexation is preferred by 29.0 and 35.3 kcal/mol, respectively.

Table S2. Computed relative energies (kcal/mol) of six-, seven-, and eight-coordinate complexes at 298.15 K. Water solvent effects included via the polarizable continuum model.

	Δ*E*		**Δ*G***	
Complex	**B3LYP**	**M11-L**	**B3LYP**	**M11-L[a]**
$[Zr(DFO)]^{+}$ (6C)	0	0	0	0
$[Zr(DFO)(H_2O)]^{+}$ (7C)	–14.5	–15.9	–3.2	–4.6
$[Zr(DFO)(H_2O)_2]^{+}$ (8C)	–17.9	–28.1	+7.2	–2.9
$Zr(TRENCAM)^{2-}$ (6C)	0	0	0	0
$[Zr(TRENCAM)(H_2O)]^{2-}$ (7C)	–5.7	–17.6	+8.5	–3.5
$Zr(TRENTAM)^{2-}$ (6C)	0	0	0	0
$[Zr(TRENTAM)(H_2O)]^{2-}$ (7C)	–4.2	–16.4	+8.4	–3.7

a M11-L electronic energies were combined with B3LYP thermochemical quantities

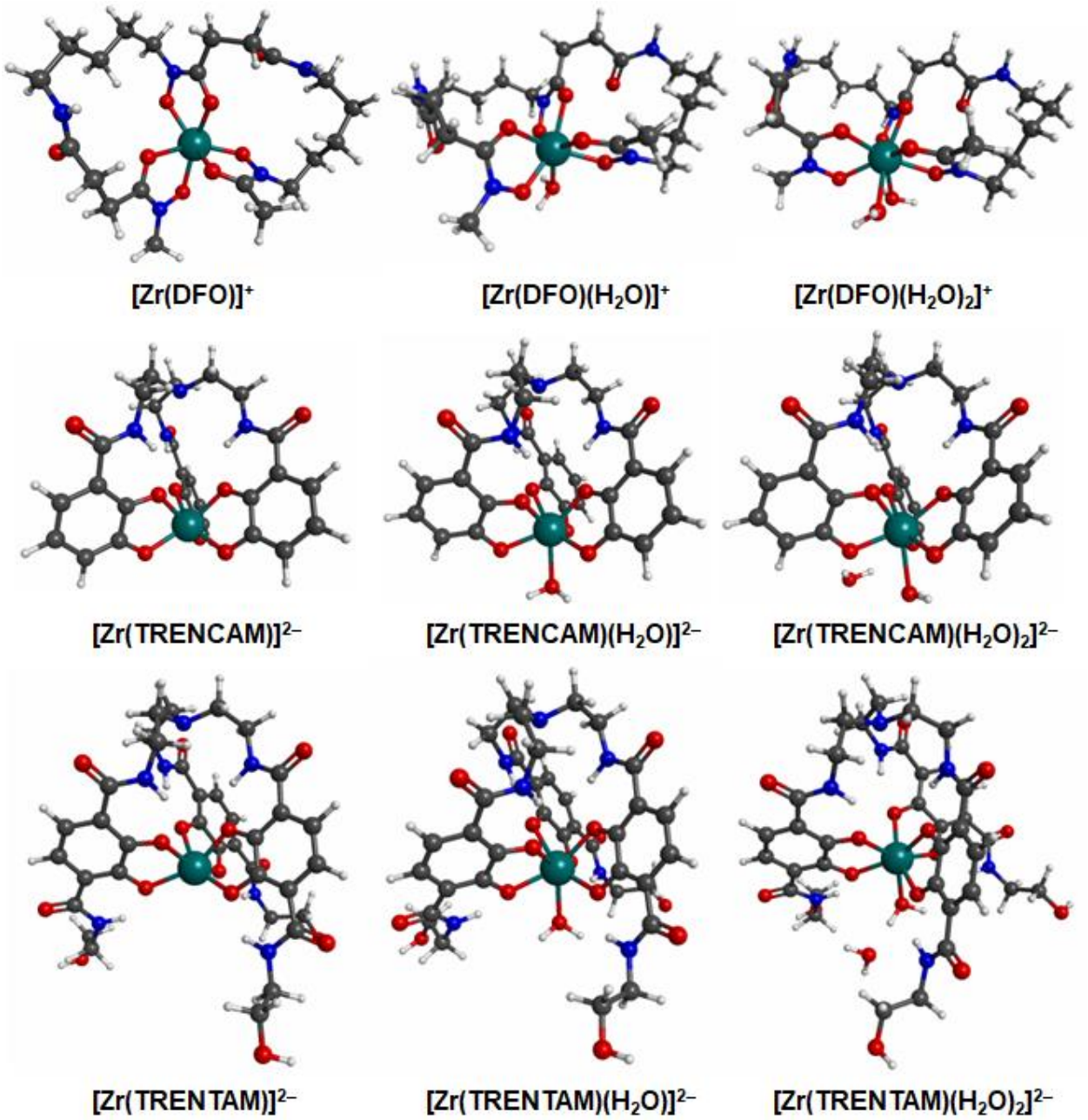


Figure S1. Illustrations of Zr(IV) complexes studied in this work. M11-L/DZVP/PCM optimized structures shown except for $[Zr(TRENCAM)(H_2O)_2]^{2-}$ and $[Zr(TRENTAM)(H_2O)_2]^{2-}$ (B3LYP/DZVP/PCM).

Table S3. Computed reaction energetics (kcal/mol) for the replacement of DFO^{3-} with $TRENCAM^{6-}$ and $TRENTAM^{6-}$ in Zr(IV) complexes at 298.15 K. Water solvent effects included via the polarizable continuum model.

	Δ*G*	
Reaction	**B3LYP**	**M11-L[a]**
$[Zr(DFO)(H_2O)]^{+}$ + $TRENCAM^{6-}$ → $[Zr(TRENCAM)(H_2O)]^{2-}$ + DFO^{3-}	–55.7	–55.9
$[Zr(DFO)(H_2O)]^{+}$ + $TRENCAM^{6-}$ → $Zr(TRENCAM)^{2-}$ + H_2O + DFO^{3-}	–64.1	–52.4
$[Zr(DFO)(H_2O)]^{+}$ + $TRENTAM^{6-}$ → $[Zr(TRENTAM)(H_2O)]^{2-}$ + DFO^{3-}	–27.0	–29.2
$[Zr(DFO)(H_2O)]^{+}$ + $TRENTAM^{6-}$ → $Zr(TRENTAM)^{2-}$ + H_2O + DFO^{3-}	–35.3	–25.5

a M11-L electronic energies were combined with B3LYP thermochemical quantities

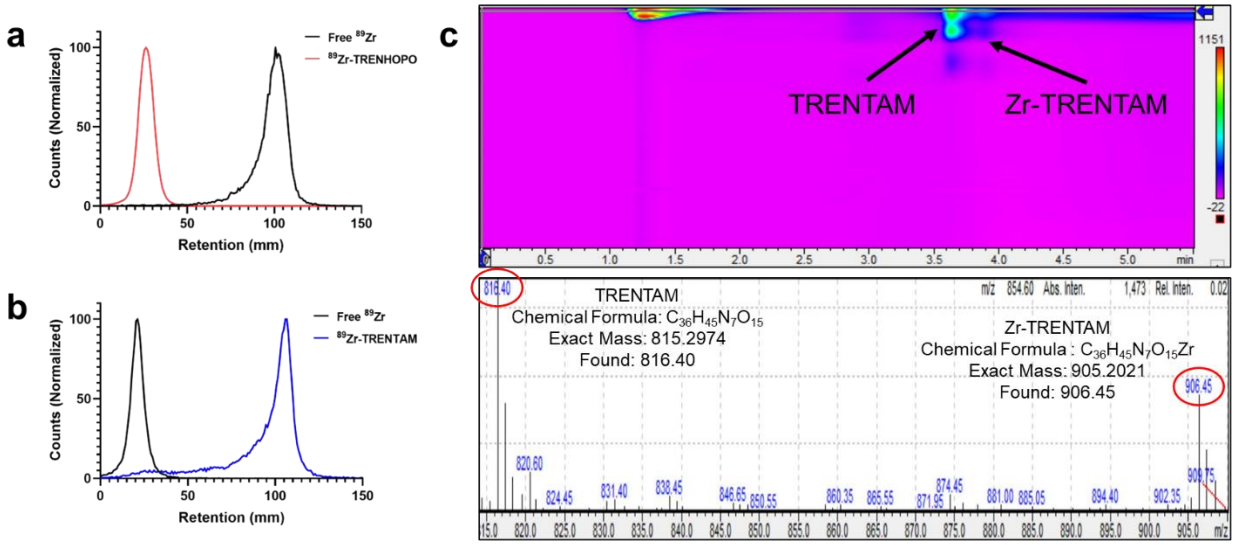


Figure S2. a. Radio-TLC (ITLC-SG) of free ^{89}Zr oxalate (black line) and TRENHOPO after radiolabeling (red line). TLC conditions: 100 mM NH_4OAc, pH 4.5, 50 mM EDTA. **b.** Radio-TLC (ITLC-SA) of free ^{89}Zr oxalate (black line) and TRENTAM after radiolabeling (blue line). TLC conditions: 50:50 MeOH/H_2O. **c.** LCMS data after incubating 1 mM TRENTAM with 1 mM $ZrCl_4$ for 10 minutes. Both m/z for TRENTAM and Zr-TRENTAM were found: 816.40 and 906.45, respectively.

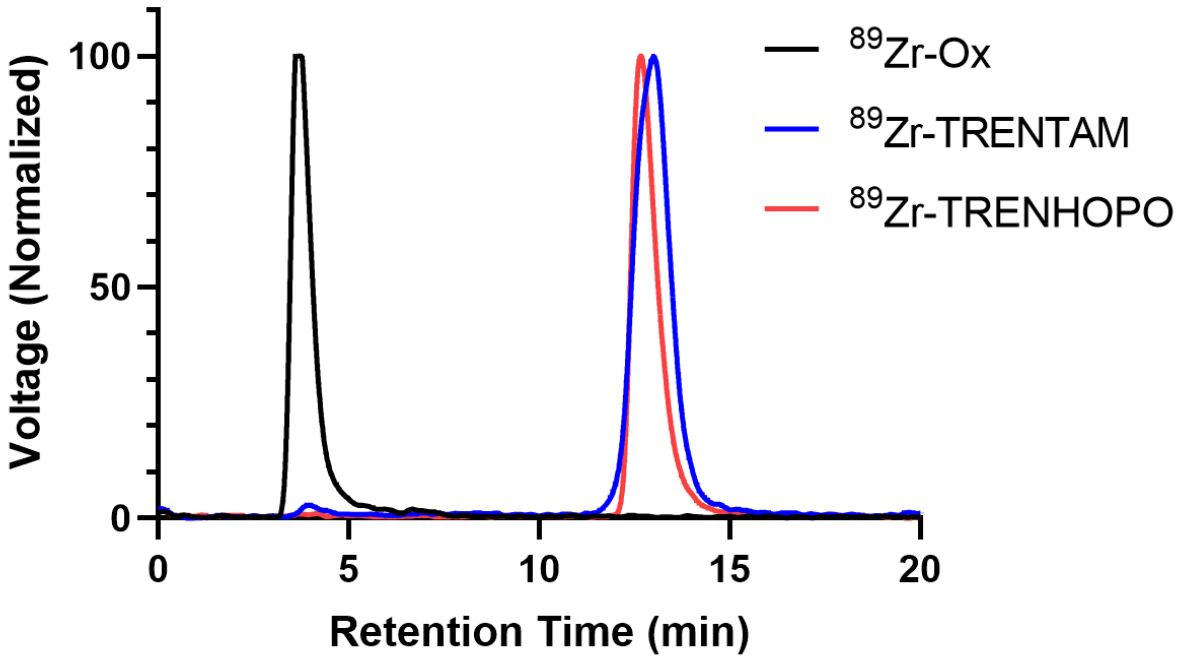


Figure S3. RP-radio-HPLC of free ^{89}Zr oxalate, ^{89}Zr-TRENTAM, and ^{89}Zr-TRENHOPO.

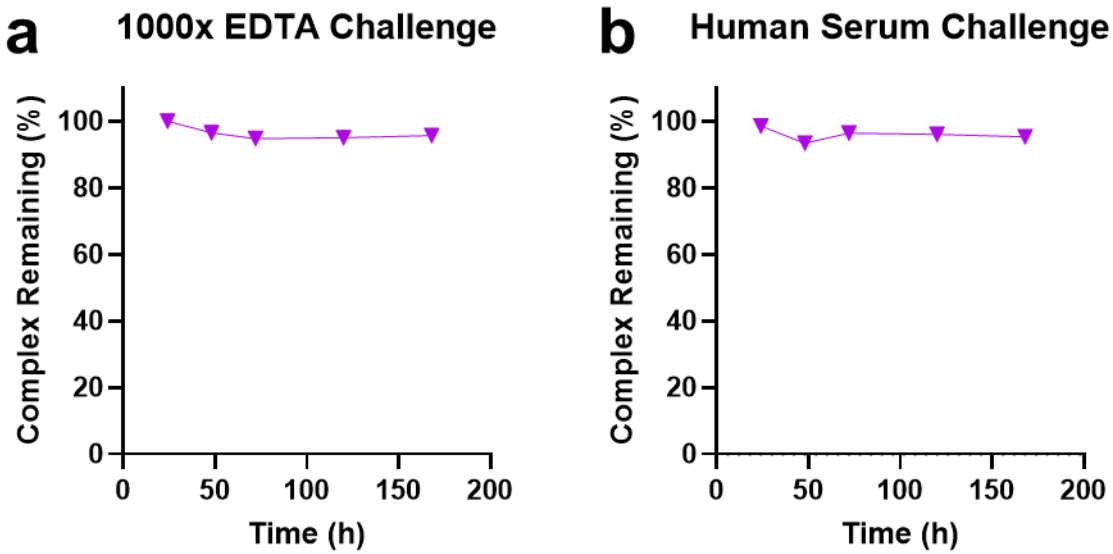


Figure S4. Stability of ^{89}Zr-TRENTAM-COOH complex in the presence of **a.** 1000 molar equivalents of EDTA or **b.** 99% human serum for 7 days, expressed as percent complex remaining after radio-TLC analysis.

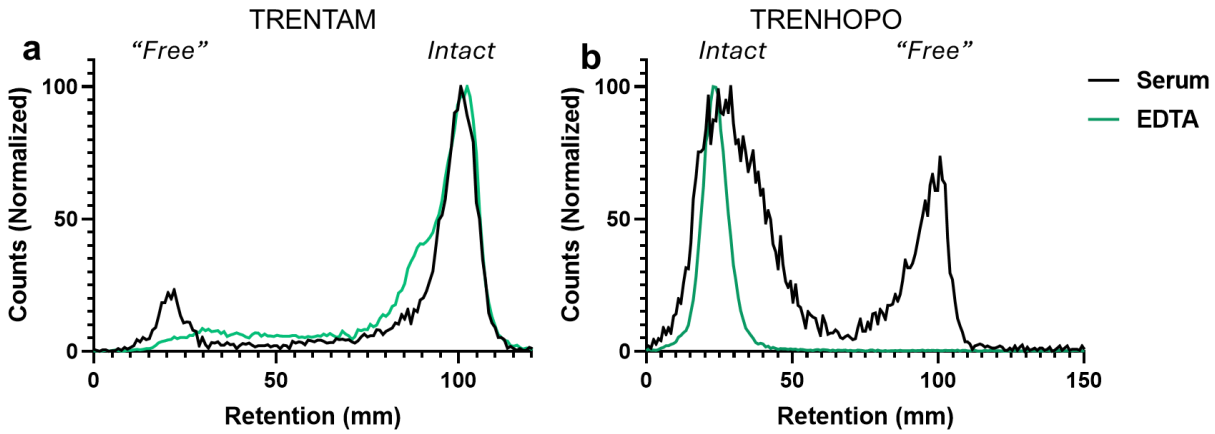


Figure S5. a. Radio-TLC of ^{89}Zr-TRENTAM in the presence of 99% serum (black line) or 1000 equivalents of EDTA (green line) after 7 days. **b.** Radio-TLC of ^{89}Zr-TRENHOPO in the presence of 99% serum or (black line) 1000 equivalents of EDTA (green line) after 7 days.

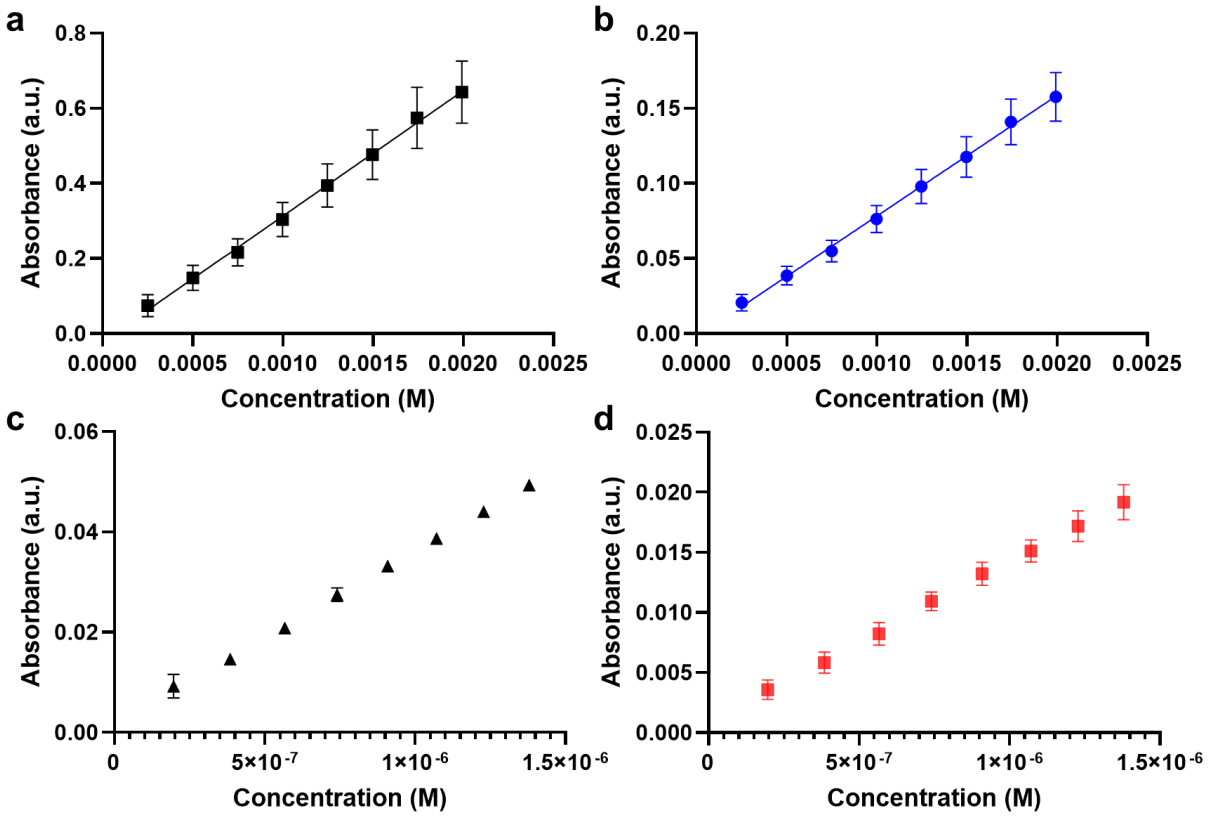


Figure S6. a. Beer's law plot for TRENTAM at 280 nm and **b.** 370 nm in PBS**. c.** Beer's law plot for Zr-TRENTAM at 280 nm and **d.** 380 nm in PBS. Error bars = SD (*n* = 3).

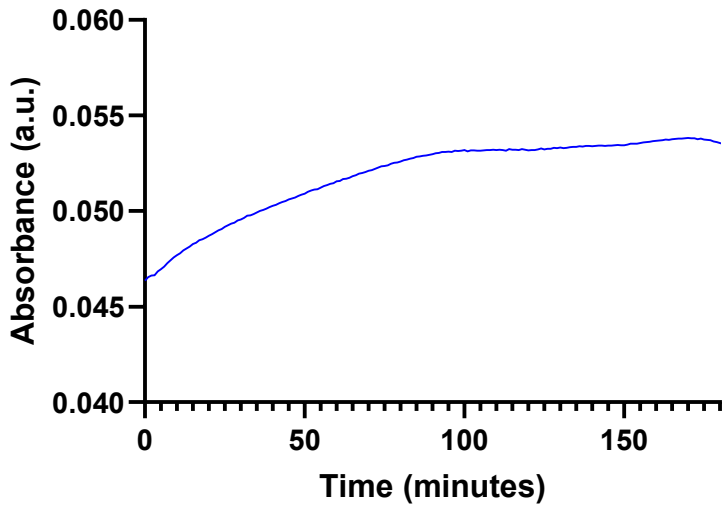


Figure S7. Kinetic absorbance measurement of TRENTAM (5 μM) in PBS with 1 eq. $ZrCl_4$. Absorbance was monitored at 370 nm.

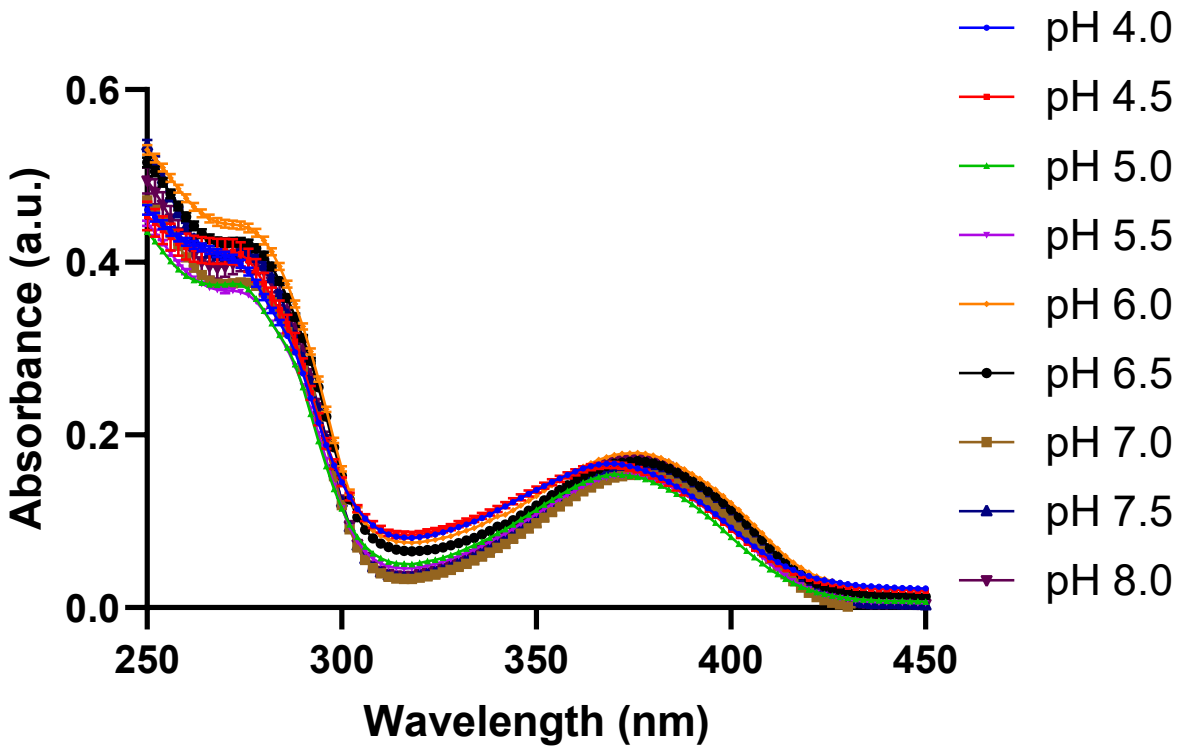


Figure S8. Absorbance plot of Zr-TRENTAM (20 μM) in PBS with pH 4.0 – 8.0. Error bars = SD (*n* = 3).

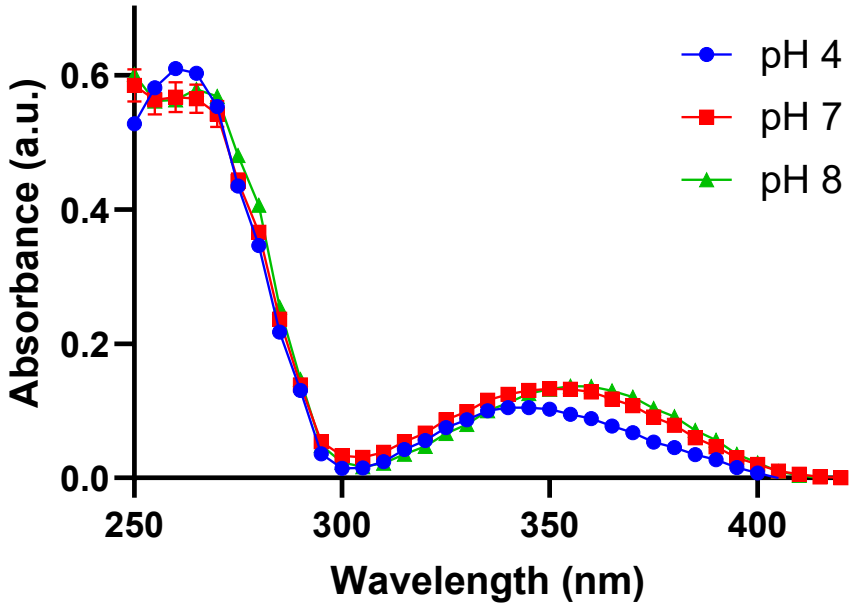


Figure S9. Absorbance spectra of TRENTAM (10 μM) in PBS at pH 4.0, 7.0, and 8.0. Error bars = SD (*n* = 3).

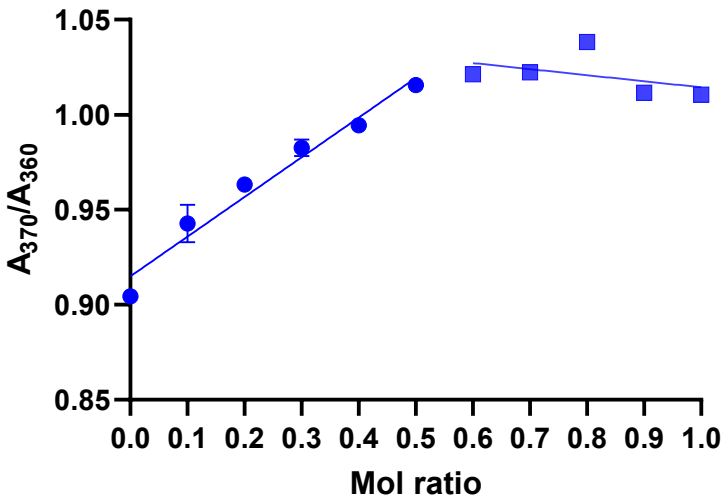


Figure S10. Job plot of TRENTAM and $ZrCl_4$ in PBS at pH 7.4. Error bars = SD (*n* = 3).

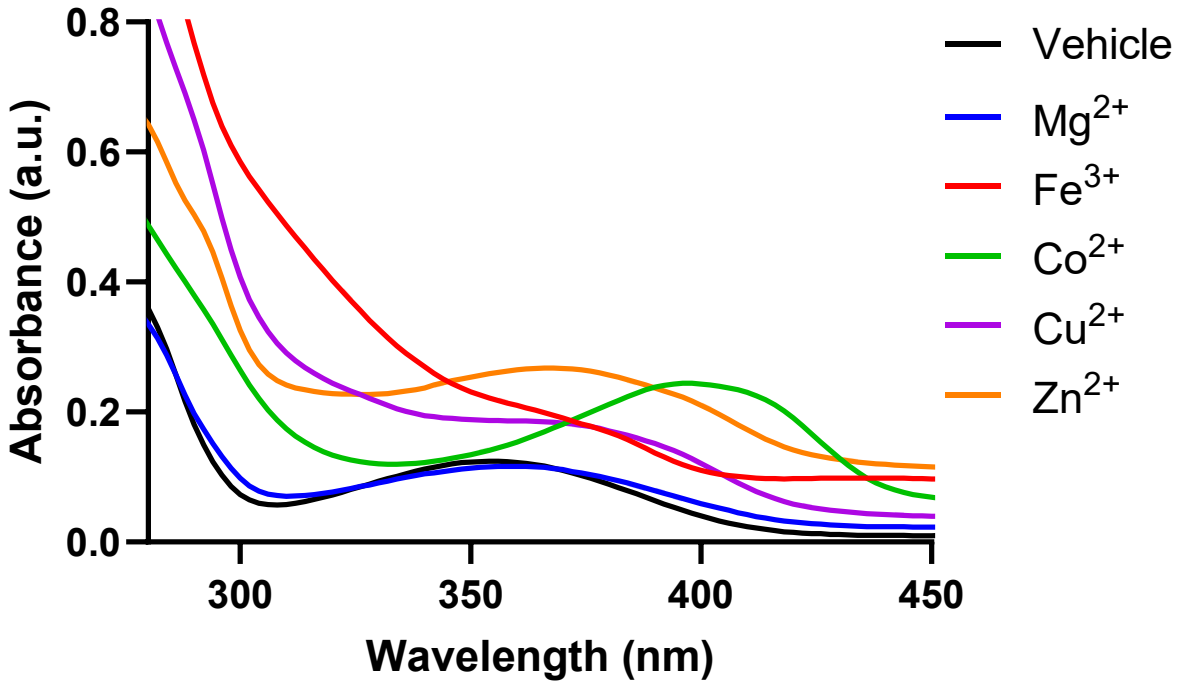


Figure S11. Absorbance plot of TRENTAM (10 μM) in PBS 24 hours post-treatment with 20 equivalents of $MgCl_2$, $FeCl_3 \cdot 6H_2O$, $CoCl_2$, $Cu(OAc)_2 \cdot H_2O$, or $Zn(OAc)_2$. Error bars not shown (*n* = 3).

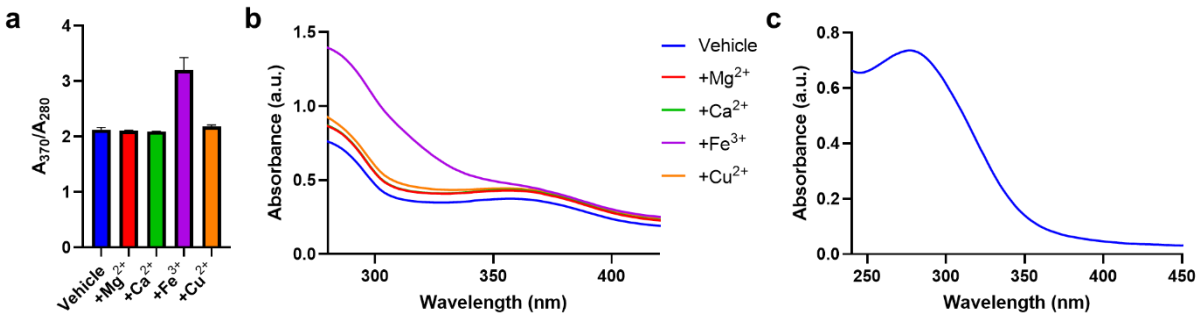
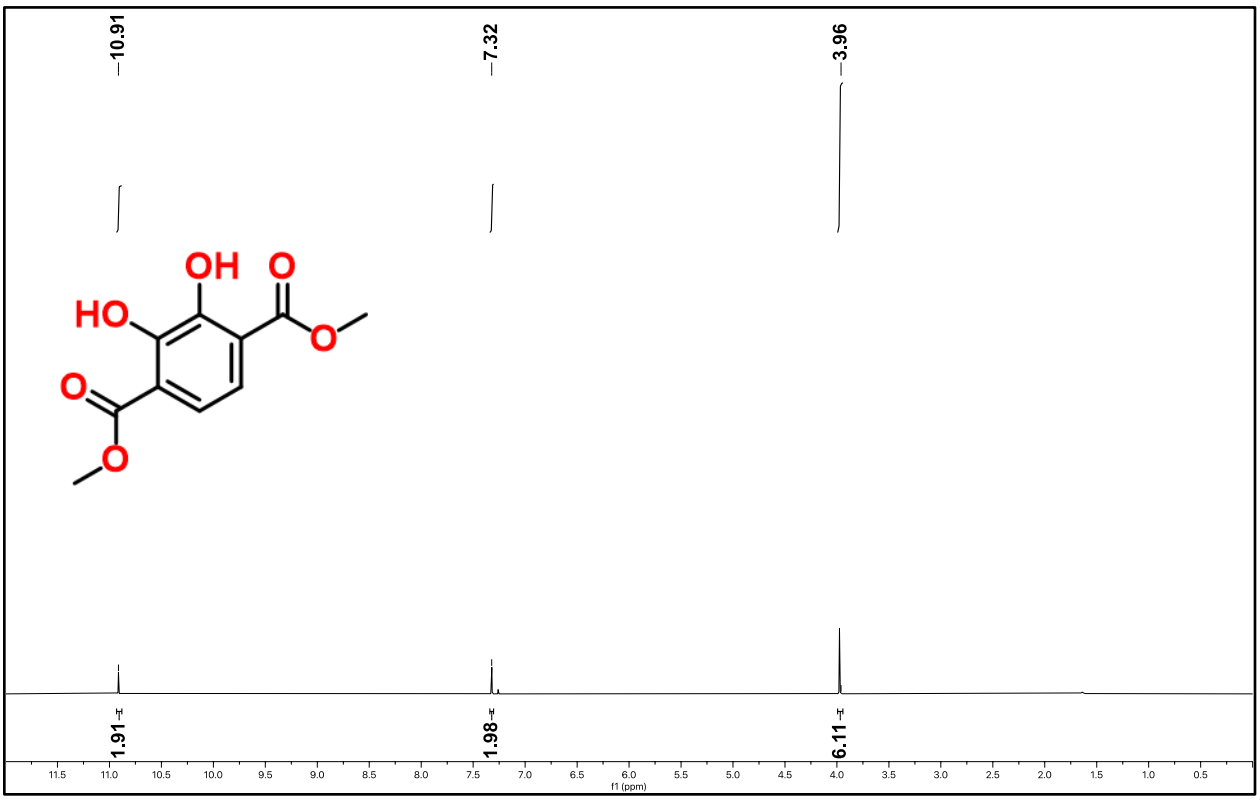
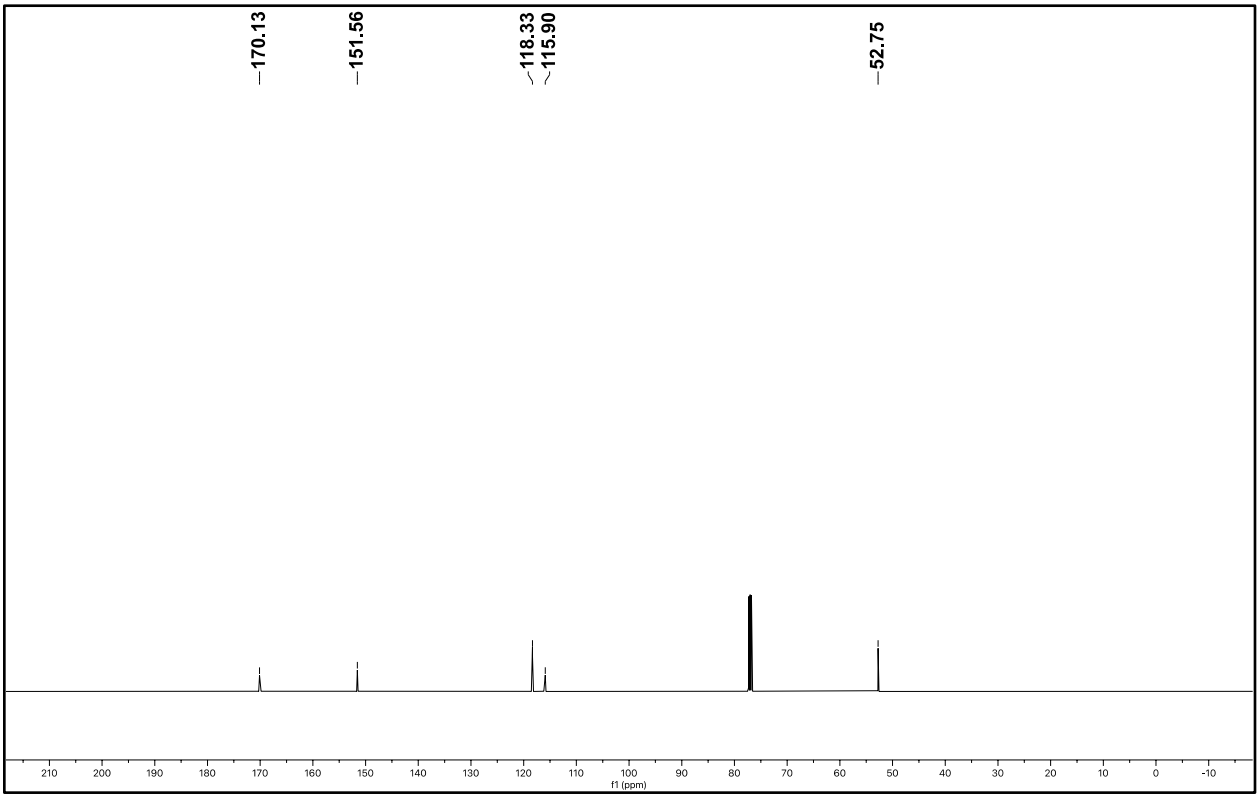


Figure S12. a. Ratiometric change in Zr-TRENTAM (10 μM) absorbance at 280 and 370 nm 24 hours post-treatment with 20 equivalents of $MgCl_2$, $CaCl_2$, $FeCl_3 \cdot 6H_2O$, or $Cu(OAc)_2 \cdot H_2O$ in PBS. Error bars = SD (*n* = 3). **b.** Absorbance spectra corresponding to **a**. Error bars not shown. **c.** Absorbance spectrum of $FeCl_3 \cdot 6H_2O$ (200 μM) in PBS indicating spectral overlap.

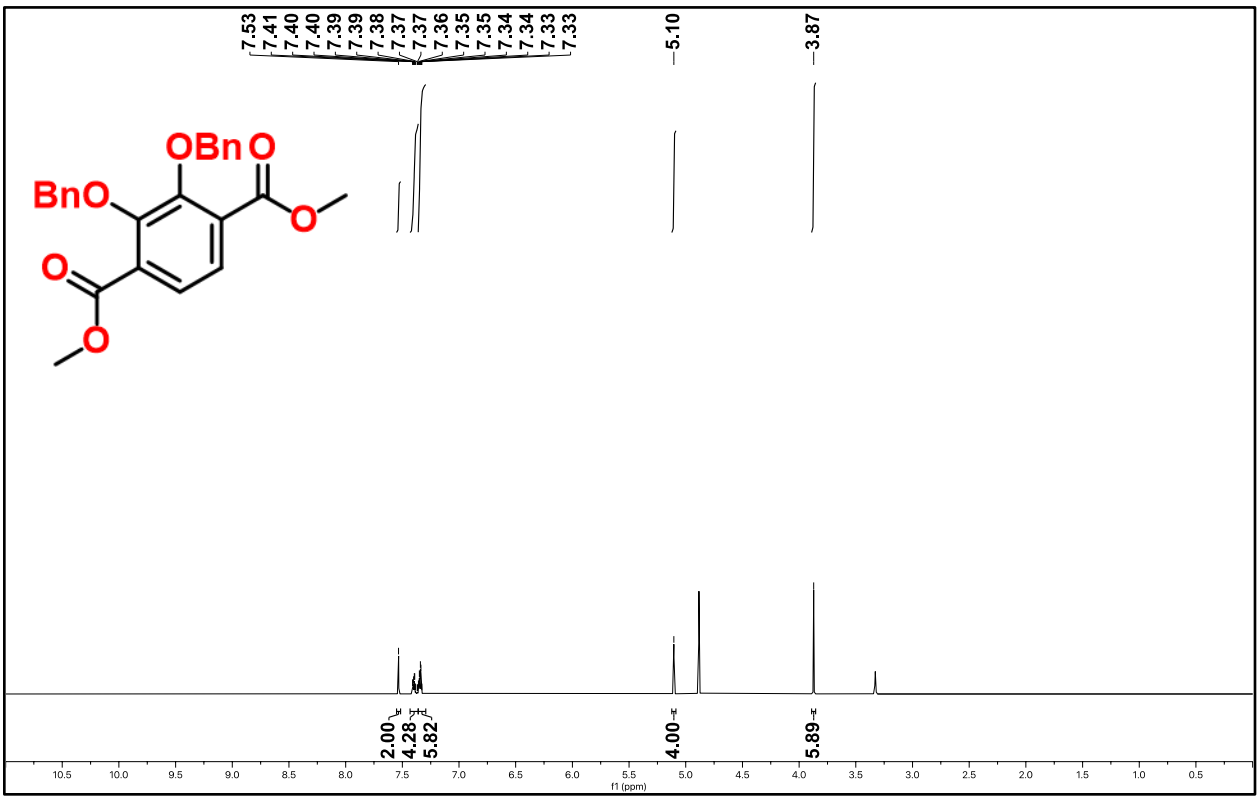
Compound Me_2TAM: ^{1}H NMR (500 MHz, $CDCl_3$)



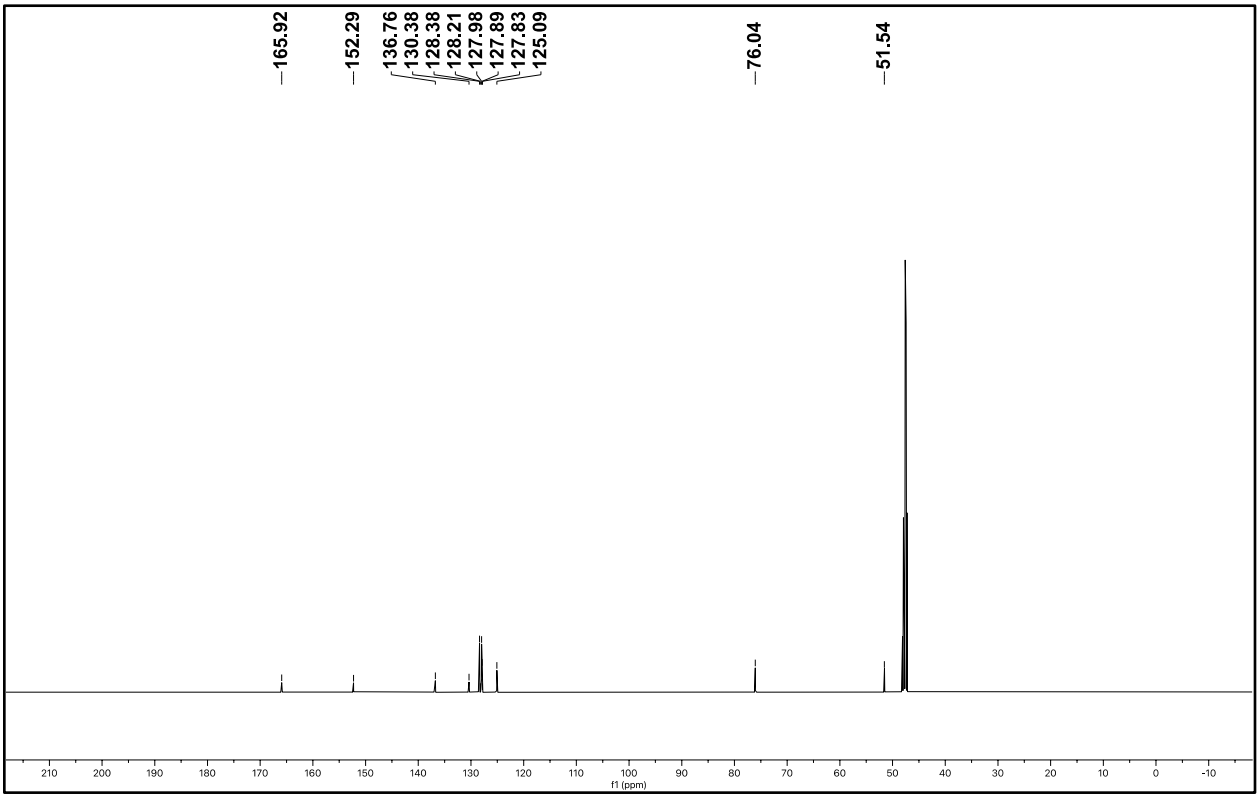
Compound Me_2TAM: ^{13}C NMR (125 MHz, $CDCl_3$)



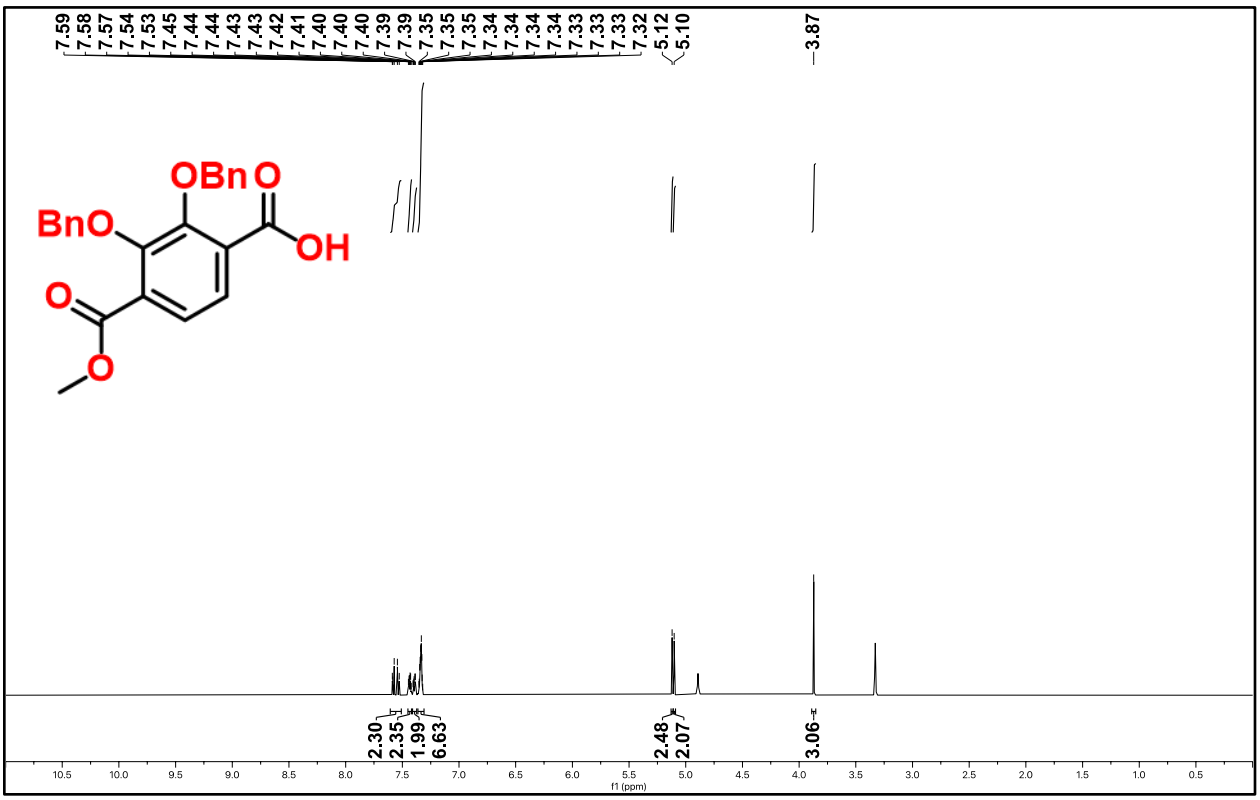
Compound Me_2Bn_2TAM: ^1H NMR (500 MHz, CD_3OD)



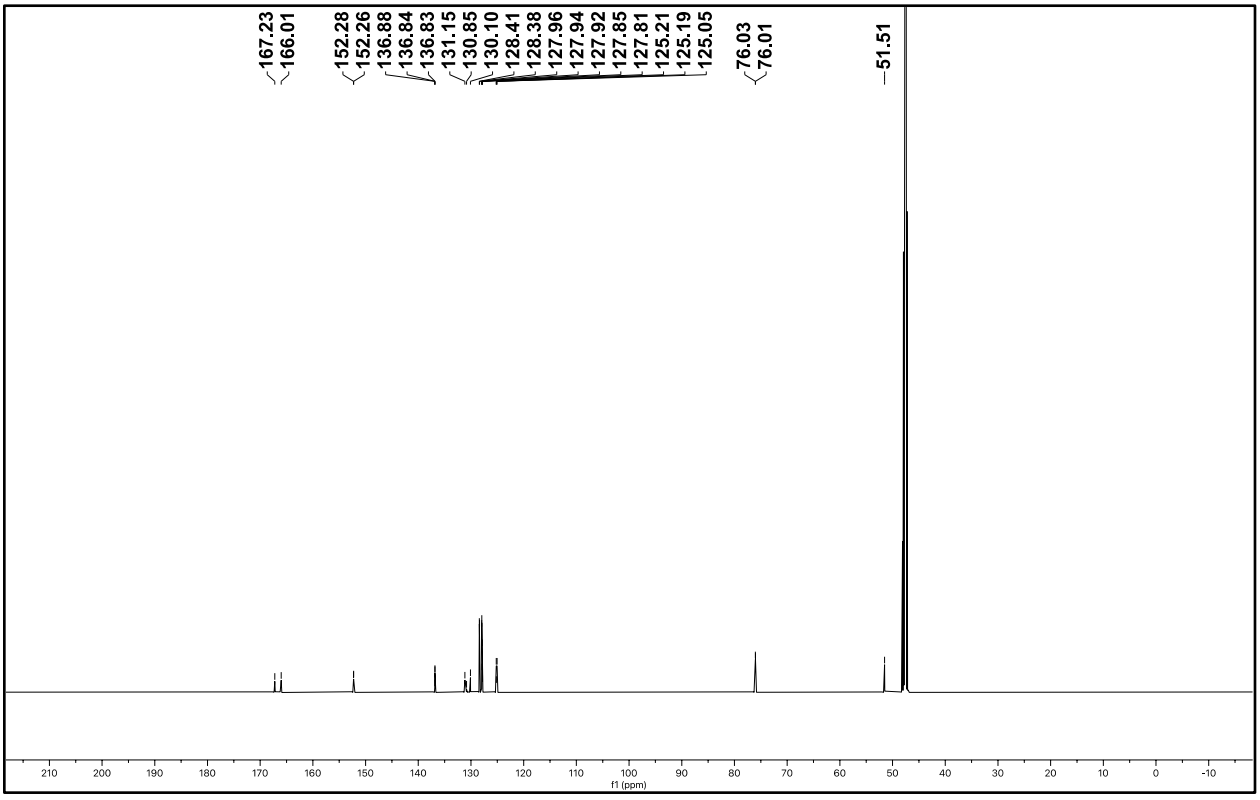
Compound Me_2Bn_2TAM: ^{13}C NMR (125 MHz, CD_3OD)



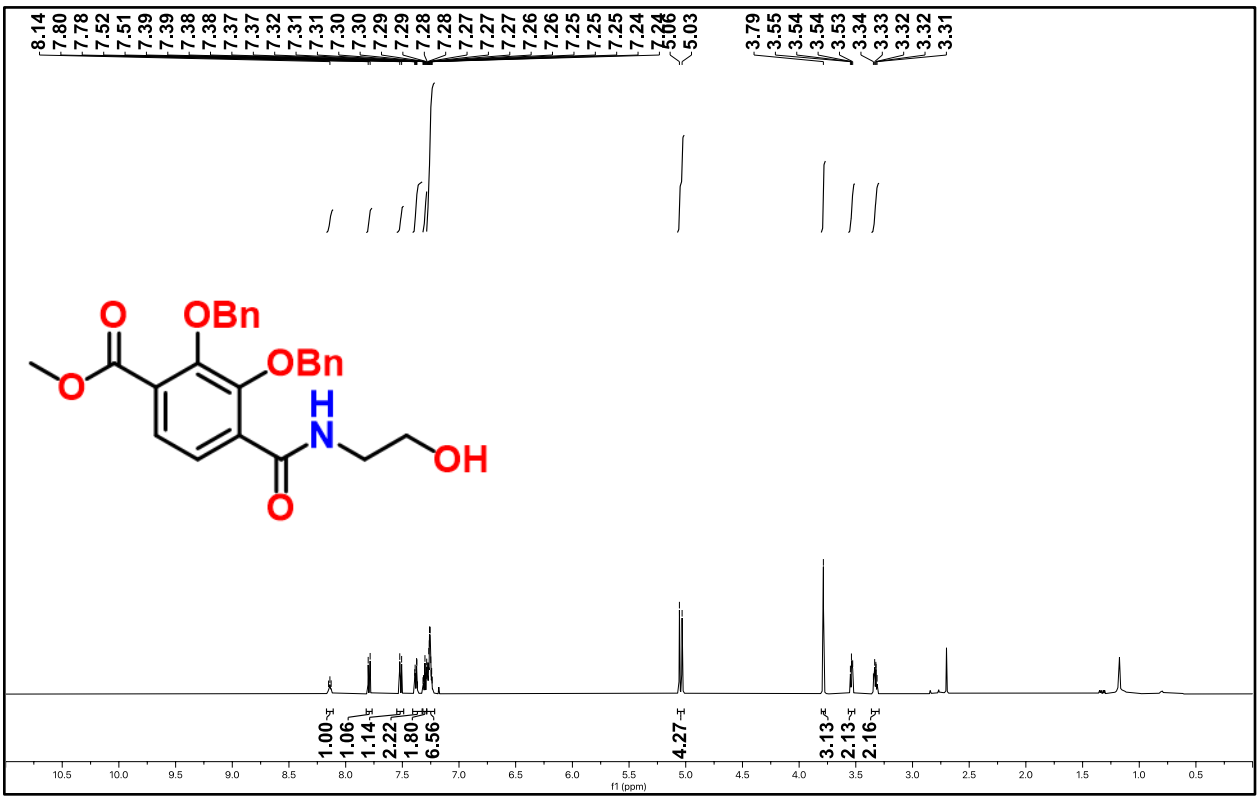
Compound MeBn$_2$TAM-COOH: ^{1}H NMR (500 MHz, CD_3OD)



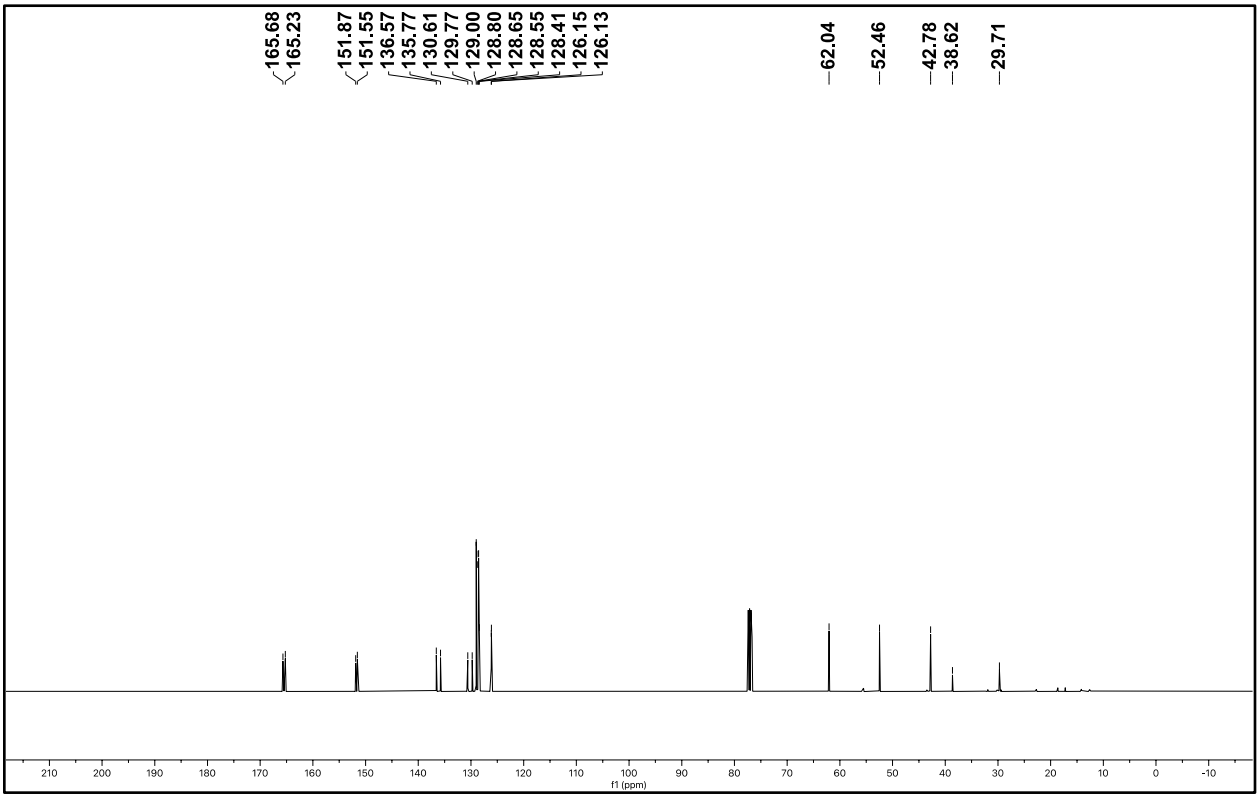
Compound MeBn$_2$TAM-COOH: ^{13}C NMR (125 MHz, CD_3OD)



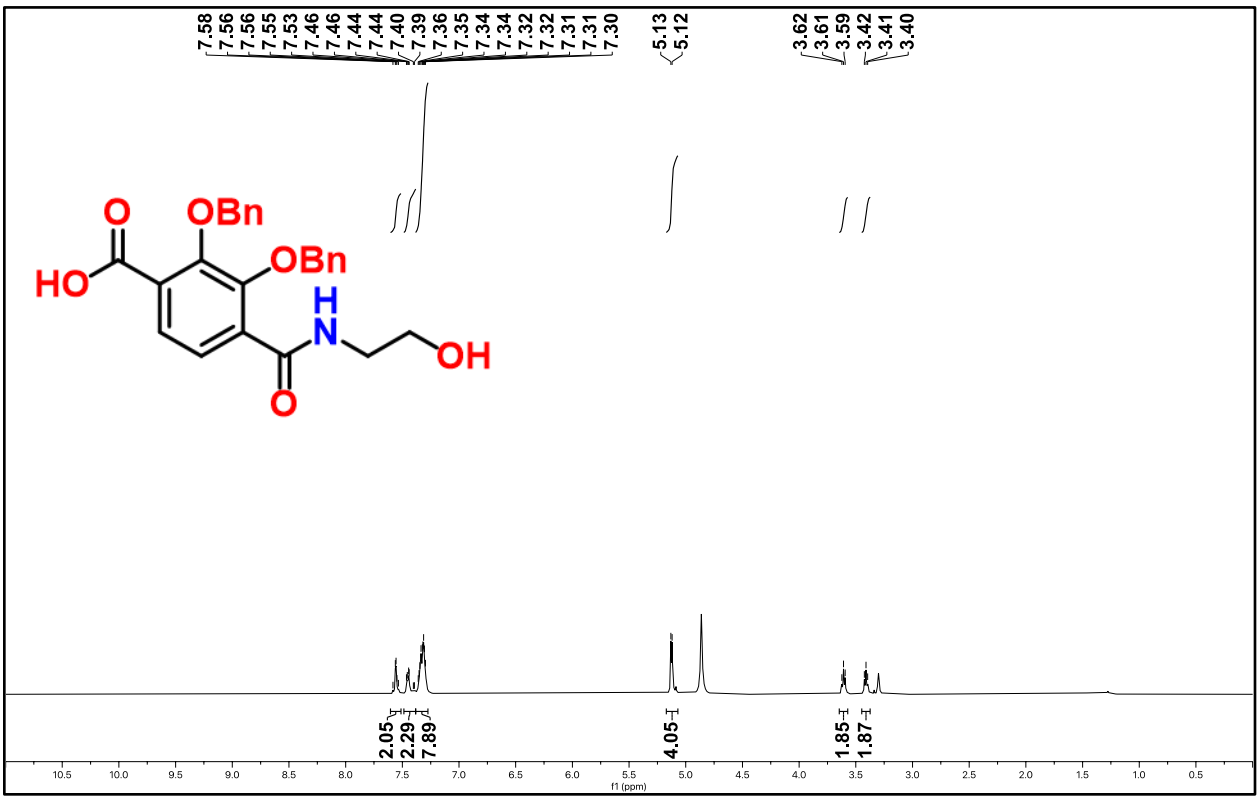
Compound MeBn$_2$TAM-EtOH: ^{1}H NMR (500 MHz, $CDCl_3$)



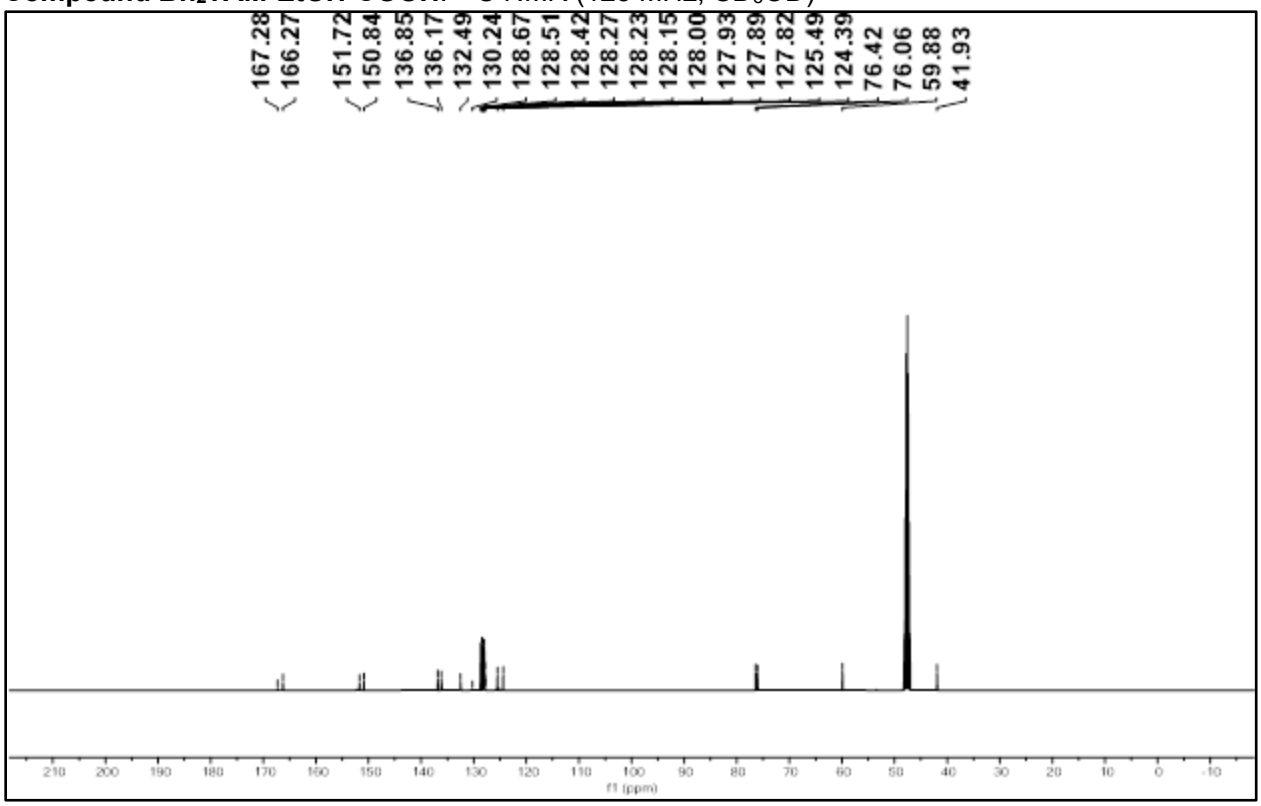
Compound MeBn$_2$TAM-EtOH: ^{13}C NMR (125 MHz, $CDCl_3$)



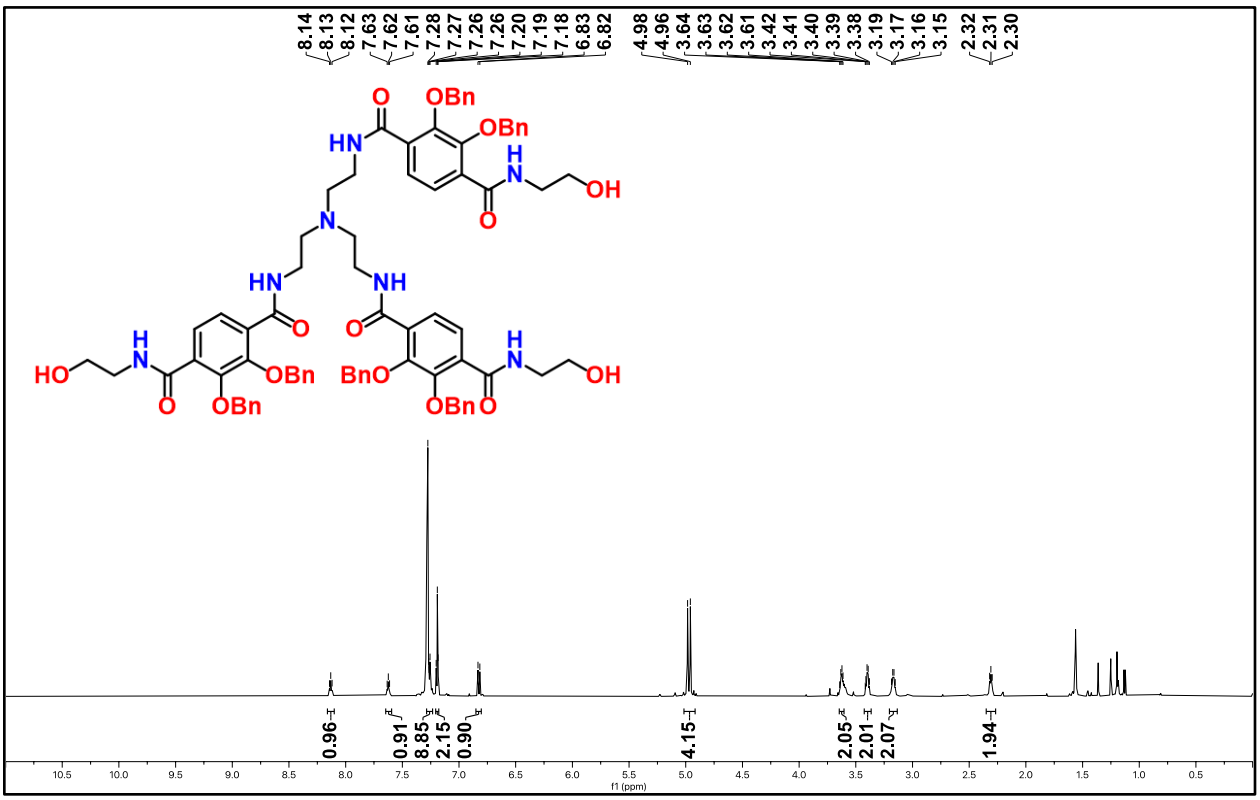
Compound Bn_2TAM-EtOH-COOH: ^{1}H NMR (400 MHz, CD_3OD)



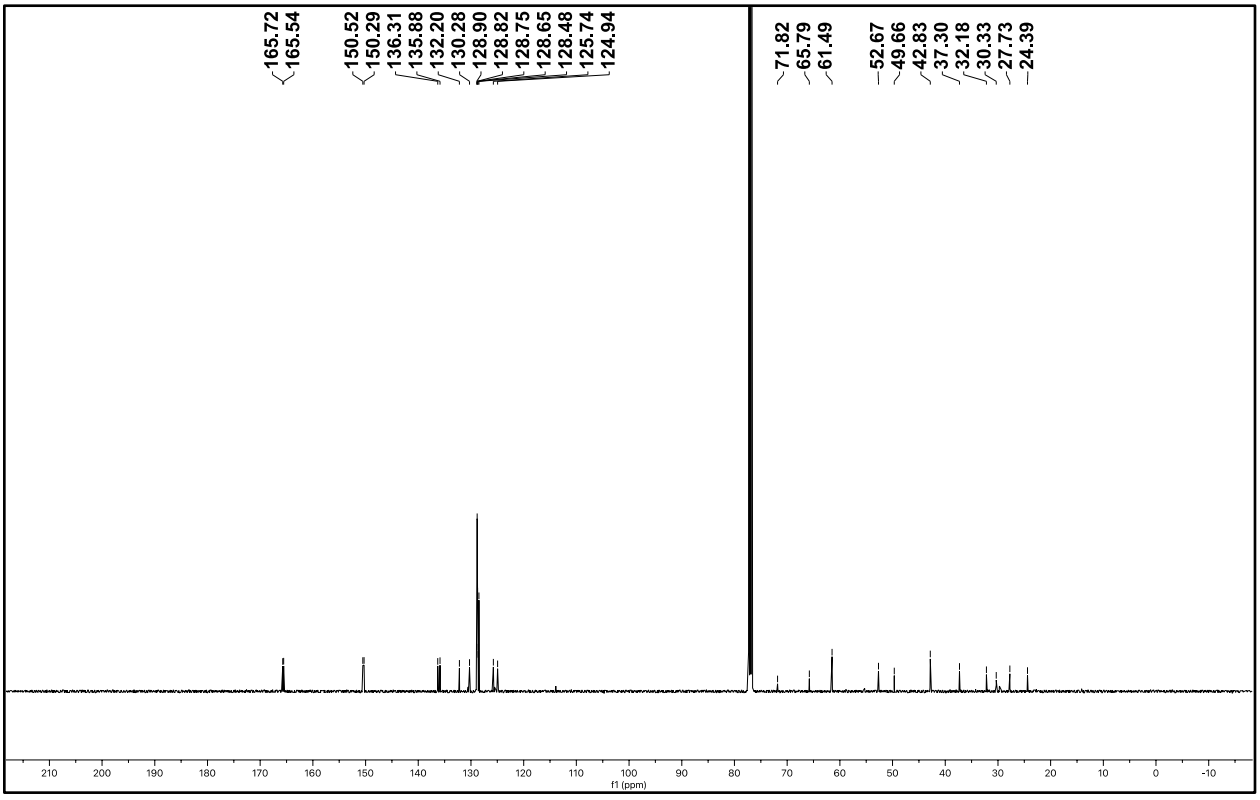
Compound Bn_2TAM-EtOH-COOH: ^{13}C NMR (125 MHz, CD_3OD)



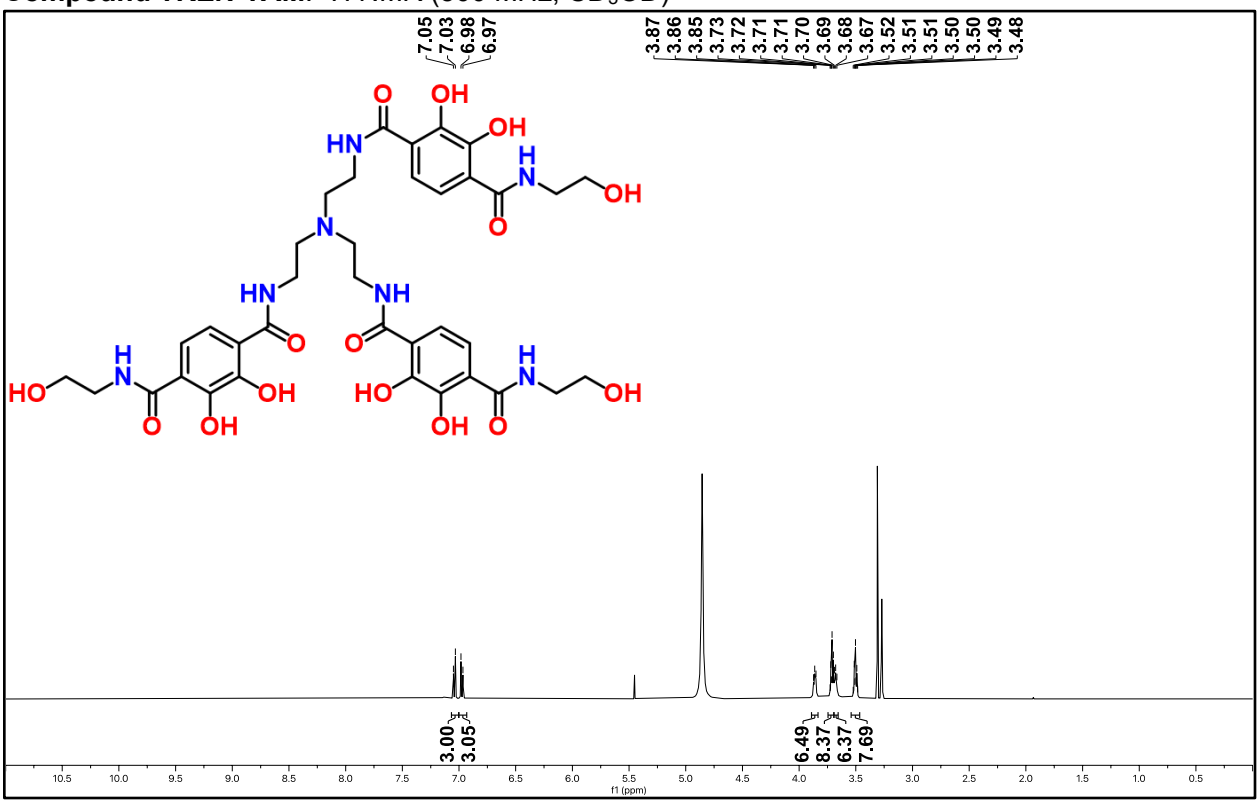
Compound TREN-TAMBn$_6$: ^{1}H NMR (500 MHz, $CDCl_3$)



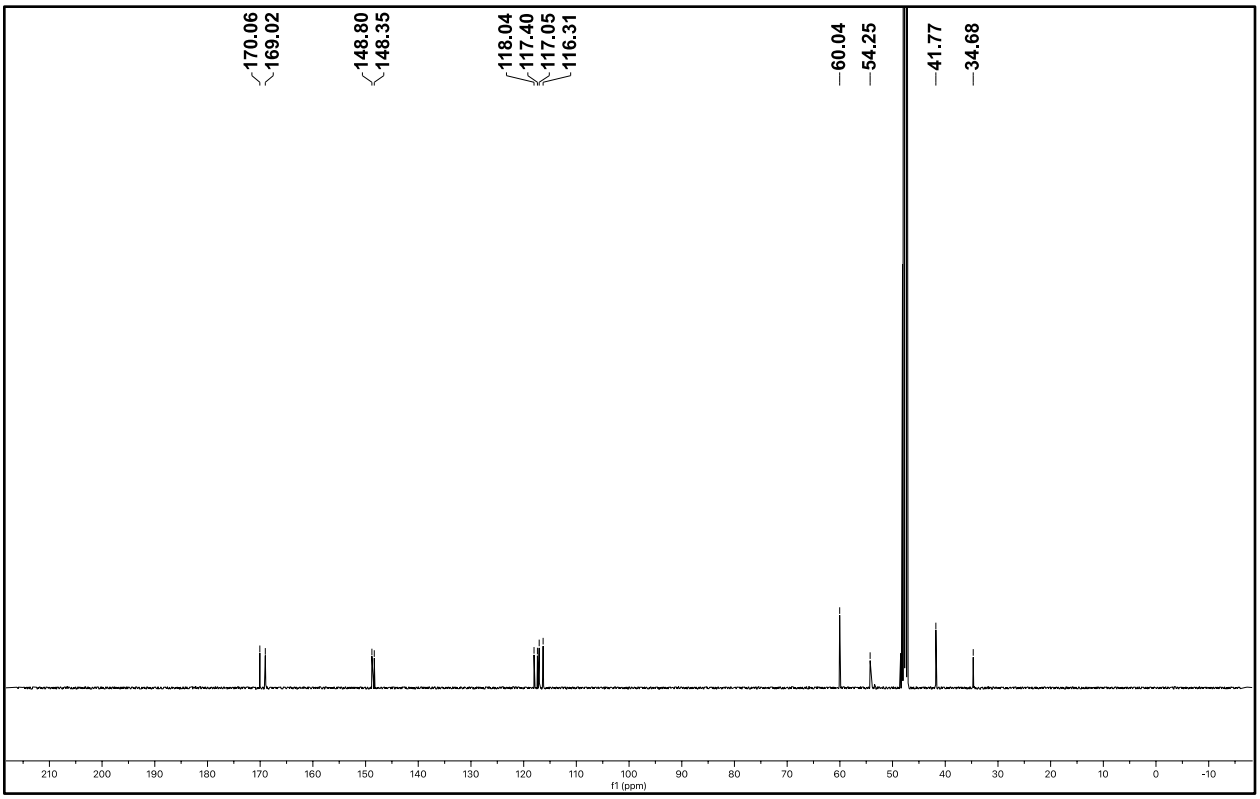
Compound TREN-TAMBn$_6$: ^{13}C NMR (125 MHz, $CDCl_3$)



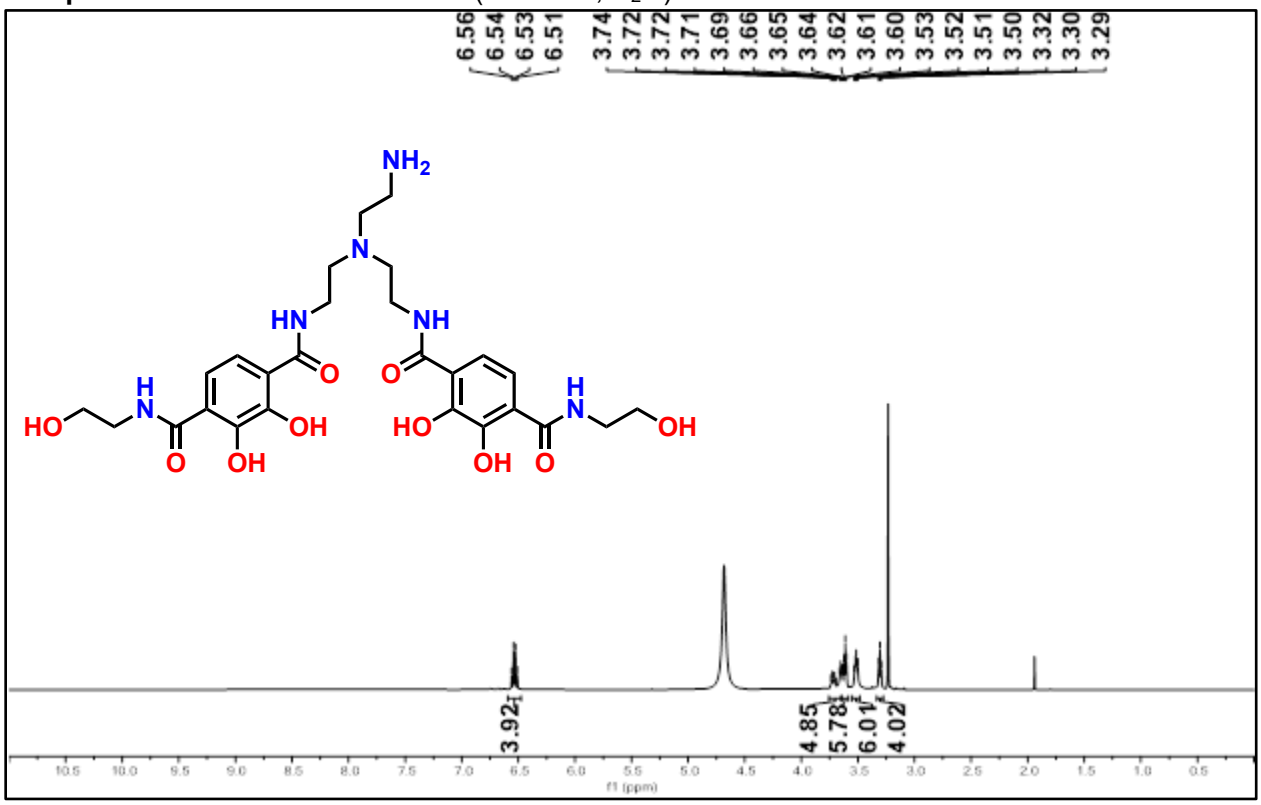
Compound TREN-TAM: ^{1}H NMR (500 MHz, CD_3OD)



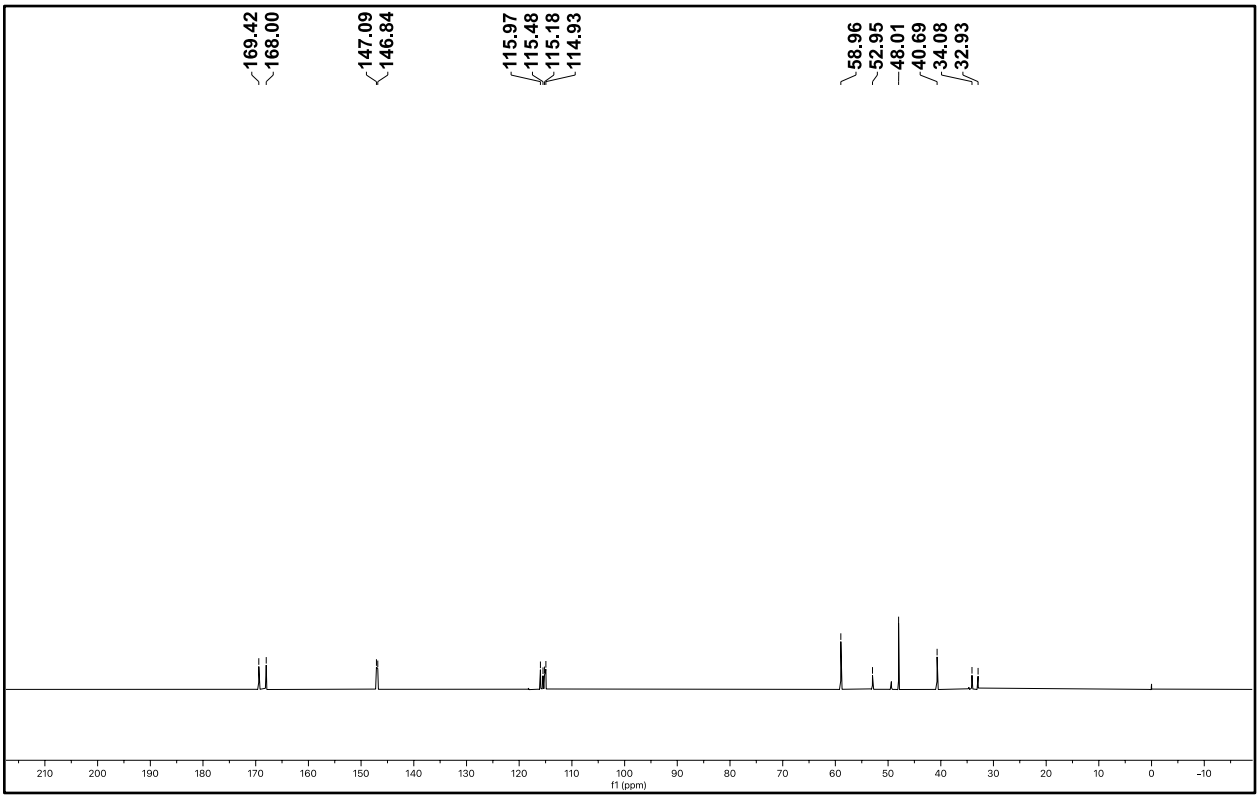
Compound TREN-TAM: ^{13}C NMR (125 MHz, CD_3OD)



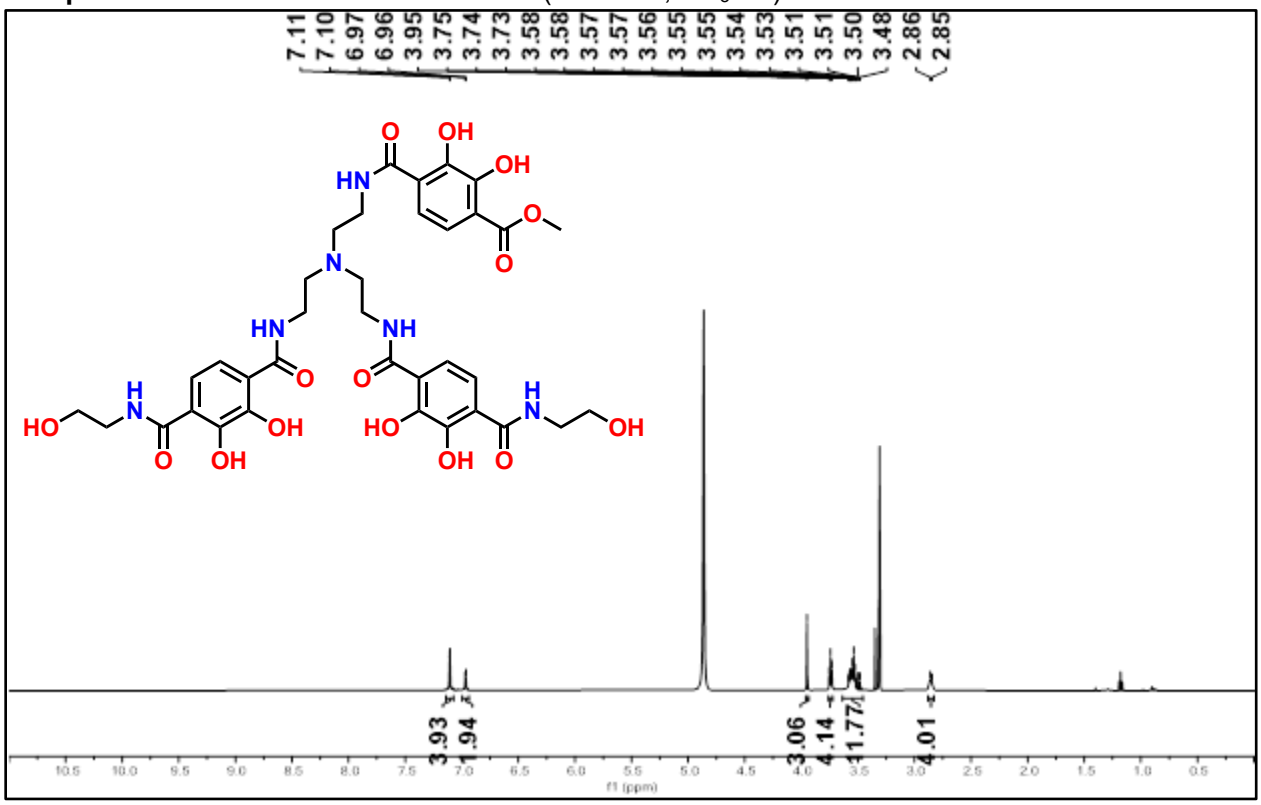
Compound TREN-BisTAM: ^{1}H NMR (500 MHz, D_2O)



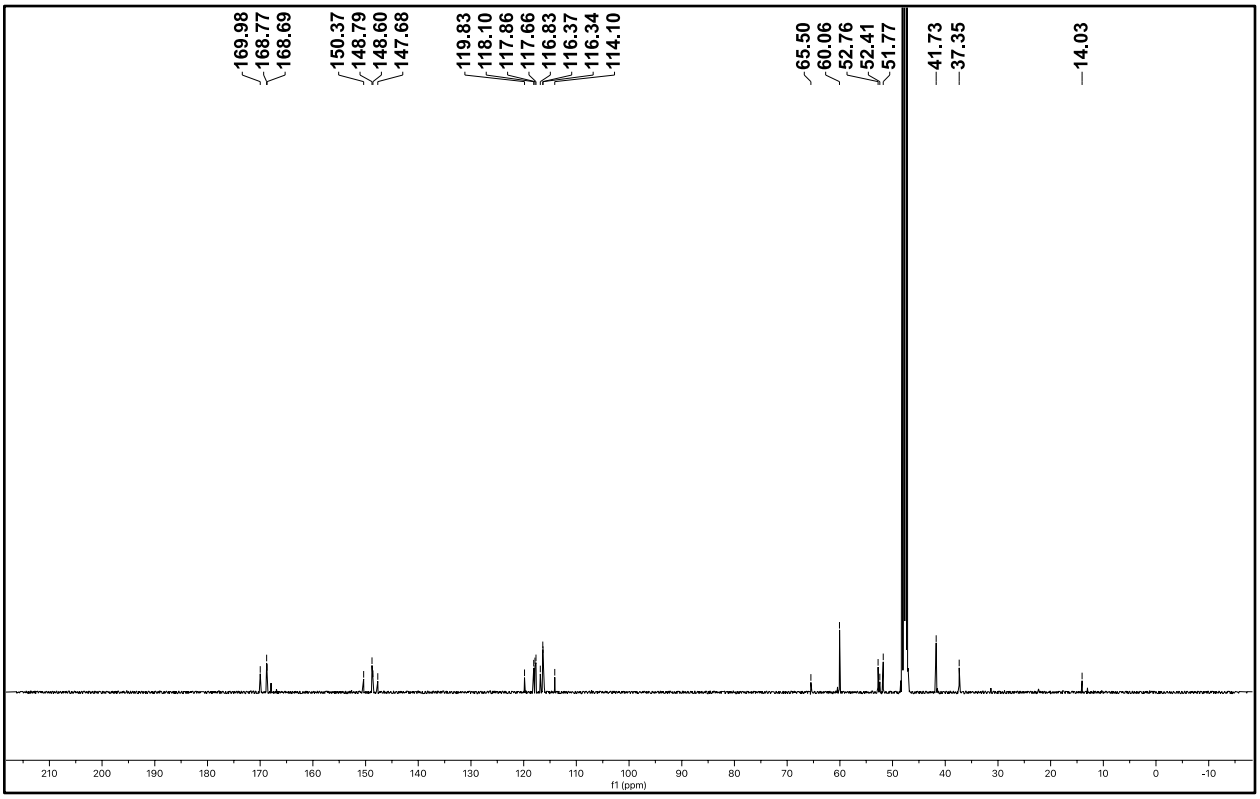
Compound TREN-BisTAM: ^{13}C NMR (125 MHz, D_2O)



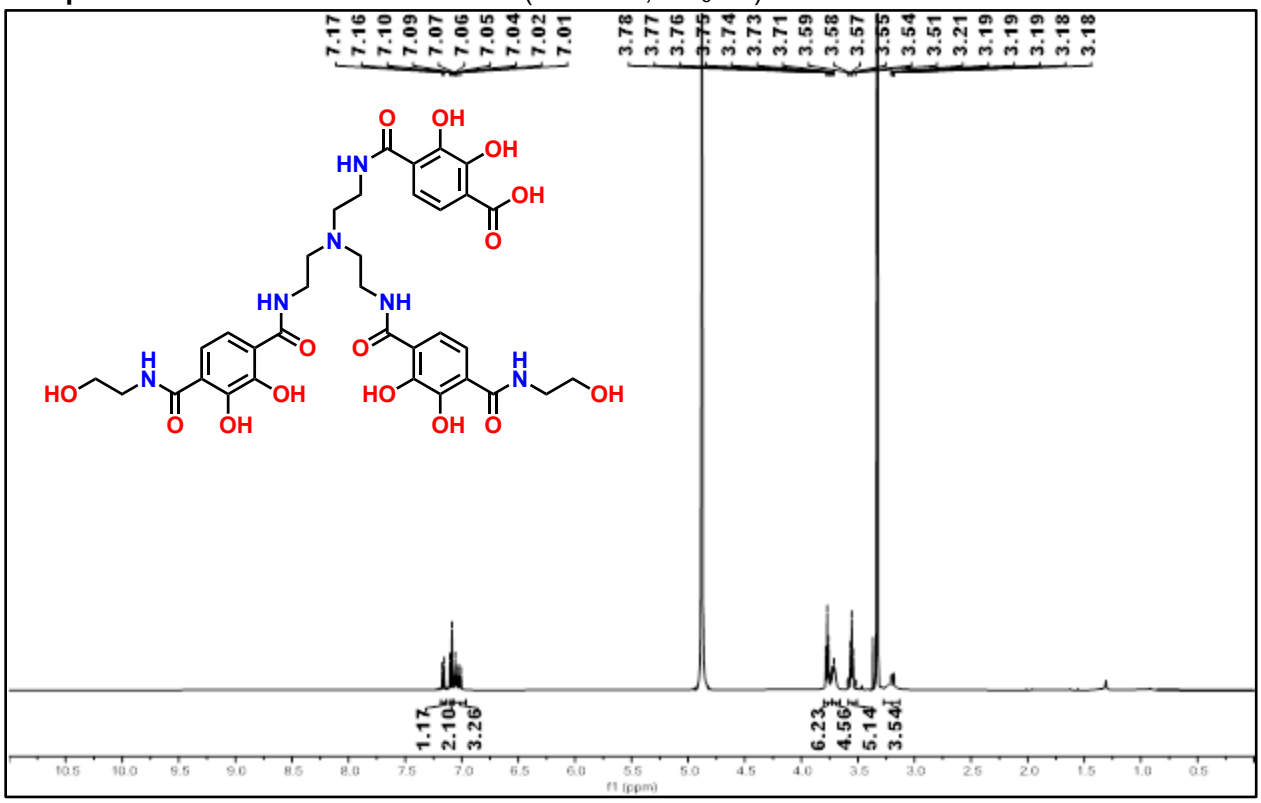
Compound TREN-TAM-COOMe: ^{1}H NMR (500 MHz, CD_3OD)



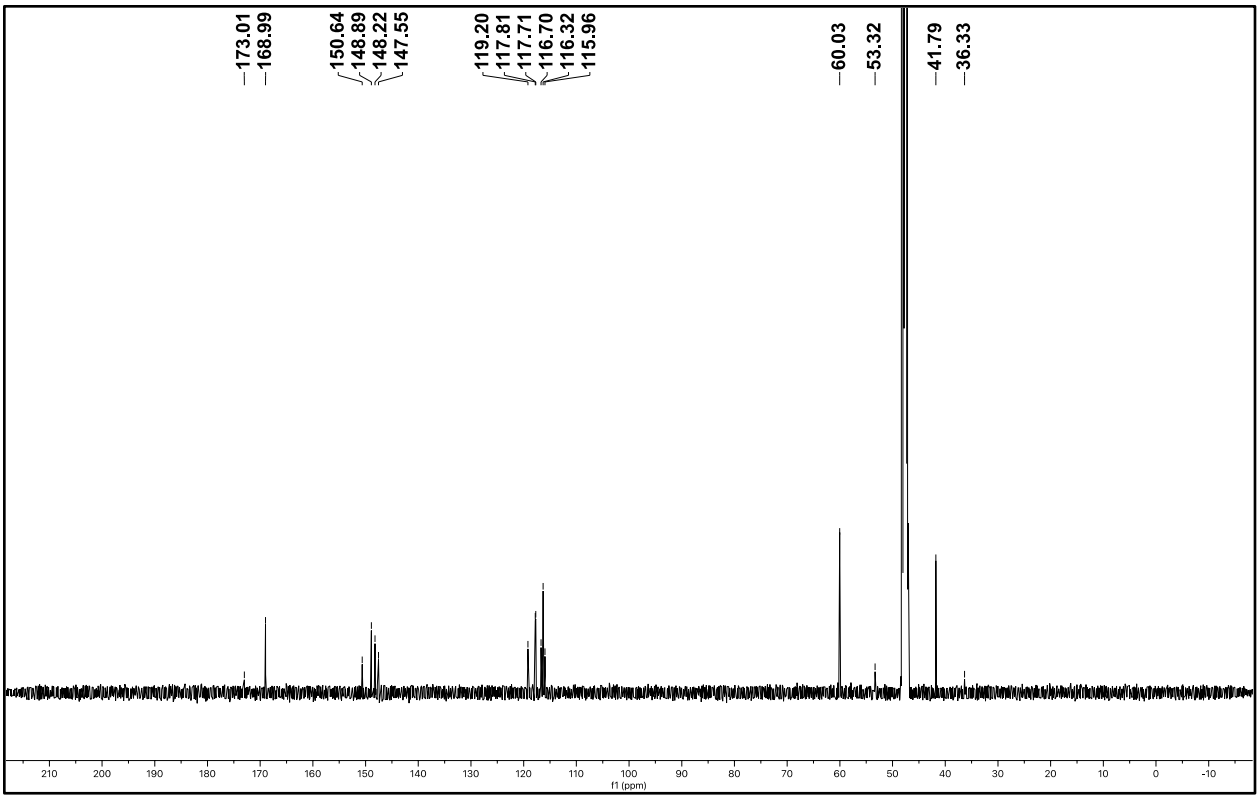
Compound TREN-TAM-COOMe: ^{13}C NMR (125 MHz, CD_3OD)



Compound TREN-TAM-COOH: ^{1}H NMR (500 MHz, CD_3OD)

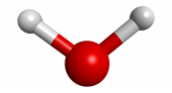


Compound TREN-TAM-COOH: ^{13}C NMR (125 MHz, CD_3OD)



Quantum Chemistry Data: Electronic energies (*E*) in hartree, thermochemical Gibbs free energies ($G_{298.15}$) in kcal/mol, and optimized structures in Angstroms (M11/DZVP/PCM geometries shown unless otherwise indicated).

1. H_2O



B3LYP/DZVP: $E = -76.398771$, $G_{298.15} = 1.833$

ATOM	CHARGE	X	Y	Z
O	8.0	-0.0784379497	-1.0925354244	-3.0336601423
H	1.0	-0.4709422182	-0.3114718106	-3.4523307996
H	1.0	-0.6344148420	-1.8374047151	-3.3083768581

M11-L/DZVP: $E = -76.388382$

ATOM	CHARGE	X	Y	Z
O	8.0	-0.0784235998	-1.0925402857	-3.0336489100
H	1.0	-0.4724477309	-0.3254789003	-3.4510129722
H	1.0	-0.6329236792	-1.8233927641	-3.3097059178

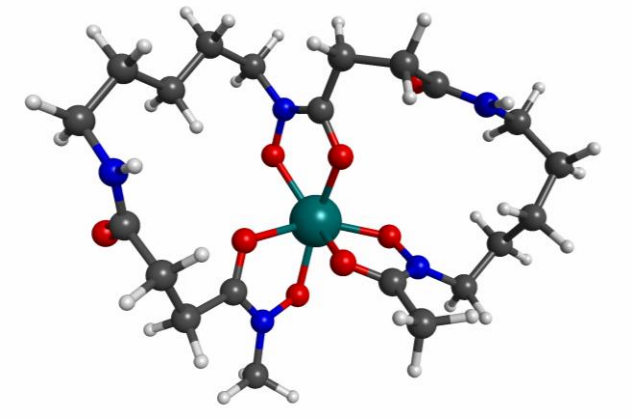
B3LYP/DZVP/PCM: $E = -76.409180$, $G_{298.15} = 1.768$

ATOM	CHARGE	X	Y	Z
O	8.0	-0.0747041216	-1.0926556294	-3.0309343572
H	1.0	-0.4730805633	-0.3140233320	-3.4534412654
H	1.0	-0.6360103252	-1.8347329886	-3.3099921773

M11-L/DZVP/PCM: $E = -76.398948$

ATOM	CHARGE	X	Y	Z
O	8.0	-0.0751532596	-1.0926556688	-3.0312597458
H	1.0	-0.4743135320	-0.3276067242	-3.4519988389
H	1.0	-0.6343282183	-1.8211495570	-3.3111092153

2. $[Zr(DFO)]^+$



B3LYP/DZVP: $E = -5237.255236$, $G_{298.15} = 332.303$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0799896353	-1.0820457408	0.4487556385
C	6.0	-3.0439172726	-3.5189181815	-1.2348916721
N	7.0	-2.2579367982	-2.7916851622	-0.2418222912
C	6.0	-2.6005513814	-2.3039305866	0.9393773502
C	6.0	-3.9288895275	-2.5464752245	1.6085089406
C	6.0	-4.6521695950	-1.2282246946	1.9377017397
C	6.0	-4.9628157423	-0.4233920890	0.6702651360
O	8.0	-4.8232311173	-0.9190133767	-0.4516411496
N	7.0	-5.3850971678	0.8548351136	0.8780421828
C	6.0	-5.7126524425	1.7917212976	-0.2022061208
C	6.0	-4.6428961858	2.8798306073	-0.4067877428
C	6.0	-3.2837458428	2.3211767270	-0.8505201045
C	6.0	-2.1774379795	3.3846013259	-0.9183046396
C	6.0	-0.7967737607	2.8193795571	-1.2884354819
N	7.0	-0.3426926064	1.7717408221	-0.3573319936
C	6.0	0.2463847344	1.8898001940	0.8186623290
C	6.0	0.6609129681	3.2084305554	1.4160862408
C	6.0	2.1583294649	3.2048540297	1.7795587845
C	6.0	3.0268219877	2.9132287848	0.5498825113
O	8.0	2.5662462216	2.9987240838	-0.5920431182
N	7.0	4.3079772750	2.5327690120	0.8131179777
C	6.0	5.2854473778	2.2097192199	-0.2300579879
C	6.0	6.1612225416	1.0067723483	0.1553926157
C	6.0	5.4120995276	-0.3198590473	0.3840977618
C	6.0	4.8462919713	-0.9558107677	-0.8953707577
C	6.0	4.1128324410	-2.2849249125	-0.6588056464
N	7.0	2.8715385593	-2.1148300177	0.1080870779
C	6.0	2.5522225787	-2.5561434303	1.3169610758
C	6.0	3.4858333675	-3.4058088711	2.1362775535
O	8.0	-0.9828711220	-2.5020517263	-0.6664796238
O	8.0	-1.7225753184	-1.5812153599	1.5593784257
O	8.0	-0.6171022651	0.4852320205	-0.7528575597
O	8.0	0.4957137785	0.7972704453	1.4679432385
O	8.0	1.9246899734	-1.3477090153	-0.5222474452

O	8.0	1.3853403042	-2.2494091230	1.7715827260
H	1.0	-4.0588399822	-3.6691696480	-0.8774197822
H	1.0	-3.0738090508	-2.9180956056	-2.1458890275
H	1.0	-4.5703513925	-3.1882511111	1.0079689135
H	1.0	-3.7122505103	-3.0710326037	2.5464520343
H	1.0	-4.0486135096	-0.6317429249	2.6294324500
H	1.0	-5.5899001665	-1.4651666703	2.4538052285
H	1.0	-5.4682542394	1.1825379357	1.8330982338
H	1.0	-5.8356191133	1.1949173691	-1.1085800768
H	1.0	-6.6785089600	2.2565251548	0.0250776897
H	1.0	-5.0252760373	3.5892032597	-1.1522005178
H	1.0	-4.5278308341	3.4490926809	0.5269763166
H	1.0	-3.3874378294	1.8342782859	-1.8281714266
H	1.0	-2.9812218915	1.5305009292	-0.1558348616
H	1.0	-2.4249391704	4.1475841625	-1.6677589933
H	1.0	-2.1068600588	3.9117308957	0.0428580838
H	1.0	-0.0277576368	3.5940969655	-1.3268720494
H	1.0	-0.8199030702	2.3302663265	-2.2641190900
H	1.0	0.4432565065	4.0292269607	0.7345485849
H	1.0	0.0745537312	3.3575638930	2.3298518649
H	1.0	2.3537357129	2.4710061499	2.5673222340
H	1.0	2.4218263692	4.1900259970	2.1821747532
H	1.0	4.6287414572	2.5589622017	1.7742645302
H	1.0	4.7165948006	2.0258413310	-1.1432181813
H	1.0	5.9283520427	3.0781448795	-0.4233189881
H	1.0	6.9123127406	0.8769385865	-0.6334572306
H	1.0	6.7242328674	1.2556130638	1.0652022002
H	1.0	4.6017219411	-0.1545138151	1.1059371810
H	1.0	6.1090381146	-1.0261572593	0.8551355552
H	1.0	4.1611912631	-0.2728816495	-1.4063327079
H	1.0	5.6630761548	-1.1676045043	-1.5964056644
H	1.0	4.7420938343	-2.9984182815	-0.1215769759
H	1.0	3.8253410900	-2.7366184035	-1.6133064358
H	1.0	3.0355757552	-3.5494075577	3.1186563290
H	1.0	3.6300895957	-4.3857614717	1.6698147712
H	1.0	4.4649407355	-2.9352283452	2.2562213177
H	1.0	-2.5575639518	-4.4771240151	-1.4336909734

M11-L/DZVP: $E = -5237.000282$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0067039169	-1.0990352516	0.0136170236
C	6.0	-3.2114219669	-3.6132893409	-1.0796021435
N	7.0	-2.3231560779	-2.8986957458	-0.2295017846
C	6.0	-2.5593201915	-2.2701878752	0.8885426910
C	6.0	-3.7791085010	-2.4522008938	1.7068818891
C	6.0	-4.3294843216	-1.1058655564	2.0953089235
C	6.0	-4.6350062601	-0.3121963288	0.8544642373
O	8.0	-4.3752963045	-0.7539235721	-0.2438821296

N	7.0	-5.1833209733	0.8903024519	1.0489677712
C	6.0	-5.5356547605	1.7660503852	-0.0320849123
C	6.0	-4.4993796059	2.8258135097	-0.3033712389
C	6.0	-3.1822258034	2.2673753708	-0.7673294881
C	6.0	-2.1512379870	3.3344383629	-1.0210575147
C	6.0	-0.8452702469	2.7848475391	-1.5332197223
N	7.0	-0.3407037183	1.7287051148	-0.7044830104
C	6.0	0.2511498299	1.7962967298	0.4531504615
C	6.0	0.6696380740	3.0760116802	1.0678270037
C	6.0	2.0265307348	2.9258350077	1.7026056432
C	6.0	3.0260928805	2.4797649952	0.6707337862
O	8.0	2.6602991256	2.0430707172	-0.3986862798
N	7.0	4.3121618491	2.5795636762	1.0192107971
C	6.0	5.3822619564	2.1814516398	0.1521039342
C	6.0	6.0343686282	0.8907172145	0.5782817735
C	6.0	5.1359731121	-0.3201116717	0.5396665884
C	6.0	4.7304338662	-0.7498750695	-0.8471551098
C	6.0	4.0532570709	-2.0943987265	-0.8698326334
N	7.0	2.7904515932	-2.0738860229	-0.1913915141
C	6.0	2.4634141583	-2.4056728014	1.0299241746
C	6.0	3.3730656611	-3.0894013774	1.9610808576
O	8.0	-1.1653668700	-2.5659031387	-0.8113385847
O	8.0	-1.6638604714	-1.4878608400	1.3037628387
O	8.0	-0.6565227506	0.4905497208	-1.0980898526
O	8.0	0.4556443622	0.7149764778	1.0647514028
O	8.0	1.8398391760	-1.4229474855	-0.8640028577
O	8.0	1.2919551431	-2.1283263897	1.3956551777
H	1.0	-4.0382912047	-4.0232933654	-0.5061430988
H	1.0	-3.5970758452	-2.9416081813	-1.8500630958
H	1.0	-4.5347744733	-3.0361570073	1.1824726651
H	1.0	-3.4917954186	-3.0076145344	2.6062377006
H	1.0	-3.6018871213	-0.5616404132	2.7075794789
H	1.0	-5.2271661470	-1.2279231723	2.7100685458
H	1.0	-5.3699644238	1.1882467225	1.9944690459
H	1.0	-5.6777939404	1.1369743952	-0.9167520181
H	1.0	-6.5029881652	2.2253079642	0.1977382603
H	1.0	-4.9037056406	3.5129458515	-1.0589598361
H	1.0	-4.3506544630	3.4340830289	0.6020609589
H	1.0	-3.3308711916	1.6643639776	-1.6746783879
H	1.0	-2.7999488831	1.5565980270	-0.0181658707
H	1.0	-2.5219779146	4.0618275881	-1.7554293876
H	1.0	-1.9754414928	3.9103360305	-0.0989492894
H	1.0	-0.0765174858	3.5589156400	-1.6296459262
H	1.0	-0.9652747001	2.3314622272	-2.5203460742
H	1.0	0.6730526940	3.8805003221	0.3288482708
H	1.0	-0.0678591898	3.3428773137	1.8338966249
H	1.0	1.9865803516	2.1729034150	2.4977961491
H	1.0	2.3296771465	3.8655434231	2.1751742855
H	1.0	4.5407492950	2.9631363720	1.9241494490
H	1.0	4.9582022509	2.1062455594	-0.8536311638
H	1.0	6.1278270898	2.9842420873	0.1215585908
H	1.0	6.9099462835	0.7212186420	-0.0625187202

H	1.0	6.4326028637	1.0120266804	1.5945911215
H	1.0	4.2386320712	-0.1270409724	1.1520284618
H	1.0	5.6615299770	-1.1497787273	1.0374872356
H	1.0	4.0674652113	-0.0098992551	-1.3120194939
H	1.0	5.6181697088	-0.8266305497	-1.4885307513
H	1.0	4.6803144625	-2.8653522806	-0.4125999803
H	1.0	3.8389657675	-2.4136647174	-1.8939290711
H	1.0	2.8594833278	-3.9636154557	2.3613676515
H	1.0	4.3192493183	-3.3961052078	1.5250444324
H	1.0	3.5709590625	-2.4250383999	2.8039139295
H	1.0	-2.6580476184	-4.4308635543	-1.5391076305

B3LYP/DZVP/PCM: $E = -5237.323975$, $G_{298.15} = 332.362$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0624256093	-0.8312975339	-0.8858091299
C	6.0	-2.2269158558	-4.5302778851	-0.9290216896
N	7.0	-1.8226381132	-3.1631216913	-0.6280731470
C	6.0	-2.3734008624	-2.2717757178	0.1835542306
C	6.0	-3.5956490815	-2.6054352853	1.0104574694
C	6.0	-4.1702902881	-1.4042319384	1.7632446323
C	6.0	-4.8468190449	-0.3864757735	0.8423100670
O	8.0	-5.2271824162	-0.6898667479	-0.3004993820
N	7.0	-5.0345190717	0.8393844863	1.3915821690
C	6.0	-5.6540444754	1.9769838341	0.7062935439
C	6.0	-4.6544333424	3.1078412218	0.4180027870
C	6.0	-3.5447605239	2.7016046927	-0.5606861186
C	6.0	-2.4628235903	3.7755070959	-0.7283847640
C	6.0	-1.2624297210	3.3130534733	-1.5666849104
N	7.0	-0.5771129225	2.1346682197	-1.0056070633
C	6.0	0.2287179586	2.0605905108	0.0415768666
C	6.0	0.6837505934	3.2858916306	0.7955634428
C	6.0	2.1004333757	3.1319403096	1.3634555873
C	6.0	3.1454718631	2.8238357522	0.2889719666
O	8.0	2.9074152187	2.9744134644	-0.9210278425
N	7.0	4.3367656725	2.3802326690	0.7601830958
C	6.0	5.4544354936	1.9544779093	-0.0864562570
C	6.0	6.2175689631	0.7794250692	0.5441375081
C	6.0	5.3846635603	-0.4963574088	0.7627566314
C	6.0	5.0385995654	-1.2496997721	-0.5299466798
C	6.0	4.0693436599	-2.4193499581	-0.3194574014
N	7.0	2.7069250789	-1.9728340757	-0.0049757256
C	6.0	1.9536214340	-2.2012834277	1.0630520591
C	6.0	2.4803319123	-2.9383785845	2.2643707435
O	8.0	-0.7150307079	-2.7214920021	-1.3098303296
O	8.0	-1.8166742323	-1.1157458919	0.2365549114
O	8.0	-0.8725907245	0.9258702092	-1.5916497517
O	8.0	0.6229402195	0.8914240071	0.3994752718
O	8.0	2.0853618332	-1.2898729067	-1.0217957900

O	8.0	0.7426170909	-1.7800805014	1.0383893639
H	1.0	-3.1054760623	-4.7929095420	-0.3417395583
H	1.0	-2.4577251371	-4.6065207497	-1.9947404953
H	1.0	-4.3642234289	-3.0260085874	0.3570221359
H	1.0	-3.3211221704	-3.3851255932	1.7300316142
H	1.0	-3.4014747368	-0.9200050434	2.3717389469
H	1.0	-4.9329421183	-1.7780677234	2.4563239898
H	1.0	-4.6705540730	0.9996371994	2.3241851906
H	1.0	-6.0861407246	1.5952786489	-0.2209769582
H	1.0	-6.4736253215	2.3524010583	1.3293848419
H	1.0	-5.2172546294	3.9641273771	0.0237681399
H	1.0	-4.2108715510	3.4413485394	1.3665039333
H	1.0	-3.9858567956	2.4739138391	-1.5399397014
H	1.0	-3.0796102555	1.7739319083	-0.2089679062
H	1.0	-2.8754597508	4.6643795748	-1.2222445556
H	1.0	-2.1090871751	4.1094991480	0.2548512869
H	1.0	-0.5281861411	4.1154690362	-1.6765580727
H	1.0	-1.5736894786	3.0121280247	-2.5687010610
H	1.0	0.6243838745	4.1647717417	0.1527072481
H	1.0	-0.0071139037	3.4486963710	1.6317852625
H	1.0	2.1197124496	2.3541204112	2.1317237973
H	1.0	2.3746291133	4.0708443695	1.8577541677
H	1.0	4.4590490531	2.3254437373	1.7652483897
H	1.0	5.0366757131	1.6881829493	-1.0596679941
H	1.0	6.1456174332	2.7914621625	-0.2498694252
H	1.0	7.0790590550	0.5568267289	-0.0974876422
H	1.0	6.6330947851	1.1051116708	1.5067778980
H	1.0	4.4631026651	-0.2331464959	1.2968522839
H	1.0	5.9440166052	-1.1688753197	1.4251441373
H	1.0	4.6065799880	-0.5772341906	-1.2771884168
H	1.0	5.9526480076	-1.6631553432	-0.9732825648
H	1.0	4.4028536923	-3.0745720598	0.4876028134
H	1.0	3.9942343622	-3.0225152296	-1.2297735143
H	1.0	1.7807099139	-2.7913782451	3.0876136471
H	1.0	2.5463862115	-4.0104419278	2.0507641326
H	1.0	3.4681172089	-2.5844218554	2.5663126547
H	1.0	-1.4062549159	-5.2072420634	-0.6804637507

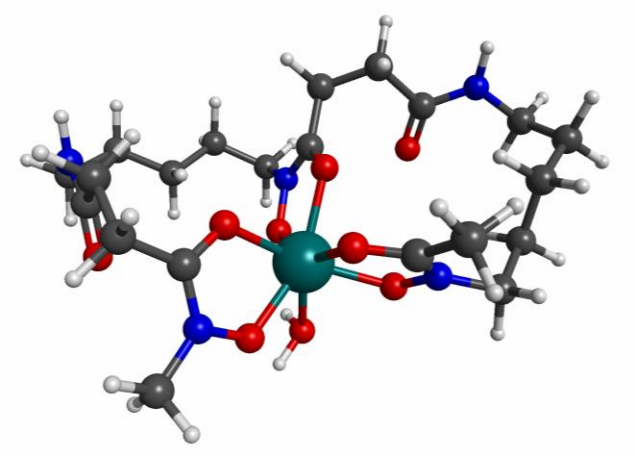
M11-L/DZVP/PCM: $E = -5237.076357$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.1053180786	-0.6525428947	-1.2909337935
C	6.0	-1.6255247299	-4.4893738225	-0.8296292078
N	7.0	-1.4083061882	-3.0903020640	-0.7277191202
C	6.0	-2.1175155951	-2.1833883047	-0.1155100409
C	6.0	-3.2284644169	-2.5643168346	0.7903353494
C	6.0	-3.6557692732	-1.4261365960	1.6662813484
C	6.0	-4.4611107919	-0.3940058515	0.9299030524
O	8.0	-5.0256230508	-0.6438762315	-0.1169763472

N	7.0	-4.5551061458	0.7783589882	1.5612855867
C	6.0	-5.2832776061	1.9030892433	1.0592743235
C	6.0	-4.3771040404	3.0419212775	0.6754388012
C	6.0	-3.4126047662	2.6833423731	-0.4203090781
C	6.0	-2.4623591524	3.8020782338	-0.7447265617
C	6.0	-1.3719377978	3.4074355195	-1.7047589734
N	7.0	-0.6327373028	2.2540046141	-1.2704628076
C	6.0	0.1560486014	2.1416036694	-0.2419232810
C	6.0	0.5658615221	3.3005565365	0.5854333925
C	6.0	1.8816210185	3.0265999640	1.2543722643
C	6.0	2.9438128279	2.6802101846	0.2504542926
O	8.0	2.7963307946	2.8899939378	-0.9389580169
N	7.0	4.0456550600	2.1355246580	0.7648504222
C	6.0	5.1797920428	1.7560187525	-0.0199013290
C	6.0	5.9396417980	0.6446608043	0.6547978754
C	6.0	5.1255538706	-0.6029082806	0.8863275204
C	6.0	4.8100968888	-1.3728702841	-0.3671695688
C	6.0	3.7431294147	-2.4081900064	-0.1535848351
N	7.0	2.4634132247	-1.8020784847	0.0491974629
C	6.0	1.5646454737	-1.9731864425	0.9856272817
C	6.0	1.8842237383	-2.6962884847	2.2301933695
O	8.0	-0.4086263268	-2.6139843882	-1.4708822470
O	8.0	-1.8041736340	-0.9829454183	-0.3134706844
O	8.0	-0.9068764778	1.0932771227	-1.8745919213
O	8.0	0.5779899555	0.9912937600	0.0251888638
O	8.0	2.0080722856	-1.1135001888	-1.0000618141
O	8.0	0.4340037996	-1.4875074295	0.7804949865
H	1.0	-2.4462577210	-4.7877936949	-0.1815822661
H	1.0	-1.8759938175	-4.7421604165	-1.8619467530
H	1.0	-4.0790019381	-2.9100465841	0.1913621143
H	1.0	-2.9138825117	-3.4090625624	1.4091496954
H	1.0	-2.7933788113	-0.9668544145	2.1592512822
H	1.0	-4.2930888424	-1.8194426497	2.4657676564
H	1.0	-4.0329485318	0.8974665135	2.4178925240
H	1.0	-5.8476732033	1.5528653009	0.1905533392
H	1.0	-6.0134264296	2.2289378654	1.8099904811
H	1.0	-4.9982483270	3.8965546253	0.3764243618
H	1.0	-3.8179044801	3.3775022850	1.5622284409
H	1.0	-3.9692186679	2.3977387487	-1.3249013413
H	1.0	-2.8458550640	1.7852540656	-0.1279286312
H	1.0	-3.0010938422	4.6535563070	-1.1796983707
H	1.0	-2.0164621624	4.1887508830	0.1825695180
H	1.0	-0.6729645697	4.2349117319	-1.8741195391
H	1.0	-1.7819446206	3.1308312929	-2.6787796414
H	1.0	0.6149023116	4.2042625329	-0.0290429551
H	1.0	-0.1945970289	3.4804903135	1.3542438307
H	1.0	1.7835581555	2.2158025558	1.9822474653
H	1.0	2.1970528366	3.9118175237	1.8161546934
H	1.0	4.1263756217	2.0827403592	1.7705494072
H	1.0	4.8071563728	1.4563246652	-1.0056544131
H	1.0	5.8449172883	2.6152053234	-0.1900053432
H	1.0	6.8244799749	0.4135418033	0.0487218818

H	1.0	6.3288224729	1.0125224569	1.6138343094
H	1.0	4.1853244450	-0.3312826133	1.3907398774
H	1.0	5.6568301986	-1.2608758927	1.5867490368
H	1.0	4.4761053801	-0.7074331351	-1.1725393436
H	1.0	5.7085770607	-1.8758485154	-0.7429900655
H	1.0	3.9608299386	-3.0397430589	0.7137793550
H	1.0	3.6565632174	-3.0708087102	-1.0237081883
H	1.0	1.1950321344	-2.3690634594	3.0046797138
H	1.0	1.7413228440	-3.7686379973	2.0852989014
H	1.0	2.9068216551	-2.5320364297	2.5672812941
H	1.0	-0.7205485474	-5.0230326714	-0.5379376334

3. $[Zr(DFO)(H_2O)]^+$



B3LYP/DZVP: $E = -5313.681374$, $G_{298.15} = 345.642$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0244592645	-1.0472902720	-0.5074280845
C	6.0	-3.0669771961	-4.1397647012	-0.6939114370
N	7.0	-2.2390610607	-3.0392824672	-0.2146957861
C	6.0	-2.4396452673	-2.2112314753	0.7989351518
C	6.0	-3.5671792016	-2.3789207564	1.7895049010
C	6.0	-4.1894207702	-1.0261067415	2.1624937548
C	6.0	-4.7390610922	-0.3026311340	0.9269937149
O	8.0	-4.7153366691	-0.8279936656	-0.1899432413
N	7.0	-5.2330036669	0.9458423712	1.1592852453
C	6.0	-5.7151620607	1.8488368381	0.1089925117
C	6.0	-4.7338861037	2.9971214088	-0.1832958687
C	6.0	-3.4094843742	2.5264941442	-0.8017432140
C	6.0	-2.3300291037	3.6184837036	-0.8241526230
C	6.0	-0.9793882942	3.1456240338	-1.3853375625
N	7.0	-0.4551322506	1.9463651183	-0.7159721989
C	6.0	0.2339994566	1.8360458724	0.4077881087
C	6.0	0.5891407220	3.0293246909	1.2618190743

C	6.0	2.0278219723	2.9323152829	1.7894325354
C	6.0	3.0300334732	2.7606943315	0.6419907745
O	8.0	2.6667783198	2.7923596122	-0.5371883430
N	7.0	4.3190471891	2.5421891589	1.0232399781
C	6.0	5.4098846995	2.2688826986	0.0848755777
C	6.0	6.2249593877	1.0307029519	0.4942934725
C	6.0	5.4334832714	-0.2872298274	0.5807939840
C	6.0	4.9974678158	-0.8660902052	-0.7737534306
C	6.0	4.2299730324	-2.1927446102	-0.6569891454
N	7.0	2.8550638452	-2.0202980576	-0.1725895595
C	6.0	2.2950797100	-2.3952740566	0.9695528269
C	6.0	3.0719871436	-3.0998013354	2.0507823946
O	8.0	-1.2144478531	-2.7034382543	-1.0697441936
O	8.0	-1.6162359100	-1.2338877045	0.9410386836
O	8.0	-0.6607594912	0.7648578504	-1.3898865106
O	8.0	0.5921303002	0.6595127607	0.7797084986
O	8.0	2.0149472035	-1.4301882162	-1.0819663934
O	8.0	1.0429639549	-2.1606998467	1.1237000580
H	1.0	-3.6510962381	-4.5600099967	0.1237342662
H	1.0	-3.7356004906	-3.7847966322	-1.4840884492
H	1.0	-4.3369747342	-3.0386301594	1.3906280415
H	1.0	-3.1553152672	-2.8449657151	2.6930099127
H	1.0	-3.4446391703	-0.3938316306	2.6560185138
H	1.0	-4.9984491771	-1.1940544341	2.8828804674
H	1.0	-5.2022054042	1.3007382086	2.1078815777
H	1.0	-5.8796429259	1.2369460901	-0.7807079999
H	1.0	-6.6853224800	2.2536471456	0.4182703952
H	1.0	-5.2324702274	3.7111709242	-0.8514981763
H	1.0	-4.5377394554	3.5427712149	0.7510652185
H	1.0	-3.5907886324	2.1608618855	-1.8205805937
H	1.0	-3.0333247601	1.6655959129	-0.2389101810
H	1.0	-2.6543477842	4.4701901247	-1.4364901330
H	1.0	-2.1822679934	4.0104058767	0.1908922955
H	1.0	-0.2215969070	3.9314126758	-1.3286542991
H	1.0	-1.0726499192	2.8587975466	-2.4347014925
H	1.0	0.4548141759	3.9541601917	0.7001417600
H	1.0	-0.1029382781	3.0534732823	2.1119014897
H	1.0	2.1203614214	2.0879385689	2.4792569155
H	1.0	2.2633336698	3.8408824948	2.3558823488
H	1.0	4.5410147782	2.5839569817	2.0112500587
H	1.0	4.9494986553	2.1499893896	-0.8975635649
H	1.0	6.0749997319	3.1395564706	0.0269034568
H	1.0	7.0544744908	0.9254976168	-0.2168121467
H	1.0	6.6932780143	1.2246074818	1.4690715643
H	1.0	4.5523739704	-0.1330314712	1.2177448403
H	1.0	6.0632843984	-1.0270130860	1.0933119676
H	1.0	4.3744077268	-0.1581763926	-1.3294601784
H	1.0	5.8830598489	-1.0614098596	-1.3917683371
H	1.0	4.7399294999	-2.8913809648	0.0112133909
H	1.0	4.1429211105	-2.6705124881	-1.6376005925
H	1.0	2.4813037106	-3.0661789694	2.9668657739
H	1.0	3.2341785680	-4.1493299955	1.7816598230

H	1.0	4.0444073111	-2.6376906346	2.2321620394
H	1.0	-2.4005177403	-4.9098912987	-1.0854271038
O	8.0	-0.0747054245	-1.2394429979	-2.8713920712
H	1.0	-0.3922426778	-0.3908503113	-3.2329278790
H	1.0	-0.7181382814	-1.9319139672	-3.1126037830

M11-L/DZVP: $E = -5313.429498$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0350487449	-0.9981060144	-0.6011710962
C	6.0	-3.0989239611	-3.9936109834	-0.5568108220
N	7.0	-2.1997994763	-2.9829169877	-0.1184561354
C	6.0	-2.3403665384	-2.1396063110	0.8650928451
C	6.0	-3.3637836558	-2.2886533496	1.9257907898
C	6.0	-3.9572868976	-0.9409412146	2.2304704989
C	6.0	-4.4936725180	-0.3257013082	0.9662457635
O	8.0	-4.3635252964	-0.8794605324	-0.1036646065
N	7.0	-5.0948773419	0.8586387184	1.1143934689
C	6.0	-5.5410909403	1.6541368619	0.0091319206
C	6.0	-4.6095752777	2.8028076784	-0.2819347017
C	6.0	-3.2498547262	2.3692896257	-0.7597451089
C	6.0	-2.2753647332	3.5140282875	-0.8456913218
C	6.0	-0.9411124836	3.1300819806	-1.4311232395
N	7.0	-0.3868695072	1.9556541201	-0.8276291225
C	6.0	0.2737723788	1.8169153311	0.2852130030
C	6.0	0.6323169903	2.9750626976	1.1369241644
C	6.0	1.9664832156	2.7498692620	1.7890747245
C	6.0	3.0192063409	2.5219699108	0.7390878929
O	8.0	2.7165419880	2.3183536129	-0.4152127268
N	7.0	4.2815983513	2.5477973699	1.1792309330
C	6.0	5.4035123590	2.2226618763	0.3514293815
C	6.0	6.0397329163	0.9139060790	0.7456184845
C	6.0	5.1390567142	-0.2904214942	0.6310258434
C	6.0	4.7921049313	-0.6770996204	-0.7837807157
C	6.0	4.0938621291	-2.0082748499	-0.8768366971
N	7.0	2.7520272607	-1.9648599122	-0.3761012673
C	6.0	2.2451922728	-2.2999069361	0.7802219217
C	6.0	3.0311472876	-2.9102357514	1.8645120986
O	8.0	-1.3069056163	-2.6046277264	-1.0422817897
O	8.0	-1.5461797409	-1.1672669860	0.9106322750
O	8.0	-0.6485535692	0.8099840415	-1.4688026463
O	8.0	0.5746486577	0.6523755147	0.6453343425
O	8.0	1.8860327292	-1.4168105144	-1.2277486900
O	8.0	1.0182387760	-2.0867957285	0.9431445418
H	1.0	-3.5668447690	-4.4840368738	0.2940581914
H	1.0	-3.8654992263	-3.5636972316	-1.2087609833
H	1.0	-4.1460775530	-2.9861778540	1.6244789925
H	1.0	-2.8797730041	-2.6954615356	2.8201014547
H	1.0	-3.1937243067	-0.2780257987	2.6520970953

H	1.0	-4.7459091257	-1.0335414004	2.9841839488
H	1.0	-5.1254949240	1.2652818075	2.0376389636
H	1.0	-5.6151018559	0.9816611587	-0.8508905063
H	1.0	-6.5513942272	2.0216500722	0.2209130269
H	1.0	-5.0801934914	3.4563437709	-1.0282975988
H	1.0	-4.5059844054	3.4206858671	0.6240240467
H	1.0	-3.3421070283	1.8733116195	-1.7370478025
H	1.0	-2.8464375919	1.5957634387	-0.0869416380
H	1.0	-2.6876631900	4.3271401933	-1.4582438391
H	1.0	-2.1299335338	3.9464112969	0.1562367930
H	1.0	-0.2137550819	3.9461719668	-1.3649336601
H	1.0	-1.0355317995	2.8804839487	-2.4916844578
H	1.0	0.6386927981	3.8977062641	0.5514510938
H	1.0	-0.1420093200	3.0876943219	1.9052039023
H	1.0	1.9229899360	1.8647865983	2.4341208067
H	1.0	2.2233452429	3.5972636436	2.4328996893
H	1.0	4.4427182774	2.7068482731	2.1630122463
H	1.0	5.0344791237	2.2052085382	-0.6781537141
H	1.0	6.1420045452	3.0312393619	0.4085987244
H	1.0	6.9378854127	0.7661667034	0.1314726431
H	1.0	6.4030939108	0.9939508754	1.7795843409
H	1.0	4.2166993457	-0.1152565798	1.2102921509
H	1.0	5.6397444160	-1.1385099564	1.1227553996
H	1.0	4.1662601184	0.0854791627	-1.2653306696
H	1.0	5.7109409154	-0.7497462879	-1.3806058277
H	1.0	4.6464952090	-2.7846905828	-0.3383173221
H	1.0	4.0062007724	-2.3348597420	-1.9171233082
H	1.0	3.0328953301	-2.2298465516	2.7176703808
H	1.0	2.5264965793	-3.8212826663	2.1869414381
H	1.0	4.0593876567	-3.1430485721	1.6012031664
H	1.0	-2.5210800259	-4.7368026210	-1.1031643394
O	8.0	-0.2901321446	-1.2012094029	-2.8582869961
H	1.0	-0.5712958185	-0.3509095903	-3.2180512756
H	1.0	-0.9873939313	-1.8401138037	-3.0515059725

B3LYP/DZVP/PCM: $E = -5313.756195$, $G_{298.15} = 345.341$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0188467620	-0.9981019679	-0.6264934660
C	6.0	-2.7406285609	-4.4104913439	-0.4632456750
N	7.0	-2.1416632215	-3.1056128199	-0.2047467778
C	6.0	-2.4313830187	-2.2085037677	0.7233257858
C	6.0	-3.5555574367	-2.3910178256	1.7154137745
C	6.0	-4.1743990325	-1.0559126132	2.1445365844
C	6.0	-4.8006330887	-0.2934456095	0.9737726388
O	8.0	-5.0434223730	-0.8490845313	-0.1106312376
N	7.0	-5.0768948224	1.0104651976	1.2238392703
C	6.0	-5.6422929620	1.9512148737	0.2529655175
C	6.0	-4.6697956634	3.0938113484	-0.0831780897

C	6.0	-3.4030691512	2.6221504279	-0.8129584488
C	6.0	-2.3093509479	3.6971685151	-0.8720760720
C	6.0	-0.9887733683	3.2136193589	-1.4901772427
N	7.0	-0.4448770862	2.0081010993	-0.8402042483
C	6.0	0.1938636960	1.8880025413	0.3111000487
C	6.0	0.5221259772	3.0778688015	1.1775216476
C	6.0	1.9401806167	2.9947919564	1.7592920993
C	6.0	3.0060591943	2.8898263822	0.6677767101
O	8.0	2.7646986349	3.2051704490	-0.5095866747
N	7.0	4.2093073939	2.4241423003	1.0821888375
C	6.0	5.3554885468	2.1974930652	0.1995415680
C	6.0	6.1562906319	0.9578854887	0.6259346798
C	6.0	5.3729013566	-0.3672644341	0.6283914542
C	6.0	5.0066578517	-0.9044908255	-0.7633325697
C	6.0	4.1884276951	-2.2043642374	-0.7201739532
N	7.0	2.8071478827	-1.9995471467	-0.2644725988
C	6.0	2.2343011628	-2.3581704449	0.8751713753
C	6.0	2.9860018527	-3.0931039051	1.9517094088
O	8.0	-1.1278847494	-2.7808100675	-1.0754578327
O	8.0	-1.7046421248	-1.1420590157	0.7642053805
O	8.0	-0.6441143570	0.8298292869	-1.5224153741
O	8.0	0.5402051075	0.7037672017	0.6807112400
O	8.0	1.9889150811	-1.3805492255	-1.1809285101
O	8.0	0.9866344844	-2.0838019028	1.0267455828
H	1.0	-3.4877495921	-4.6406643314	0.2932868048
H	1.0	-3.2011032564	-4.4050873784	-1.4548298022
H	1.0	-4.3279096847	-3.0350623401	1.2961112137
H	1.0	-3.1491154995	-2.8955948870	2.6002181558
H	1.0	-3.4310385569	-0.4299686544	2.6452616278
H	1.0	-4.9611120140	-1.2647014331	2.8788550330
H	1.0	-4.8331597898	1.3766129968	2.1377607212
H	1.0	-5.8936956761	1.3755722263	-0.6403659500
H	1.0	-6.5736900531	2.3619211861	0.6599363726
H	1.0	-5.2072571777	3.8321529699	-0.6917341080
H	1.0	-4.3921178810	3.6079128658	0.8474278405
H	1.0	-3.6629125594	2.2993619237	-1.8293935544
H	1.0	-3.0060846012	1.7392878234	-0.3000353973
H	1.0	-2.6447212859	4.5572544965	-1.4657811480
H	1.0	-2.1163151663	4.0779992641	0.1384456530
H	1.0	-0.2259138282	3.9952239347	-1.4557382838
H	1.0	-1.1232769336	2.9294070370	-2.5353740673
H	1.0	0.4009946008	4.0030897105	0.6147537828
H	1.0	-0.1965831490	3.0982504027	2.0049344804
H	1.0	2.0255895163	2.1498777790	2.4471985908
H	1.0	2.1244479751	3.9035286989	2.3438675191
H	1.0	4.3338660221	2.2486896640	2.0734012591
H	1.0	4.9647376966	2.0962041277	-0.8148121990
H	1.0	6.0146203268	3.0753303253	0.2057290763
H	1.0	7.0272061281	0.8793953422	-0.0370268189
H	1.0	6.5587484781	1.1295319946	1.6331313309
H	1.0	4.4610495451	-0.2410990476	1.2252292814
H	1.0	5.9810113452	-1.1204958705	1.1456524499

H	1.0	4.4484524730	-0.1625459041	-1.3433277110
H	1.0	5.9227250733	-1.1199056243	-1.3271705198
H	1.0	4.6522711726	-2.9426213950	-0.0625744795
H	1.0	4.1146970213	-2.6478856216	-1.7172812945
H	1.0	2.3751886708	-3.0943337387	2.8546510761
H	1.0	3.1633271387	-4.1301540644	1.6477625018
H	1.0	3.9498199464	-2.6309471705	2.1726026689
H	1.0	-1.9512601800	-5.1650443807	-0.4299988907
O	8.0	-0.1407817445	-1.2328782277	-2.9661771388
H	1.0	-0.5115926306	-0.4305169695	-3.3826984941
H	1.0	-0.7026628001	-1.9838057600	-3.2387796253

M11-L/DZVP/PCM: E = –5313.500576

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0666652352	-0.9958823144	-0.6340301100
C	6.0	-2.9952107652	-4.1208619465	-0.5043387427
N	7.0	-2.2053241560	-3.0016992044	-0.1293184523
C	6.0	-2.3801056703	-2.1395180201	0.8297028955
C	6.0	-3.4098902869	-2.2785241337	1.8837361379
C	6.0	-3.9863710887	-0.9274403996	2.1997390466
C	6.0	-4.5501828258	-0.3001276174	0.9564900646
O	8.0	-4.5011895472	-0.8750915756	-0.1154188442
N	7.0	-5.0889917065	0.9080005171	1.1193144783
C	6.0	-5.5453253146	1.7277377420	0.0371138908
C	6.0	-4.6042134295	2.8721067698	-0.2381571326
C	6.0	-3.2615191875	2.4303092050	-0.7534936601
C	6.0	-2.2571642797	3.5499402470	-0.7923955735
C	6.0	-0.9388367414	3.1529673305	-1.4008905378
N	7.0	-0.3967821978	1.9604350644	-0.8164596401
C	6.0	0.2537607777	1.8031769668	0.2993312300
C	6.0	0.6200325032	2.9443258770	1.1666912108
C	6.0	1.9796415622	2.7362598464	1.7700260960
C	6.0	3.0097320061	2.5452542198	0.6941252478
O	8.0	2.6848807400	2.3747139691	-0.4656849564
N	7.0	4.2781328820	2.5678436025	1.1053556024
C	6.0	5.3854594205	2.2401317468	0.2598394363
C	6.0	6.0548690980	0.9576092950	0.6839673411
C	6.0	5.1722298846	-0.2636236109	0.6349742998
C	6.0	4.8178017863	-0.7229929087	-0.7556867100
C	6.0	4.0873067599	-2.0401297714	-0.7764122539
N	7.0	2.7315663629	-1.9303461969	-0.3316134621
C	6.0	2.1912713249	-2.3023258520	0.7953163405
C	6.0	2.9776609551	-2.9560288224	1.8577630471
O	8.0	-1.2898937171	-2.6467834815	-1.0403441638
O	8.0	-1.6067939230	-1.1437335969	0.8486466417
O	8.0	-0.6535208989	0.8248637861	-1.4798651119
O	8.0	0.5500615885	0.6280174053	0.6392912565
O	8.0	1.8903346485	-1.3904589834	-1.2173614448

O	8.0	0.9556667210	-2.1016900433	0.9236529730
H	1.0	-3.6016853244	-4.4566225068	0.3322468665
H	1.0	-3.6386666115	-3.8570822862	-1.3472498598
H	1.0	-4.1986353427	-2.9661874624	1.5787316445
H	1.0	-2.9350384765	-2.6970650024	2.7773136373
H	1.0	-3.2160373414	-0.2694225456	2.6131526317
H	1.0	-4.7614447164	-1.0186836468	2.9662661319
H	1.0	-5.0672675433	1.3183469679	2.0420214269
H	1.0	-5.6371848895	1.0787750477	-0.8391629277
H	1.0	-6.5484835365	2.1021794263	0.2703991309
H	1.0	-5.0779000813	3.5540012903	-0.9564963784
H	1.0	-4.4747127822	3.4572879753	0.6851872779
H	1.0	-3.3767506882	1.9946060875	-1.7568143979
H	1.0	-2.8730253882	1.6122738658	-0.1261688684
H	1.0	-2.6465404946	4.3987080533	-1.3699230295
H	1.0	-2.0949192543	3.9322499935	0.2263338440
H	1.0	-0.1976674646	3.9553161918	-1.3274277211
H	1.0	-1.0501100644	2.9213785857	-2.4635434927
H	1.0	0.5822531537	3.8827019098	0.6091798215
H	1.0	-0.1268900563	3.0187393510	1.9653283187
H	1.0	1.9808305242	1.8465517991	2.4097467123
H	1.0	2.2401726162	3.5802373329	2.4150092887
H	1.0	4.4588019268	2.6980576072	2.0911654236
H	1.0	4.9961500701	2.1777849552	-0.7603042744
H	1.0	6.1107883978	3.0627118523	0.2743247174
H	1.0	6.9401438716	0.8032210124	0.0528659946
H	1.0	6.4383373934	1.0822769175	1.7056090836
H	1.0	4.2538441451	-0.0741333388	1.2152669091
H	1.0	5.6909689272	-1.0811589486	1.1566885413
H	1.0	4.2091690022	0.0263165621	-1.2787536358
H	1.0	5.7348128393	-0.8473682616	-1.3458612517
H	1.0	4.5907085560	-2.7830941247	-0.1482190868
H	1.0	4.0434368240	-2.4515884302	-1.7898681450
H	1.0	2.3703305351	-2.9994915286	2.7575574540
H	1.0	3.2417509330	-3.9751535676	1.5690906946
H	1.0	3.9006290141	-2.4215909084	2.0800795849
H	1.0	-2.3284704346	-4.9313335670	-0.7972708225
O	8.0	-0.2491810288	-1.1813900357	-2.8934777670
H	1.0	-0.6326065230	-0.3748161726	-3.2635505359
H	1.0	-0.8326612277	-1.9017069814	-3.1658965917

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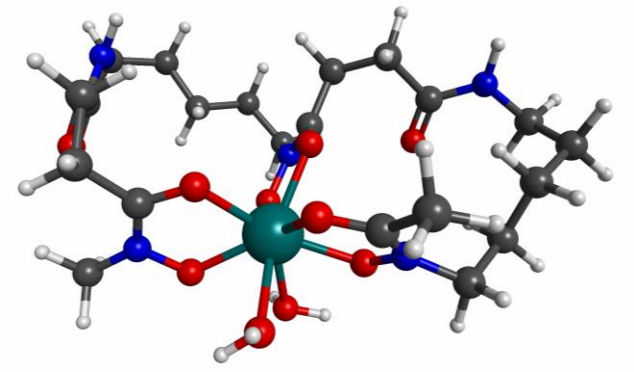
4. $[Zr(DFO)(H_2O)_2]^+$



B3LYP/DZVP/PCM: $E = -5390.170923$, $G_{298.15} = 361.104$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0116724849	-1.2438514177	0.4670031689
C	6.0	4.1721769480	-2.6285051743	1.1237832621
N	7.0	2.9589761435	-2.1315354272	0.4779969853
C	6.0	2.7458897462	-1.8040600106	-0.7825654940
C	6.0	3.7964773921	-1.9013874775	-1.8609951591
C	6.0	4.2569835117	-0.5258964811	-2.3826579236
C	6.0	5.0057276381	0.2730188230	-1.3154239550
O	8.0	5.7452669920	-0.2942221638	-0.4924229136
N	7.0	4.8061310248	1.6123033342	-1.3349788875
C	6.0	5.3778534757	2.5513008993	-0.3660764277
C	6.0	4.3012767811	3.4800971687	0.2147093183
C	6.0	3.2106127413	2.7441485227	1.0096258528
C	6.0	1.9953577017	3.6337350414	1.3057565397
C	6.0	0.7870348359	2.8887668899	1.8937792514
N	7.0	0.3307469556	1.7517923581	1.0739064111
C	6.0	-0.2794630532	1.7557778166	-0.0980981998
C	6.0	-0.6559366704	3.0284239483	-0.8149290059
C	6.0	-2.0586308322	2.9673972023	-1.4285827256
C	6.0	-3.1530282627	2.8083968544	-0.3717055811
O	8.0	-2.8995966928	2.8460956322	0.8428447587
N	7.0	-4.4016300282	2.6204581150	-0.8685379643
C	6.0	-5.5869591863	2.3585210348	-0.0510410274
C	6.0	-6.3889343904	1.1545081061	-0.5710869574
C	6.0	-5.5998734855	-0.1604908598	-0.6936106644
C	6.0	-5.0992415593	-0.7376981195	0.6380784239
C	6.0	-4.3177890133	-2.0504379243	0.4790372978
N	7.0	-2.9413688173	-1.8559186102	-0.0007462228
C	6.0	-2.4023339146	-2.1265060030	-1.1800877582
C	6.0	-3.1992768793	-2.6108912701	-2.3581400721
O	8.0	1.8764340876	-2.0606572546	1.3160092913
O	8.0	1.5576926147	-1.3968760854	-1.0961823776
O	8.0	0.6176035077	0.5006457631	1.5680147733
O	8.0	-0.5260680796	0.6120271858	-0.6320589276
O	8.0	-2.0769683257	-1.4176534181	0.9750890596
O	8.0	-1.1300530783	-1.9783240679	-1.3183284047

H	1.0	5.0422412356	-2.4077441015	0.5102933136
H	1.0	4.2716733359	-2.1075016864	2.0779919797
H	1.0	4.6586920996	-2.4767598884	-1.5271490552
H	1.0	3.3346883613	-2.4497704614	-2.6878763996
H	1.0	3.4065962827	0.0366024942	-2.7780296969
H	1.0	4.9480127213	-0.6944760755	-3.2166223471
H	1.0	4.2154626142	1.9962354433	-2.0643226333
H	1.0	5.8485316883	1.9523186848	0.4164174268
H	1.0	6.1634246947	3.1441599730	-0.8499614724
H	1.0	4.8000863774	4.2256782275	0.8462992560
H	1.0	3.8391030535	4.0413037213	-0.6093431058
H	1.0	3.6299291727	2.3563355436	1.9471475466
H	1.0	2.8800952707	1.8703385432	0.4359581097
H	1.0	2.2602419281	4.4253106300	2.0182597815
H	1.0	1.6909247770	4.1468027412	0.3859938837
H	1.0	-0.0573925841	3.5688348912	2.0387229641
H	1.0	1.0314077737	2.4523564983	2.8636490611
H	1.0	-0.5769735738	3.8832728884	-0.1442077942
H	1.0	0.0694570226	3.1746063180	-1.6243742643
H	1.0	-2.1245437478	2.1451112613	-2.1468354829
H	1.0	-2.2356828767	3.8921837422	-1.9892542571
H	1.0	-4.5163206250	2.6286020824	-1.8760669166
H	1.0	-5.2364988494	2.1982190883	0.9697659801
H	1.0	-6.2321367259	3.2460781756	-0.0377977382
H	1.0	-7.2504762331	1.0151822330	0.0951018767
H	1.0	-6.8058801295	1.4050924440	-1.5555397052
H	1.0	-4.7507054726	-0.0060785330	-1.3711572369
H	1.0	-6.2499151299	-0.9004729233	-1.1785660320
H	1.0	-4.4626788921	-0.0209401176	1.1665243001
H	1.0	-5.9538503927	-0.9472367552	1.2935546683
H	1.0	-4.8278594215	-2.7386133958	-0.1970620758
H	1.0	-4.2181760752	-2.5551883957	1.4438604811
H	1.0	-2.9475696063	-1.9855317375	-3.2190676927
H	1.0	-2.8938761818	-3.6352532366	-2.5944782827
H	1.0	-4.2766564431	-2.5869243676	-2.2073319921
H	1.0	4.0784556694	-3.7033247027	1.3037678334
O	8.0	-0.2556413203	-1.7880428427	2.7609795875
H	1.0	-1.2062350772	-1.7324795053	2.9810723629
H	1.0	0.2024010334	-1.1472525360	3.3365704005
O	8.0	-0.1962031395	-3.6681418336	0.6293030206
H	1.0	-0.2588752320	-4.1533374204	-0.2127758376
H	1.0	0.5865087041	-4.0221941592	1.0919356797

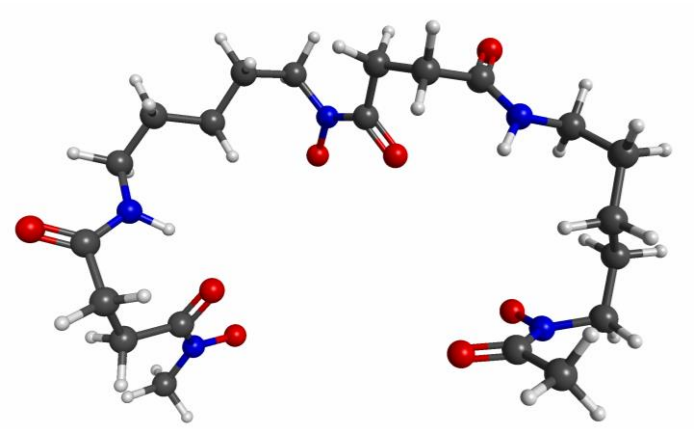
M11-L/DZVP/PCM: E = –5389.918972

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0559933399	-1.3265976799	0.5177909643
C	6.0	4.1390181603	-2.5704229193	1.1948207929
N	7.0	2.9439012648	-2.1551300921	0.5472344135

C	6.0	2.7335567843	-1.8257704627	-0.6896994172
C	6.0	3.7637008940	-1.8527902590	-1.7530491178
C	6.0	4.0320551112	-0.4662610311	-2.2757141352
C	6.0	4.6804427217	0.3859768522	-1.2221207978
O	8.0	5.1461721993	-0.1048930115	-0.2115662509
N	7.0	4.7159480462	1.6934123686	-1.4850512693
C	6.0	5.1824588527	2.6633827806	-0.5414359723
C	6.0	4.0552359743	3.4635343325	0.0555582742
C	6.0	3.0487794852	2.6433078753	0.8179034744
C	6.0	1.8927634990	3.4835643649	1.2883597574
C	6.0	0.7687519541	2.7092161796	1.9273833940
N	7.0	0.3202348427	1.5923162607	1.1434161067
C	6.0	-0.2617060641	1.5949831929	-0.0190055253
C	6.0	-0.6280589678	2.8530116814	-0.7099499749
C	6.0	-1.9530399488	2.7351416351	-1.4055543730
C	6.0	-3.0486325497	2.5283520976	-0.4022672157
O	8.0	-2.7980497138	2.1954331093	0.7399766615
N	7.0	-4.2865918779	2.7360077872	-0.8556347502
C	6.0	-5.4614891634	2.4264898565	-0.0995505972
C	6.0	-6.1921253479	1.2263390547	-0.6477494024
C	6.0	-5.3642008755	-0.0302002443	-0.7241998484
C	6.0	-4.9436279400	-0.5876094018	0.6097911729
C	6.0	-4.2202779006	-1.9013409486	0.4921456479
N	7.0	-2.8662980118	-1.7634265493	0.0362043049
C	6.0	-2.3375230558	-2.0341841534	-1.1254909674
C	6.0	-3.1424013484	-2.3858714433	-2.3069235403
O	8.0	1.8855782202	-2.0948890881	1.3605544034
O	8.0	1.5613096500	-1.4551808202	-0.9981548722
O	8.0	0.6381083797	0.3783122837	1.6090177308
O	8.0	-0.4718687508	0.4824746711	-0.5620632221
O	8.0	-2.0021248244	-1.4490929092	1.0055590911
O	8.0	-1.0824084361	-1.9914054817	-1.2237180280
H	1.0	4.9640520806	-2.6164331330	0.4914181831
H	1.0	4.3847438352	-1.8475501940	1.9740328890
H	1.0	4.6911687405	-2.3171050188	-1.4222692525
H	1.0	3.3566927538	-2.4697744477	-2.5602529093
H	1.0	3.1047512189	-0.0003898349	-2.6258058295
H	1.0	4.6945246489	-0.5209314558	-3.1459184982
H	1.0	4.2633063528	2.0250300999	-2.3249005949
H	1.0	5.7233945647	2.1139084785	0.2342492073
H	1.0	5.9018308238	3.3291316429	-1.0316959593
H	1.0	4.4852955274	4.2349760211	0.7080140688
H	1.0	3.5398422999	4.0114772530	-0.7481614285
H	1.0	3.5318482218	2.1460656448	1.6714279416
H	1.0	2.6749530539	1.8269310461	0.1772474613
H	1.0	2.2335454566	4.2280547843	2.0195615691
H	1.0	1.5095829421	4.0699350062	0.4418065503
H	1.0	-0.0870991914	3.3595859711	2.1459688436
H	1.0	1.0860420144	2.2695986157	2.8756323436
H	1.0	-0.6458104072	3.6879471210	-0.0051477282
H	1.0	0.1540946150	3.0686079445	-1.4483683235
H	1.0	-1.9480617063	1.8825859153	-2.0945841706

H	1.0	-2.1423235786	3.6236914746	-2.0145477829
H	1.0	-4.3999448439	2.9786261010	-1.8296563980
H	1.0	-5.1366189276	2.2638502126	0.9322189064
H	1.0	-6.1265629934	3.2981284657	-0.0898199793
H	1.0	-7.0817189373	1.0521776267	-0.0276290363
H	1.0	-6.5713522068	1.4670447676	-1.6499042841
H	1.0	-4.4750578076	0.1546295879	-1.3491452400
H	1.0	-5.9460742004	-0.7930861425	-1.2622480921
H	1.0	-4.3007233416	0.1177961263	1.1512045782
H	1.0	-5.8306765016	-0.7511199469	1.2360644548
H	1.0	-4.7500504963	-2.5904017306	-0.1727240039
H	1.0	-4.1442165118	-2.3967952299	1.4649636887
H	1.0	-2.8782760080	-1.7044842786	-3.1164056222
H	1.0	-2.8727477239	-3.3914323949	-2.6335016064
H	1.0	-4.2163333271	-2.3410082854	-2.1494477377
H	1.0	3.9737712588	-3.5499554910	1.6469891885
O	8.0	-0.2239507080	-1.9495723292	2.6821081435
H	1.0	-1.1673237150	-1.8773042074	2.8865710786
H	1.0	0.2252437184	-1.3649856351	3.3058277820
O	8.0	-0.1630117733	-3.6396945353	0.6112405990
H	1.0	-0.2193393867	-4.1118188211	-0.2270130018
H	1.0	0.5855539640	-4.0322628030	1.0785103296

5. DFO^{3-}



B3LYP/DZVP/PCM: $E = -1697.032016$, $G_{298.15} = 325.004$

ATOM	CHARGE	X	Y	Z
C	6.0	-4.5647123444	-4.4124252971	-1.4211186492
N	7.0	-3.7823796265	-3.2254300286	-1.0903789773
C	6.0	-3.9724669817	-2.4591746121	-0.0092359741
C	6.0	-5.1319252936	-2.8113107495	0.9444459964
C	6.0	-5.2825906368	-1.8214082772	2.1187474824
C	6.0	-5.9703853529	-0.4959193374	1.7810341515
O	8.0	-7.1207355293	-0.2507143135	2.2060819319

N	7.0	-5.2534216163	0.3711494518	1.0302918762
C	6.0	-5.7636833161	1.6740855397	0.6028603877
C	6.0	-4.7009762415	2.7838037651	0.6326332749
C	6.0	-3.6745890242	2.7456629275	-0.5126368268
C	6.0	-2.6676638370	3.9008080627	-0.4172568648
C	6.0	-1.6086943078	3.9585340729	-1.5349722930
N	7.0	-0.7521869021	2.7689940668	-1.6465476601
C	6.0	0.3638924322	2.5858318265	-0.9217128697
C	6.0	0.8398468280	3.7496620893	-0.0331996009
C	6.0	2.0461773034	3.3656305599	0.8300316884
C	6.0	3.3560212519	3.2553887246	0.0569107391
O	8.0	3.6830935972	4.0978950307	-0.8008262708
N	7.0	4.1821780105	2.2488039277	0.4380543168
C	6.0	5.5142221131	2.0278905236	-0.1283039187
C	6.0	6.4413196373	1.3133924118	0.8652625100
C	6.0	6.1009356589	-0.1617348258	1.1575353071
C	6.0	6.4329745190	-1.1207016634	0.0043838675
C	6.0	6.0545040466	-2.5861039732	0.2767583662
N	7.0	4.6062951538	-2.8096353643	0.2632279964
C	6.0	3.8792976024	-3.1554053048	1.3388461722
C	6.0	4.6052148890	-3.4236337663	2.6622999156
O	8.0	-2.8149357727	-2.9609513480	-2.0112626077
O	8.0	-3.2344599662	-1.4552881781	0.2556389386
O	8.0	-1.2288958464	1.8118487057	-2.4973581662
O	8.0	1.0541642473	1.5200137544	-0.9604277600
O	8.0	4.0282868261	-2.5853746589	-0.9568252887
O	8.0	2.6155464433	-3.2854468433	1.3079427896
H	1.0	-5.2960399941	-4.6659183708	-0.6537465179
H	1.0	-5.0877871477	-4.2490069880	-2.3710044812
H	1.0	-6.0821582806	-2.8756969227	0.4017844239
H	1.0	-4.9618546377	-3.8040834886	1.3786681417
H	1.0	-4.2964751195	-1.6242678947	2.5485620706
H	1.0	-5.9020148781	-2.2899385714	2.8875795785
H	1.0	-4.3693091339	0.0005363179	0.6617682600
H	1.0	-6.1934318247	1.5980345398	-0.4069590859
H	1.0	-6.5819700894	1.9275332572	1.2801788320
H	1.0	-5.2335505919	3.7439821896	0.5931987141
H	1.0	-4.1883374417	2.7556342699	1.6037203166
H	1.0	-4.2101589974	2.8104082408	-1.4692808901
H	1.0	-3.1297059451	1.7958849237	-0.5273287703
H	1.0	-3.2117024904	4.8569957083	-0.4350314006
H	1.0	-2.1640328216	3.8587969082	0.5576892274
H	1.0	-0.9955856101	4.8553886736	-1.3956870830
H	1.0	-2.0998703956	4.0493316372	-2.5080661942
H	1.0	1.1149875936	4.6126615122	-0.6508793630
H	1.0	0.0419252079	4.0912989878	0.6338041094
H	1.0	1.8429431730	2.4437594857	1.3801542370
H	1.0	2.2040597830	4.1597686964	1.5719177836
H	1.0	3.7969255347	1.5378806828	1.0469417600
H	1.0	5.4394910348	1.4651295664	-1.0683542163
H	1.0	5.9242671983	3.0095145145	-0.3780180436
H	1.0	7.4632690977	1.3712128821	0.4689533670

H	1.0	6.4405395548	1.8845031251	1.8025827954
H	1.0	5.0403551561	-0.2641350200	1.4250573898
H	1.0	6.6629445503	-0.4705348757	2.0489226039
H	1.0	5.9272316185	-0.8165558420	-0.9171870754
H	1.0	7.5126756887	-1.0808795799	-0.1935613340
H	1.0	6.4850655521	-2.9145897816	1.2250939442
H	1.0	6.4814477246	-3.2173589258	-0.5131749741
H	1.0	3.8448453513	-3.7047308058	3.3937881012
H	1.0	5.3281726816	-4.2440185897	2.5886406144
H	1.0	5.1371089525	-2.5466964567	3.0463230780
H	1.0	-3.8767612483	-5.2559103048	-1.5483378498

M11-L/DZVP/PCM: $E = -1696.965236$

ATOM	CHARGE	X	Y	Z
C	6.0	-5.1869932623	-4.4360313332	-1.2642169994
N	7.0	-4.2706659837	-3.3648547550	-1.0771364048
C	6.0	-4.2278697359	-2.5896565525	-0.0146161126
C	6.0	-5.2873241160	-2.7771586175	1.0489078043
C	6.0	-5.2247421394	-1.7127152761	2.1212924140
C	6.0	-5.8477051994	-0.4063548802	1.7114828092
O	8.0	-6.9301009385	-0.0485550294	2.1532224503
N	7.0	-5.1342803911	0.3049661701	0.8383623401
C	6.0	-5.6169643953	1.5139499207	0.2490773465
C	6.0	-4.6471306409	2.6599643138	0.3650198913
C	6.0	-3.4338670721	2.5516199906	-0.5209439134
C	6.0	-2.5331817503	3.7497925596	-0.3864615349
C	6.0	-1.4211151311	3.8420836705	-1.4015190028
N	7.0	-0.5629869379	2.6954508613	-1.4713613555
C	6.0	0.5231372481	2.5721188005	-0.7333512170
C	6.0	0.8947721494	3.7297967928	0.1625244824
C	6.0	2.0691507841	3.3613815107	1.0211430438
C	6.0	3.3446556535	3.2582425966	0.2415554487
O	8.0	3.6441642188	4.0795112107	-0.6080348699
N	7.0	4.1853788914	2.2923486437	0.6332399924
C	6.0	5.4536298835	2.0895861499	0.0002428598
C	6.0	6.4042354216	1.3472989235	0.9014573874
C	6.0	6.0926596871	-0.1171984211	1.1087405366
C	6.0	6.4441448797	-0.9924457658	-0.0656900797
C	6.0	6.1010752850	-2.4475233615	0.1402445974
N	7.0	4.6913362156	-2.6850184510	0.1265380220
C	6.0	3.9726996156	-2.9739638557	1.1977605534
C	6.0	4.6990361823	-3.2161625566	2.4935630866
O	8.0	-3.3961330908	-3.2528066845	-2.0644093541
O	8.0	-3.3471799799	-1.7186702495	0.1361533908
O	8.0	-0.9745332814	1.7408675429	-2.2979498247
O	8.0	1.2553118844	1.5668671250	-0.7447850269
O	8.0	4.1301454634	-2.4558204439	-1.0578622149
O	8.0	2.7343217594	-3.0802895093	1.1753522175

H	1.0	-5.8757901567	-4.5684129958	-0.4298884249
H	1.0	-5.7668831192	-4.2671806167	-2.1788358866
H	1.0	-6.2967347737	-2.7949833105	0.6176160906
H	1.0	-5.1627048792	-3.7547053397	1.5348791291
H	1.0	-4.1817299357	-1.5567373819	2.4133906336
H	1.0	-5.7779248525	-2.0513979181	3.0004176120
H	1.0	-4.3024465666	-0.1601590068	0.4722466562
H	1.0	-5.8581993957	1.3423486221	-0.8124268659
H	1.0	-6.5580258352	1.7561375322	0.7486311001
H	1.0	-5.1860386912	3.5847299887	0.1124082799
H	1.0	-4.3435294613	2.7644996756	1.4174834332
H	1.0	-3.7549029755	2.4499691128	-1.5679118444
H	1.0	-2.8585260266	1.6407513725	-0.3021709341
H	1.0	-3.1362323230	4.6673272885	-0.4767039742
H	1.0	-2.1178690539	3.7755093664	0.6327057740
H	1.0	-0.8388774262	4.7546681883	-1.2182879691
H	1.0	-1.8528902353	3.9443461398	-2.4045081743
H	1.0	1.1615145209	4.6175465042	-0.4278440210
H	1.0	0.0640344369	4.0403355743	0.8075620351
H	1.0	1.8740079232	2.4412281363	1.5790396269
H	1.0	2.2359366448	4.1533357814	1.7630718426
H	1.0	3.7752229102	1.5179301711	1.1353991765
H	1.0	5.3389895032	1.5708566479	-0.9648793411
H	1.0	5.8549544279	3.0797166491	-0.2352273044
H	1.0	7.4152766883	1.4383922711	0.4825316610
H	1.0	6.4296677209	1.8666138556	1.8685549287
H	1.0	5.0295941369	-0.2573754623	1.3647070289
H	1.0	6.6443554227	-0.4724801793	1.9914470084
H	1.0	5.9399457605	-0.6552019296	-0.9798695509
H	1.0	7.5228411547	-0.9137809062	-0.2610601777
H	1.0	6.5528440362	-2.8097535757	1.0705975474
H	1.0	6.5331891944	-3.0415222926	-0.6782052093
H	1.0	3.9490266988	-3.4966113059	3.2332560811
H	1.0	5.4332890672	-4.0256369879	2.4401189137
H	1.0	5.2243935855	-2.3343825366	2.8740324317
H	1.0	-4.6200825329	-5.3638715720	-1.4001840270

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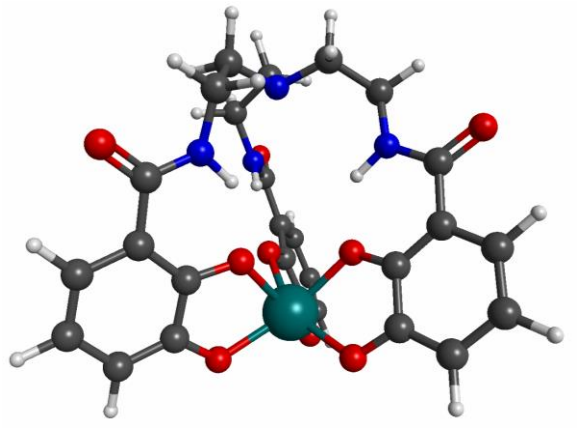
6. [Zr(TRENCAM)]$^{2-}$



B3LYP/DZVP/PCM: $E = -5479.699576$, $G_{298.15} = 268.713$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0842402743	-0.0062956594	0.1098015751
O	8.0	1.7153402723	-0.4504454203	-0.9179852174
C	6.0	2.8810099180	-0.3495007588	-0.2361242254
C	6.0	4.1348873832	-0.6832532542	-0.7459895061
C	6.0	5.2690758626	-0.5963285038	0.0903522373
C	6.0	5.1436104723	-0.1755602586	1.4117477654
C	6.0	3.8825188594	0.1688089358	1.9560241464
C	6.0	2.7549403138	0.1120906307	1.1096133542
O	8.0	1.5126078098	0.4639343764	1.4721068145
C	6.0	3.8087062739	0.5370012484	3.4109825222
N	7.0	2.5656873090	0.5880617630	3.9629868885
C	6.0	2.3198371831	0.9210380353	5.3594403353
C	6.0	1.3823651844	-0.0706756290	6.0626562419
N	7.0	-0.0166698515	-0.0927111867	5.5794445174
C	6.0	-0.7379452613	1.1026114156	6.0729905056
C	6.0	-2.0460979439	1.4420075173	5.3410851943
N	7.0	-1.8468081871	1.9033743766	3.9738172402
C	6.0	-2.3165407850	3.0874755771	3.4918671290
C	6.0	-2.0429799651	3.3788655322	2.0409319844
C	6.0	-1.4990084820	2.4338014739	1.1465913668
C	6.0	-1.1440632401	2.7964112587	-0.1891528410
C	6.0	-1.4186367091	4.0859698929	-0.6454297305
C	6.0	-2.0091791772	5.0230278374	0.2320283673
C	6.0	-2.3116714693	4.6780837157	1.5475553119
H	1.0	-2.7396807942	5.4088218040	2.2271308408
H	1.0	-2.2187706863	6.0294945902	-0.1236663537
H	1.0	-1.1627085184	4.3628750489	-1.6663615769
O	8.0	-0.5382837186	1.8204742498	-0.9084277048
O	8.0	-1.2702126272	1.1488775215	1.4533193304
O	8.0	-2.9188569569	3.9141527630	4.2134377319
H	1.0	-1.4355798875	1.2651515637	3.2920260246
H	1.0	-2.5430017801	2.2423868933	5.8917166257
H	1.0	-2.7270263597	0.5818842390	5.3410908219

H	1.0	-0.0790822357	1.9692572852	5.9815705403
H	1.0	-0.9694248378	0.9933207022	7.1493928792
C	6.0	-0.6918462022	-1.3190032550	6.0646327025
C	6.0	-0.3223569319	-2.6168406792	5.3328129634
N	7.0	-0.7856607751	-2.6482435819	3.9527588429
C	6.0	-1.4763874403	-3.6884766915	3.4135090466
C	6.0	-1.8358923602	-3.5758198499	1.9598845778
C	6.0	-1.3579742860	-2.5489022508	1.1188493516
C	6.0	-1.8000422480	-2.4557094981	-0.2360264054
C	6.0	-2.6693851063	-3.4131629744	-0.7563507112
C	6.0	-3.1272737767	-4.4576863026	0.0774661755
C	6.0	-2.7156793677	-4.5370969000	1.4050761592
H	1.0	-3.0742265498	-5.3324342587	2.0517787793
H	1.0	-3.8089844684	-5.2030286846	-0.3259642760
H	1.0	-2.9999561146	-3.3351572472	-1.7902291538
O	8.0	-1.3344533785	-1.3768298524	-0.9118809786
O	8.0	-0.4924374757	-1.5975109308	1.4952854818
O	8.0	-1.8205076826	-4.6850293853	4.0899250825
H	1.0	-0.4913122137	-1.9108021114	3.3108725538
H	1.0	-0.7917025639	-3.4524595875	5.8563734219
H	1.0	0.7610583679	-2.7899670134	5.3634391536
H	1.0	-1.7716442238	-1.1830643132	5.9641047601
H	1.0	-0.4911778214	-1.4673138830	7.1423041638
H	1.0	1.8088649584	-1.0689264308	5.9345599467
H	1.0	1.4129975812	0.1475196912	7.1470259099
H	1.0	3.2824306973	0.8996425249	5.8747831050
H	1.0	1.9397633730	1.9475627977	5.4388586910
H	1.0	1.7750108319	0.4991962092	3.3237781318
O	8.0	4.8469657871	0.7455840529	4.0792980336
H	1.0	6.0119128289	-0.1275354581	2.0616666438
H	1.0	6.2469844466	-0.8645789844	-0.3034264576
H	1.0	4.2240998711	-1.0253305585	-1.7752420222

M11-L/DZVP/PCM: $E = -5479.454300$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0622983754	0.0013772170	0.0470310294
O	8.0	1.7272605151	-0.4785344188	-0.8932243793
C	6.0	2.8467243113	-0.4215710768	-0.1988486357
C	6.0	4.0930883982	-0.7765870079	-0.6605500653
C	6.0	5.1878268096	-0.6975184609	0.1961284374
C	6.0	5.0331117560	-0.2612534768	1.4888526537
C	6.0	3.7795860399	0.0974453968	1.9870291361
C	6.0	2.6894656837	0.0452960658	1.1235740225
O	8.0	1.4732494971	0.4187659282	1.4287244338
C	6.0	3.6787931034	0.5006492903	3.4044028090
N	7.0	2.4375419854	0.6233524720	3.8946229205
C	6.0	2.1838686690	1.0379169925	5.2328450218
C	6.0	1.3359303076	0.0550285589	5.9935096749

N	7.0	-0.0214774506	-0.0704290983	5.5083545091
C	6.0	-0.8078368581	1.0360914697	6.0099919672
C	6.0	-2.0844357041	1.2840408923	5.2524473628
N	7.0	-1.8589818732	1.7387270084	3.9228603250
C	6.0	-2.2505201681	2.9486268226	3.5016286552
C	6.0	-1.9671434099	3.2703758340	2.0881464836
C	6.0	-1.4187288780	2.3632126276	1.1866356441
C	6.0	-1.0767750853	2.7697394440	-0.1208879732
C	6.0	-1.3550012293	4.0521906444	-0.5350883823
C	6.0	-1.9429226073	4.9473696690	0.3556122531
C	6.0	-2.2398037073	4.5634445207	1.6401910696
H	1.0	-2.6781938647	5.2650318758	2.3460865651
H	1.0	-2.1607236653	5.9621898336	0.0291718614
H	1.0	-1.1000123923	4.3539850914	-1.5497414151
O	8.0	-0.4919545045	1.8357934458	-0.8453673543
O	8.0	-1.1877470971	1.1013857271	1.4437453955
O	8.0	-2.7909682465	3.7575167397	4.2449302745
H	1.0	-1.4432882836	1.1145262489	3.2381022721
H	1.0	-2.6601867789	2.0521966013	5.7752571011
H	1.0	-2.7109518084	0.3814363567	5.2309701338
H	1.0	-0.2069153614	1.9511853164	5.9533091510
H	1.0	-1.0437402608	0.8881036646	7.0849309123
C	6.0	-0.5855842398	-1.3094224313	5.9997244212
C	6.0	-0.1795227469	-2.5303283254	5.2217119619
N	7.0	-0.6882417381	-2.5264041876	3.8915313471
C	6.0	-1.4001205084	-3.5460059321	3.3943688001
C	6.0	-1.7946222247	-3.4390482281	1.9763204219
C	6.0	-1.3298629361	-2.4465183417	1.1192452287
C	6.0	-1.8161678007	-2.3619998895	-0.2030084246
C	6.0	-2.6923324727	-3.3100725988	-0.6790963352
C	6.0	-3.1276891699	-4.3246879038	0.1702207502
C	6.0	-2.6859649363	-4.3860170149	1.4683962263
H	1.0	-3.0336076567	-5.1675072056	2.1408329579
H	1.0	-3.8243548468	-5.0729171484	-0.2017246800
H	1.0	-3.0502694086	-3.2417108353	-1.7050501977
O	8.0	-1.3653864890	-1.3243060179	-0.8824251480
O	8.0	-0.4365537903	-1.5433526642	1.4319472764
O	8.0	-1.7347128693	-4.5063463887	4.0778110684
H	1.0	-0.3947278713	-1.8012932142	3.2437771944
H	1.0	-0.5732299154	-3.4165275553	5.7260702453
H	1.0	0.9146998676	-2.6418209137	5.2041020305
H	1.0	-1.6788932087	-1.2407593704	5.9586413832
H	1.0	-0.3261870271	-1.4568485482	7.0690107588
H	1.0	1.8260583555	-0.9237398643	5.9288794875
H	1.0	1.3388580487	0.3302365766	7.0692919201
H	1.0	3.1473506913	1.1347665425	5.7399095196
H	1.0	1.7273052849	2.0386389167	5.2364227422
H	1.0	1.6649326305	0.5378234662	3.2405003368
O	8.0	4.6762763792	0.6791935689	4.0922165898
H	1.0	5.8840014523	-0.2095642410	2.1637632619
H	1.0	6.1736316623	-0.9820894850	-0.1656355186
H	1.0	4.2043828686	-1.1293948115	-1.6846446862

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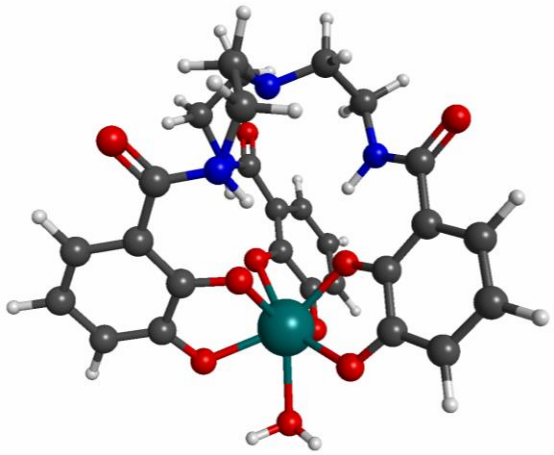
7. [Zr(TRENCAM)(H_2O)]$^{2-}$



B3LYP/DZVP/PCM: E = –5556.117865, $G_{298.15}$ = 284.659

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0035701102	0.1147474951	-0.2465166655
O	8.0	1.8459959506	-0.7266760520	-1.0368531312
C	6.0	2.9011689211	-0.7811143013	-0.2000204796
C	6.0	4.0855880534	-1.4735778122	-0.4558945915
C	6.0	5.1136407575	-1.4731119206	0.5114014082
C	6.0	4.9464152030	-0.8040529651	1.7202112969
C	6.0	3.7539082365	-0.0954767815	2.0093235652
C	6.0	2.7439667824	-0.0554981274	1.0217755955
O	8.0	1.5930115668	0.6217408073	1.1248647735
C	6.0	3.6122952446	0.5145042150	3.3736765039
N	7.0	2.3730622847	0.9572804160	3.7145088205
C	6.0	2.0331730911	1.4674838947	5.0352408765
C	6.0	1.3912219668	0.4098965402	5.9481501077
N	7.0	0.0458887684	-0.0132492381	5.5168565384
C	6.0	-0.9831216033	0.9277516350	5.9965387613
C	6.0	-2.2830376306	0.9041966970	5.1769117273
N	7.0	-2.1302117113	1.4565300858	3.8394286837
C	6.0	-2.5258329325	2.7139383444	3.5052073335
C	6.0	-2.1829677009	3.1757367784	2.1216547654
C	6.0	-1.5431746882	2.3584768764	1.1575761994
C	6.0	-1.1575438160	2.9242050327	-0.0956842019
C	6.0	-1.4589346453	4.2493064793	-0.4047728964
C	6.0	-2.1273020407	5.0500772639	0.5460820947
C	6.0	-2.4774451810	4.5204269821	1.7833834791
H	1.0	-2.9740252814	5.1341600653	2.5288890461
H	1.0	-2.3597374837	6.0860451482	0.3083083868
H	1.0	-1.1576703039	4.6542780196	-1.3690891506
O	8.0	-0.4834271989	2.0899560821	-0.9140268452

O	8.0	-1.2382605770	1.0667748130	1.3195836670
O	8.0	-3.1339748960	3.4571034109	4.3115372475
H	1.0	-1.6248157772	0.9295307581	3.1239916008
H	1.0	-3.0364747335	1.4962628343	5.6999330215
H	1.0	-2.6680106093	-0.1176227845	5.0919185655
H	1.0	-0.5805491855	1.9438289114	5.9471458081
H	1.0	-1.2301015915	0.7378341417	7.0582645329
C	6.0	-0.2467938525	-1.3884424751	5.9616033938
C	6.0	0.3725314207	-2.4764618901	5.0703989134
N	7.0	-0.2018410043	-2.5249541920	3.7330168258
C	6.0	-1.1033553699	-3.4646526136	3.3414352072
C	6.0	-1.6782428990	-3.3147410828	1.9647784210
C	6.0	-1.2410910469	-2.3436242831	1.0306137282
C	6.0	-1.9325423543	-2.1994872033	-0.2136754251
C	6.0	-2.9873412940	-3.0499447979	-0.5411756698
C	6.0	-3.3967705844	-4.0405730853	0.3780506332
C	6.0	-2.7615002176	-4.1574883863	1.6101937958
H	1.0	-3.0839372331	-4.9017549670	2.3326801005
H	1.0	-4.2244746474	-4.6997782105	0.1250992221
H	1.0	-3.4948111577	-2.9245969971	-1.4959428857
O	8.0	-1.5156233214	-1.1777631952	-0.9927453107
O	8.0	-0.2195055450	-1.5043754840	1.2148042220
O	8.0	-1.4541064757	-4.4043257604	4.0940457964
H	1.0	0.0254567775	-1.7967931720	3.0540568108
H	1.0	0.2039847276	-3.4467286344	5.5420832778
H	1.0	1.4552730886	-2.3332687706	4.9835914582
H	1.0	-1.3298967362	-1.5375280604	5.9598704733
H	1.0	0.0908079167	-1.5486103539	7.0026463919
H	1.0	2.0502549626	-0.4622231065	5.9568362979
H	1.0	1.3717558284	0.7981245673	6.9834419686
H	1.0	2.9497887654	1.8285086020	5.5076932868
H	1.0	1.3637253129	2.3257051048	4.9114181646
H	1.0	1.6406342134	0.8506366777	3.0131756030
O	8.0	4.5854364470	0.5813354359	4.1595934582
H	1.0	5.7224056493	-0.8312130331	2.4792263548
H	1.0	6.0347145061	-2.0188000689	0.3167381444
H	1.0	4.1981028861	-2.0151356094	-1.3934059278
O	8.0	0.1653142997	0.3127398924	-2.6896753475
H	1.0	0.1324445422	1.2720370776	-2.8655203158
H	1.0	1.0958828563	0.0361978801	-2.8087647421

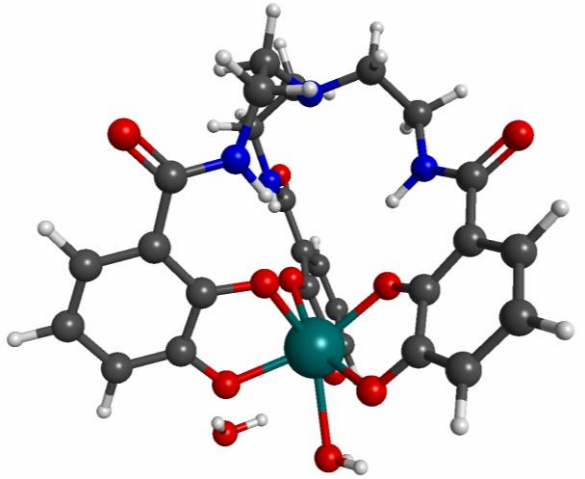
M11-L/DZVP/PCM: E = –5555.881343

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0396609745	0.0622401279	-0.3771621943
O	8.0	1.9157761508	-0.6959043389	-1.0145933574
C	6.0	2.8644644958	-0.7754335060	-0.1068937703
C	6.0	4.0407181367	-1.4799413741	-0.2326707612
C	6.0	4.9470425013	-1.5007956771	0.8250541197

C	6.0	4.6793966656	-0.8233106137	1.9878892260
C	6.0	3.5012362357	-0.0903578774	2.1409450876
C	6.0	2.6021483860	-0.0503301466	1.0779456650
O	8.0	1.4835533094	0.6204607108	1.0709093013
C	6.0	3.2620828282	0.5689398604	3.4361500722
N	7.0	2.0824312433	1.1858660965	3.5894650042
C	6.0	1.6859480188	1.6783023378	4.8681038918
C	6.0	1.2541764398	0.5749504454	5.7996224250
N	7.0	0.0611812809	-0.0871665010	5.3432370541
C	6.0	-1.1198465943	0.6049729779	5.7853779084
C	6.0	-2.2882756134	0.4077520316	4.8526771290
N	7.0	-2.1028225097	1.0453546901	3.5914202566
C	6.0	-2.3316748519	2.3567167884	3.4389559993
C	6.0	-1.9810901308	2.9378967128	2.1291564024
C	6.0	-1.4019280780	2.2030682522	1.0950410678
C	6.0	-1.0018301678	2.8410903320	-0.1003234968
C	6.0	-1.2387814022	4.1859373138	-0.2716766056
C	6.0	-1.8543680714	4.9113320438	0.7474955803
C	6.0	-2.2048459815	4.3013240502	1.9260468991
H	1.0	-2.6595342946	4.8681854901	2.7356940905
H	1.0	-2.0379136684	5.9753914584	0.6120598682
H	1.0	-0.9380563731	4.6696565660	-1.2000635246
O	8.0	-0.4080433124	2.0469490833	-0.9676010136
O	8.0	-1.1873351494	0.9204089536	1.1213280308
O	8.0	-2.8120485776	3.0349763898	4.3408590289
H	1.0	-1.6069621730	0.5671797111	2.8441372648
H	1.0	-3.1957121414	0.8010863975	5.3226467919
H	1.0	-2.4610621006	-0.6614881246	4.6681420182
H	1.0	-0.9092471574	1.6812856340	5.8284010797
H	1.0	-1.4055891187	0.3068448898	6.8159519118
C	6.0	0.0455106962	-1.4654101261	5.7562276550
C	6.0	0.8024394392	-2.3543367285	4.8017857714
N	7.0	0.1720483069	-2.4427069253	3.5254192338
C	6.0	-0.9393414878	-3.1751806956	3.3701770673
C	6.0	-1.6537800159	-3.0292346247	2.0913121011
C	6.0	-1.2222991703	-2.1963687247	1.0597395028
C	6.0	-2.0273184619	-2.0163505188	-0.0890035040
C	6.0	-3.2153017543	-2.7015853610	-0.2137519301
C	6.0	-3.6284670476	-3.5538159294	0.8081530167
C	6.0	-2.8601357190	-3.7143622245	1.9341786852
H	1.0	-3.1829238782	-4.3658201704	2.7436081920
H	1.0	-4.5695291841	-4.0918473985	0.7117849684
H	1.0	-3.8247168269	-2.5544923910	-1.1046422400
O	8.0	-1.5390884653	-1.1720291717	-0.9692339984
O	8.0	-0.1068979192	-1.5256080601	1.0518701710
O	8.0	-1.3424476105	-3.9217911350	4.2552429289
H	1.0	0.3807272304	-1.7575974017	2.8041763535
H	1.0	0.8889256657	-3.3584216044	5.2315298576
H	1.0	1.8234926924	-1.9801789378	4.6470766448
H	1.0	-0.9916720550	-1.8210996606	5.7879063599
H	1.0	0.4426780776	-1.5887863624	6.7851429535
H	1.0	2.0728347270	-0.1539976303	5.8509493198

H	1.0	1.1336271392	0.9723124229	6.8287272603
H	1.0	2.5207687208	2.2266704203	5.3179671141
H	1.0	0.8722431877	2.3989989164	4.7140517016
H	1.0	1.3871161939	1.0434666368	2.8628116985
O	8.0	4.0994458689	0.5570387875	4.3312214843
H	1.0	5.3731524729	-0.8498107416	2.8258743820
H	1.0	5.8693978769	-2.0705456634	0.7292249517
H	1.0	4.2407700983	-2.0277580087	-1.1526194897
O	8.0	0.1921124951	0.2148149370	-2.6862875372
H	1.0	0.0721032917	1.1422885267	-2.9269478803
H	1.0	1.1075038056	0.0038179130	-2.9117084761

8. $[Zr(TRENCAM)(H_2O)_2]^{2-}$ (B3LYP/DZVP/PCM optimized geometry)



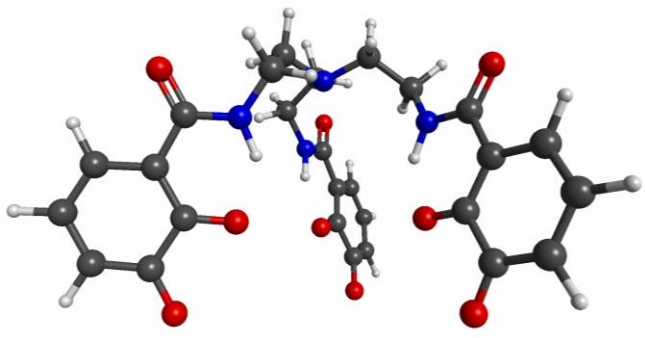
B3LYP/DZVP/PCM: $E = -5632.535749$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0144714135	0.0893021216	-0.1725387960
O	8.0	1.8303108863	-0.7596606886	-0.9656308180
C	6.0	2.8995399115	-0.7854212315	-0.1472356123
C	6.0	4.0892501198	-1.4643776830	-0.4153957635
C	6.0	5.1360719767	-1.4277703652	0.5299222694
C	6.0	4.9783293949	-0.7445782818	1.7322531939
C	6.0	3.7795889506	-0.0516048930	2.0334886045
C	6.0	2.7517692037	-0.0432093270	1.0641979630
O	8.0	1.5903358215	0.6188361672	1.1752776838
C	6.0	3.6487155944	0.5583458986	3.3987541591
N	7.0	2.4066318894	0.9756661228	3.7623526355
C	6.0	2.0805899836	1.4502380270	5.1002112820
C	6.0	1.4623731158	0.3647013210	5.9968610841
N	7.0	0.1101672736	-0.0523091494	5.5825336742
C	6.0	-0.9091623872	0.8876408495	6.0852792745
C	6.0	-2.2110695335	0.8889782988	5.2699531668

N	7.0	-2.0545508547	1.4501232745	3.9363081473
C	6.0	-2.4572469862	2.7051603771	3.6034769334
C	6.0	-2.1542100992	3.1559455200	2.2060202851
C	6.0	-1.5480655656	2.3293591224	1.2278789818
C	6.0	-1.2469418242	2.8691741277	-0.0575152048
C	6.0	-1.5754654149	4.1851752189	-0.3758789971
C	6.0	-2.1955094544	5.0000513088	0.5949494355
C	6.0	-2.4746550376	4.4914543448	1.8592455485
H	1.0	-2.9413267514	5.1136906385	2.6170496088
H	1.0	-2.4477801043	6.0298243916	0.3509968006
H	1.0	-1.3372345795	4.5709040409	-1.3653989440
O	8.0	-0.6271717851	2.0181739811	-0.9109357538
O	8.0	-1.2135649346	1.0467418403	1.4032309222
O	8.0	-3.0490536874	3.4528559412	4.4170452036
H	1.0	-1.5675071409	0.9172114614	3.2130747470
H	1.0	-2.9555754015	1.4860207289	5.8001657594
H	1.0	-2.6087845852	-0.1274973181	5.1770095053
H	1.0	-0.4996394001	1.9014967807	6.0552609393
H	1.0	-1.1537818994	0.6784883771	7.1437104774
C	6.0	-0.1806328649	-1.4298617435	6.0223241294
C	6.0	0.4168093278	-2.5154976910	5.1134107203
N	7.0	-0.1847570519	-2.5538853375	3.7877466985
C	6.0	-1.1103662180	-3.4766701419	3.4132987258
C	6.0	-1.7081106839	-3.3155870911	2.0469517666
C	6.0	-1.2730850248	-2.3500610300	1.1066311308
C	6.0	-1.9807642279	-2.2004155820	-0.1258735504
C	6.0	-3.0486021572	-3.0377196702	-0.4410017727
C	6.0	-3.4553257604	-4.0234983209	0.4834993044
C	6.0	-2.8030932554	-4.1470198277	1.7064129046
H	1.0	-3.1230026801	-4.8886996785	2.4325779489
H	1.0	-4.2925289859	-4.6745612135	0.2417367141
H	1.0	-3.5638421252	-2.9111929720	-1.3913416169
O	8.0	-1.5458669755	-1.1948135653	-0.9218331630
O	8.0	-0.2325942264	-1.5288829118	1.2749646881
O	8.0	-1.4651799106	-4.4097151171	4.1710026028
H	1.0	0.0454463968	-1.8311481599	3.1045139502
H	1.0	0.2544354185	-3.4875682792	5.5836564013
H	1.0	1.4979459622	-2.3761790708	5.0042515332
H	1.0	-1.2644565427	-1.5737784003	6.0382169899
H	1.0	0.1740053855	-1.5988036264	7.0561985674
H	1.0	2.1248594859	-0.5046550688	5.9695861265
H	1.0	1.4631601914	0.7252390664	7.0424322515
H	1.0	3.0012698659	1.8069239998	5.5672133403
H	1.0	1.4028823096	2.3058091896	5.0090866407
H	1.0	1.6622973269	0.8567471896	3.0758875894
O	8.0	4.6323044954	0.6410790065	4.1691379610
H	1.0	5.7683226778	-0.7466513806	2.4769433097
H	1.0	6.0633020651	-1.9592699545	0.3259002619
H	1.0	4.1921331611	-2.0176788658	-1.3470250759
O	8.0	0.1829306744	0.2461340732	-2.6268032456
H	1.0	0.1265105796	1.1910746969	-2.8601137713
H	1.0	1.1247948883	-0.0077526300	-2.7018528022

O	8.0	-3.0652702539	0.7346360443	-2.3802485299
H	1.0	-2.4422907345	1.4320415364	-2.1049377630
H	1.0	-2.6622087544	-0.0728040863	-1.9900885629

9. TRENCAM^{6-}



B3LYP/DZVP/PCM: $E = -1939.306059$, $G_{298.15} = 264.997$

ATOM	CHARGE	X	Y	Z
O	8.0	4.1280446368	-0.3935674293	-1.4262698015
C	6.0	4.7259556809	-0.4443351538	-0.2692457157
C	6.0	6.0710055688	-0.8665897929	-0.1203960797
C	6.0	6.7516015976	-0.8737912224	1.1270116538
C	6.0	6.1014257094	-0.4569628667	2.2761119067
C	6.0	4.7338939219	-0.0320406351	2.2172189277
C	6.0	4.0052108131	-0.0327724012	0.9742749669
O	8.0	2.7527678173	0.3270987835	0.8793891599
C	6.0	4.1212473082	0.3983700996	3.5023262192
N	7.0	2.8072463891	0.7661925487	3.4666930704
C	6.0	2.1036999004	1.2781173194	4.6310439057
C	6.0	1.3489984469	0.2090209320	5.4471170426
N	7.0	-0.0159405899	-0.0897060409	4.9613318113
C	6.0	-0.9536124515	0.9449644909	5.4516138200
C	6.0	-2.2510388554	1.0869533619	4.6290617206
N	7.0	-2.1513901693	1.9799118997	3.4860876248
C	6.0	-2.3955301411	3.3196773343	3.5703878410
C	6.0	-2.3172388090	4.0933538035	2.3025177253
C	6.0	-1.9927839422	3.4815115698	1.0420334631
C	6.0	-1.8760451580	4.3539041427	-0.1622851028
C	6.0	-2.1652170182	5.7288663530	0.0046432223
C	6.0	-2.5158937055	6.2951071122	1.2594069270
C	6.0	-2.5847730184	5.4978757987	2.3883752806
H	1.0	-2.8492568154	5.9136312336	3.3568694760
H	1.0	-2.7296504474	7.3627782963	1.3285566579
H	1.0	-2.0972619750	6.3675094314	-0.8784412152
O	8.0	-1.5362756807	3.8294833694	-1.3076219855
O	8.0	-1.7961102911	2.1976163496	0.8902802002

O	8.0	-2.6779316410	3.8558997983	4.6807641259
H	1.0	-1.9638735674	1.6565015174	2.5231322311
H	1.0	-3.0344826006	1.4691608780	5.2913233105
H	1.0	-2.5732423089	0.1049150064	4.2676169722
H	1.0	-0.4513609698	1.9154356987	5.4399699578
H	1.0	-1.2156192538	0.7458146777	6.5086972124
C	6.0	-0.4413846842	-1.4192276465	5.4482267271
C	6.0	0.1002474023	-2.6075107322	4.6290848998
N	7.0	-0.6888335448	-2.9564885968	3.4588900810
C	6.0	-1.7249264043	-3.8434067529	3.5113283724
C	6.0	-2.4204987014	-4.1402289037	2.2312329672
C	6.0	-2.0627101254	-3.5045075367	0.9895754276
C	6.0	-2.8223169538	-3.8797722868	-0.2401790228
C	6.0	-3.8618459916	-4.8280001659	-0.0898810960
C	6.0	-4.1749093106	-5.4488947256	1.1481891876
C	6.0	-3.4776637422	-5.1039334586	2.2921104941
H	1.0	-3.7004967734	-5.5623531398	3.2511140687
H	1.0	-4.9831371673	-6.1801347494	1.1943143058
H	1.0	-4.4354850986	-5.0938204009	-0.9793325362
O	8.0	-2.5203328053	-3.3423789226	-1.3900926760
O	8.0	-1.1087923071	-2.6170857728	0.8854594430
O	8.0	-2.0541628801	-4.3881054714	4.6053580469
H	1.0	-0.5523328140	-2.5331466311	2.5267941489
H	1.0	0.1332420091	-3.4847564536	5.2814321292
H	1.0	1.1244854141	-2.3992952530	4.3024421531
H	1.0	-1.5325392385	-1.4755128825	5.4249088261
H	1.0	-0.1457834491	-1.5454846892	6.5078440130
H	1.0	1.9471955564	-0.7051985125	5.4161199891
H	1.0	1.3123908396	0.5207233857	6.5089464547
H	1.0	2.8406920724	1.7497103326	5.2879862693
H	1.0	1.4083006748	2.0569320309	4.2996497521
H	1.0	2.3908914066	0.7160995192	2.5229176678
O	8.0	4.7716686811	0.4322402866	4.5864728008
H	1.0	6.6004965150	-0.4531769737	3.2412009799
H	1.0	7.7895269997	-1.2071869633	1.1723120863
H	1.0	6.6119911642	-1.1466243684	-1.0253292578

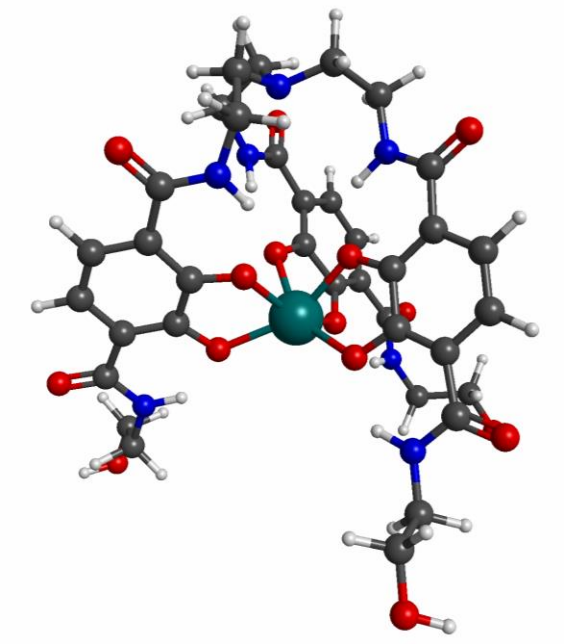
M11-L/DZVP/PCM: E = –1939.258065

ATOM	CHARGE	X	Y	Z
O	8.0	4.1111894302	-0.3474443841	-1.3682024262
C	6.0	4.6717786091	-0.4404587349	-0.2296852694
C	6.0	5.9931175608	-0.8760368805	-0.0602500973
C	6.0	6.6425519246	-0.9064031481	1.1813855838
C	6.0	5.9887254455	-0.4925326076	2.3089591877
C	6.0	4.6447786223	-0.0609944871	2.2293758195
C	6.0	3.9400622337	-0.0469939909	0.9927947243
O	8.0	2.7228597447	0.3115596409	0.8792761719
C	6.0	4.0282038260	0.3602403429	3.4880482506

N	7.0	2.7320019524	0.7139085724	3.4402964593
C	6.0	2.0681552989	1.2439198157	4.5799050914
C	6.0	1.3110991228	0.2138246137	5.3861497008
N	7.0	-0.0104095560	-0.0809961970	4.8762453071
C	6.0	-0.9264888596	0.9309037603	5.3558829378
C	6.0	-2.2021457350	1.0453601742	4.5513128882
N	7.0	-2.1075659612	1.9087535991	3.4253720582
C	6.0	-2.3341322431	3.2282627557	3.5399353983
C	6.0	-2.2787894145	4.0140193964	2.3074219538
C	6.0	-1.9709228392	3.4377717157	1.0462622671
C	6.0	-1.8818325849	4.3277687814	-0.1247523815
C	6.0	-2.1762123595	5.6807761741	0.0775345659
C	6.0	-2.5033175372	6.2088926178	1.3335455183
C	6.0	-2.5606714038	5.3937854907	2.4291246111
H	1.0	-2.8108648711	5.7827053271	3.4152178728
H	1.0	-2.7310372486	7.2728135682	1.4293307917
H	1.0	-2.1263507864	6.3391561150	-0.7948016068
O	8.0	-1.5795962301	3.8313357664	-1.2561550388
O	8.0	-1.7694002549	2.1936128667	0.8569097492
O	8.0	-2.5803070609	3.7262807941	4.6454462043
H	1.0	-1.9272968436	1.5881407833	2.4717449796
H	1.0	-2.9964051773	1.4172627764	5.2099027460
H	1.0	-2.5133285460	0.0529515256	4.2012443326
H	1.0	-0.4322049101	1.9096641123	5.3287825850
H	1.0	-1.1668313239	0.7454797317	6.4260164797
C	6.0	-0.4326159038	-1.3681113142	5.3829172861
C	6.0	0.1031343443	-2.5448122561	4.6002133309
N	7.0	-0.6545710176	-2.8817626624	3.4456478872
C	6.0	-1.6814225059	-3.7470909789	3.5108765457
C	6.0	-2.3604910288	-4.0557380170	2.2508955826
C	6.0	-2.0087487988	-3.4354022780	1.0194217625
C	6.0	-2.7660448320	-3.8148749377	-0.1897880710
C	6.0	-3.7957015595	-4.7489511063	-0.0261471820
C	6.0	-4.0939870209	-5.3588054586	1.1987604030
C	6.0	-3.4041405248	-5.0047492848	2.3234635360
H	1.0	-3.6192675972	-5.4616730657	3.2868565540
H	1.0	-4.9034873379	-6.0895529836	1.2560488623
H	1.0	-4.3728447531	-5.0216779440	-0.9138395424
O	8.0	-2.4692469239	-3.2990857287	-1.3157366772
O	8.0	-1.0741710307	-2.5772944511	0.8977852033
O	8.0	-2.0032220565	-4.2591874479	4.5912108972
H	1.0	-0.5099205541	-2.4580235841	2.5267318190
H	1.0	0.1290024712	-3.4185560925	5.2599479831
H	1.0	1.1380566152	-2.3462923984	4.2917362452
H	1.0	-1.5279562775	-1.4262787238	5.3584308877
H	1.0	-0.1508779680	-1.4648633102	6.4547705421
H	1.0	1.9115603354	-0.7043055219	5.3907312228
H	1.0	1.2432437387	0.5358580901	6.4486267471
H	1.0	2.8176114732	1.7097588763	5.2296701913
H	1.0	1.3850048125	2.0395897502	4.2528658186
H	1.0	2.3187710418	0.6856823824	2.5054998593
O	8.0	4.6506466553	0.3994584140	4.5563619382

H	1.0	6.4673040237	-0.5143652758	3.2861080421
H	1.0	7.6735243404	-1.2613978638	1.2421469877
H	1.0	6.5519909397	-1.1354053858	-0.9630988432

10. [Zr(TRENTAM)]$^{2-}$



B3LYP/DZVP/PCM: E = –6447.010447, $G_{298.15}$ = 420.514

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0811010019	-0.0977371218	0.2675664363
O	8.0	1.8925066054	-0.5653872739	-0.7530645542
C	6.0	3.0562207166	-0.5264044007	-0.0640222659
C	6.0	4.3216971275	-0.8588555641	-0.5779287882
C	6.0	5.4320530560	-0.7914604763	0.3017839839
C	6.0	5.2878180713	-0.4092287057	1.6260271570
C	6.0	4.0209434971	-0.0760415454	2.1634739237
C	6.0	2.9132215713	-0.1205995520	1.2997100425
O	8.0	1.6638795784	0.2111897493	1.6572820043
C	6.0	3.9309996032	0.2926991681	3.6202972226
N	7.0	2.6824814618	0.3751753162	4.1531192136
C	6.0	2.4213422500	0.7460059286	5.5381486590
C	6.0	1.4123762870	-0.1816728518	6.2291098629
N	7.0	0.0242444756	-0.1241108909	5.7155649148
C	6.0	-0.6400701848	1.1042741327	6.2084831298
C	6.0	-1.9278884423	1.5058344635	5.4760713208
N	7.0	-1.6931096570	1.9213698641	4.0991191504
C	6.0	-2.2233487699	3.0482256529	3.5541267786
C	6.0	-1.8982014401	3.3206253714	2.1100091232

C	6.0	-1.3103126905	2.3778575735	1.2501114335
C	6.0	-0.9400718593	2.7246570986	-0.0876924535
C	6.0	-1.2325731805	4.0057867763	-0.5900815673
C	6.0	-1.8612696960	4.9337596776	0.2788365466
C	6.0	-2.1815494262	4.6047802850	1.5864176108
H	1.0	-2.6485243643	5.3345260681	2.2403581010
H	1.0	-2.0851879405	5.9213872895	-0.1110511624
O	8.0	-0.2999717196	1.7437244261	-0.7624840758
O	8.0	-1.0566714699	1.1056211604	1.5941110785
O	8.0	-2.9206771827	3.8506580115	4.2129443397
H	1.0	-1.2328949156	1.2723487000	3.4616206198
H	1.0	-2.3704631291	2.3515495575	6.0059567916
H	1.0	-2.6662592524	0.6945861620	5.4977344648
H	1.0	0.0609833996	1.9373911671	6.1160425933
H	1.0	-0.8778138652	1.0076937921	7.2842762106
C	6.0	-0.7268889653	-1.3166770403	6.1707897071
C	6.0	-0.4291482909	-2.6199940428	5.4148858417
N	7.0	-0.8886299538	-2.6134633300	4.0322099405
C	6.0	-1.8155379584	-3.4766690935	3.5376106736
C	6.0	-2.1794526194	-3.3228766372	2.0845860942
C	6.0	-1.5364213588	-2.4391213507	1.2030440180
C	6.0	-2.0005380482	-2.2480734180	-0.1364498461
C	6.0	-3.0781852864	-3.0138004782	-0.6193595610
C	6.0	-3.6922236229	-3.9322418305	0.2701399713
C	6.0	-3.2664536215	-4.0770687890	1.5805753533
H	1.0	-3.7643828816	-4.7713531641	2.2505482691
H	1.0	-4.5240033331	-4.5196080886	-0.1048774053
O	8.0	-1.3349199274	-1.2952731516	-0.8280930899
O	8.0	-0.4605341246	-1.7048286121	1.5275598947
O	8.0	-2.3734729251	-4.3429720461	4.2449163021
H	1.0	-0.4694249350	-1.9608768692	3.3712336199
H	1.0	-0.9445498471	-3.4336748142	5.9289585534
H	1.0	0.6425529333	-2.8511601531	5.4360148750
H	1.0	-1.7956470705	-1.1154301597	6.0657139293
H	1.0	-0.5442660303	-1.4996304420	7.2463142401
H	1.0	1.7815906153	-1.2046665448	6.1194678191
H	1.0	1.4327920889	0.0451179815	7.3115423119
H	1.0	3.3678401564	0.6827677321	6.0791671255
H	1.0	2.0956956749	1.7929020921	5.5891383136
H	1.0	1.8996870852	0.3010148324	3.5039372856
O	8.0	4.9650084984	0.4840762996	4.2965950149
H	1.0	6.1496923694	-0.3708716859	2.2847650145
H	1.0	6.4084771066	-1.0549792841	-0.0923227782
C	6.0	-3.6203718334	-2.9348327386	-2.0175797219
N	7.0	-3.0289307700	-2.0425616665	-2.8554215913
H	1.0	-2.2739356911	-1.4750235297	-2.4719893855
O	8.0	-4.5586192004	-3.6714033117	-2.3892844353
C	6.0	-3.4308847879	-1.8809458529	-4.2461332365
C	6.0	-4.5207685023	-0.8110650250	-4.4174748033
O	8.0	-4.9120554401	-0.6687449294	-5.7911766221
H	1.0	-5.3786071391	-1.4788289484	-6.0567235192
H	1.0	-2.5505409028	-1.6032200746	-4.8339108668

H	1.0	-3.7979720215	-2.8428363571	-4.6153350515
H	1.0	-4.1391636689	0.1673857720	-4.1120992737
H	1.0	-5.3844672667	-1.0536391499	-3.7860813085
C	6.0	4.5816160964	-1.2841170892	-1.9956659504
N	7.0	3.5173547997	-1.2660304317	-2.8424227057
H	1.0	2.6158627992	-1.0092989649	-2.4420025729
C	6.0	3.5969547302	-1.6552312683	-4.2430969499
C	6.0	3.0414149463	-3.0687700393	-4.4787823857
H	1.0	3.0300949034	-0.9398968751	-4.8485760405
H	1.0	4.6442221700	-1.6087862835	-4.5498612100
O	8.0	5.7260490853	-1.6158737807	-2.3689776190
O	8.0	3.0506382162	-3.4183199046	-5.8705372281
H	1.0	3.9744329245	-3.5239671254	-6.1526921640
H	1.0	3.6040251771	-3.7994925510	-3.8837654090
H	1.0	1.9933799116	-3.1163935264	-4.1685870978
C	6.0	-0.9329903330	4.4611332896	-1.9901518320
N	7.0	-0.4180010901	3.5324836074	-2.8395638086
O	8.0	-1.1745366174	5.6312084030	-2.3545967612
H	1.0	-0.2135315675	2.6131706277	-2.4510616420
C	6.0	-0.1119256175	3.8164808079	-4.2346246129
C	6.0	1.3641010755	4.1889743930	-4.4472153557
H	1.0	-0.7508127054	4.6406533903	-4.5629638613
H	1.0	-0.3544741545	2.9351148895	-4.8370272915
O	8.0	1.6501341317	4.4433023504	-5.8306038365
H	1.0	1.1797950667	5.2525089715	-6.0923134104
H	1.0	2.0092835514	3.3544813768	-4.1580626855
H	1.0	1.6262422187	5.0536899344	-3.8246906400

M11-L/DZVP/PCM: $E = -6446.697150$

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0751457752	-0.3309901820	-0.3150314384
O	8.0	1.8268355810	-0.8086250211	-1.0148938680
C	6.0	2.8920984429	-0.5694106367	-0.2762171012
C	6.0	4.2095635113	-0.7807194269	-0.6496468141
C	6.0	5.2086736372	-0.4921967228	0.2858920733
C	6.0	4.9063906609	-0.0219105081	1.5329228390
C	6.0	3.5855460164	0.2166734129	1.9197118900
C	6.0	2.5809551800	-0.0416798892	0.9961697975
O	8.0	1.3118689993	0.1737645591	1.1953990404
C	6.0	3.3395231221	0.7423557332	3.2786791862
N	7.0	2.0654458287	1.0031920822	3.5943076306
C	6.0	1.6881072972	1.4796166501	4.8829799460
C	6.0	1.1619285453	0.3861335284	5.7755986922
N	7.0	-0.0964424196	-0.1496615464	5.3222729560
C	6.0	-1.1922400708	0.6857140813	5.7437156829
C	6.0	-2.3786021617	0.5819275405	4.8197506888
N	7.0	-2.1088985395	1.1138969151	3.5242116592
C	6.0	-2.1426603314	2.4337178872	3.3044176738

C	6.0	-1.6804082130	2.8955355895	1.9804843794
C	6.0	-1.2300926622	2.0440114963	0.9813292622
C	6.0	-0.6849782452	2.5626120242	-0.2146206875
C	6.0	-0.7043984880	3.9267421408	-0.4605658926
C	6.0	-1.2189041679	4.7656874656	0.5332259034
C	6.0	-1.6654791169	4.2695434882	1.7256452805
H	1.0	-2.0264207292	4.9344717221	2.5071973200
H	1.0	-1.2230751129	5.8351374443	0.3352275402
O	8.0	-0.1984775326	1.6363791187	-1.0103712660
O	8.0	-1.2612845484	0.7408765757	1.0332982119
O	8.0	-2.5354953214	3.2205535661	4.1553046337
H	1.0	-1.6787379083	0.5293117043	2.8150891238
H	1.0	-3.2260833245	1.1197531063	5.2567588049
H	1.0	-2.6900770047	-0.4637572715	4.6970878398
H	1.0	-0.8681479022	1.7337088013	5.7493611053
H	1.0	-1.5018133138	0.4560587571	6.7839343365
C	6.0	-0.2750843554	-1.4974678366	5.8011375540
C	6.0	0.3531123505	-2.5200831484	4.8910223732
N	7.0	-0.2943232749	-2.5880093507	3.6217501484
C	6.0	-1.4471064572	-3.2498594186	3.4731739155
C	6.0	-2.1129047175	-3.1372911435	2.1594161563
C	6.0	-1.5997725727	-2.4112585676	1.0954467155
C	6.0	-2.3416232282	-2.2402254520	-0.0954791843
C	6.0	-3.5502099167	-2.9023831896	-0.2581369282
C	6.0	-4.0270803226	-3.6745310542	0.8064584380
C	6.0	-3.3434766881	-3.7730385486	1.9855833276
H	1.0	-3.7411517988	-4.3499689743	2.8175814935
H	1.0	-4.9807610154	-4.1789628621	0.6732860756
O	8.0	-1.7715079513	-1.4314174644	-0.9609130771
O	8.0	-0.4318944911	-1.8280248271	1.0892497684
O	8.0	-1.9324777727	-3.9144676282	4.3789316370
H	1.0	0.0049784995	-1.9842739934	2.8629750422
H	1.0	0.3094907712	-3.5049523974	5.3677998618
H	1.0	1.4117866329	-2.2919236842	4.7173847278
H	1.0	-1.3477263107	-1.7208761996	5.8585613123
H	1.0	0.1163300185	-1.6170966738	6.8319626623
H	1.0	1.9062349596	-0.4209240824	5.7893613452
H	1.0	1.0910456962	0.7565108902	6.8196503044
H	1.0	2.5631376435	1.9380756724	5.3510556064
H	1.0	0.9377423372	2.2728514581	4.7567904301
H	1.0	1.3506221618	0.7502234710	2.9186704842
O	8.0	4.2620921390	0.9400947803	4.0586700042
H	1.0	5.6933185935	0.1950306654	2.2520819545
H	1.0	6.2408723184	-0.6670714250	-0.0066748592
C	6.0	-4.3691506884	-2.8576356008	-1.4847450943
N	7.0	-3.8984610102	-2.1087675806	-2.4883442186
H	1.0	-3.0302282982	-1.6074465825	-2.3390076145
O	8.0	-5.4115367811	-3.4884134276	-1.5857793338
C	6.0	-4.5813440853	-2.0381211643	-3.7362387124
C	6.0	-5.6519295639	-0.9763692981	-3.7466376690
O	8.0	-6.3391986971	-0.9423140063	-4.9605267219
H	1.0	-6.8710443520	-1.7412204211	-5.0208764130

H	1.0	-3.8550428646	-1.8422775518	-4.5314350806
H	1.0	-5.0360896180	-3.0150387415	-3.9436011526
H	1.0	-5.2003950265	0.0129960049	-3.6197927831
H	1.0	-6.3314317488	-1.1329414342	-2.8948638850
C	6.0	4.6371395077	-1.2575162497	-1.9808355658
N	7.0	3.6610142620	-1.5851220445	-2.8350347716
H	1.0	2.7036622701	-1.4732014107	-2.5231047179
C	6.0	3.9431650686	-2.0013533640	-4.1677832926
C	6.0	4.2039411900	-3.4831262507	-4.2603712730
H	1.0	3.0955322658	-1.7376841713	-4.8083724153
H	1.0	4.8150344213	-1.4489757158	-4.5387182770
O	8.0	5.8178115481	-1.3304238028	-2.2881847263
O	8.0	4.4574720435	-3.8870585282	-5.5718457530
H	1.0	5.3095255969	-3.5263254548	-5.8334722975
H	1.0	5.0249117509	-3.7567765625	-3.5802444118
H	1.0	3.3172428170	-4.0363199041	-3.9333572276
C	6.0	-0.2240209751	4.5597610818	-1.7043748575
N	7.0	0.2557385599	3.7369350676	-2.6439527537
O	8.0	-0.2805147155	5.7682287722	-1.8729993259
H	1.0	0.3013128392	2.7481236348	-2.4278712072
C	6.0	0.7534863458	4.2337929484	-3.8825259536
C	6.0	2.1926301796	4.6721238461	-3.7804317710
H	1.0	0.1309171981	5.0778920280	-4.2034254280
H	1.0	0.6609718171	3.4512140426	-4.6423241080
O	8.0	2.6995163830	5.1128012302	-5.0039154432
H	1.0	2.2683799648	5.9430248774	-5.2254215251
H	1.0	2.8157426602	3.8236235126	-3.4789684930
H	1.0	2.2891803020	5.4389143295	-2.9965030606

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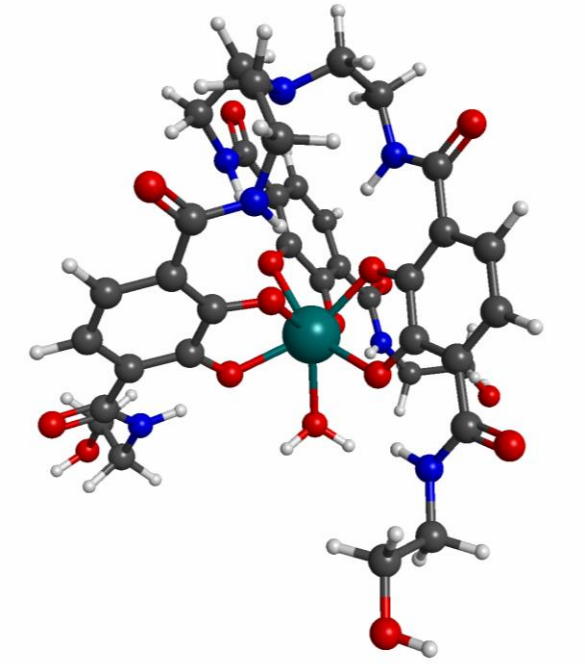
11. [Zr(TRENTAM)(H_2O)]$^{2-}$



B3LYP/DZVP/PCM: E = –6523.426393, $G_{298.15}$ = 434.897

ATOM	CHARGE	X	Y	Z
ZR	40.0	-0.0400295959	-0.2480161634	-0.4179958110
O	8.0	1.9308439552	-0.7808495911	-1.0461255203
C	6.0	2.9788073409	-0.5438805699	-0.2361449607
C	6.0	4.3050711543	-0.9244884351	-0.5077282813
C	6.0	5.2901238434	-0.6398008139	0.4722352743
C	6.0	4.9629368639	-0.0044046587	1.6574527984
C	6.0	3.6344797522	0.3997566991	1.9413496760
C	6.0	2.6413483720	0.1492061220	0.9723109373
O	8.0	1.3598112619	0.5078892263	1.0800115527
C	6.0	3.3633393132	1.0191141866	3.2812841746
N	7.0	2.0637517478	1.2772784861	3.5818997113
C	6.0	1.6260489887	1.7192430142	4.8988497256
C	6.0	1.1077158416	0.5688024113	5.7764650687
N	7.0	-0.1418755030	-0.0407268035	5.2854787579
C	6.0	-1.3165538562	0.7690330016	5.6590969860
C	6.0	-2.5032124557	0.6307129829	4.6894825066
N	7.0	-2.2467112650	1.2020360796	3.3732983727
C	6.0	-2.4993499609	2.5006723062	3.0622934451
C	6.0	-2.0151663487	2.9843534632	1.7222900502
C	6.0	-1.4385645152	2.1492304764	0.7464202170
C	6.0	-0.8255544637	2.6960698019	-0.4288582707
C	6.0	-0.8658082860	4.0874007761	-0.6529794047
C	6.0	-1.5074071448	4.9073197890	0.3106062099
C	6.0	-2.0563500312	4.3767551035	1.4654882361
H	1.0	-2.5062288577	5.0220705772	2.2136365773
H	1.0	-1.5299209086	5.9773441796	0.1289461513
O	8.0	-0.2317739558	1.7911850580	-1.2286397465
O	8.0	-1.3927976398	0.8150517380	0.8357337774
O	8.0	-3.0685549405	3.2765690403	3.8610802827
H	1.0	-1.7661847586	0.6465206142	2.6670227709
H	1.0	-3.3690335573	1.1379630719	5.1225966294
H	1.0	-2.7698259207	-0.4225809240	4.5550869674
H	1.0	-1.0279776363	1.8230387555	5.6768179807
H	1.0	-1.6621331120	0.5219244038	6.6793880300
C	6.0	-0.2724251725	-1.4303113849	5.7621021812
C	6.0	0.5135400146	-2.4498999088	4.9200933598
N	7.0	-0.0547271753	-2.6527903825	3.5942412086
C	6.0	-0.9956400206	-3.5972918697	3.3316681118
C	6.0	-1.6513421349	-3.5413343802	1.9806398747
C	6.0	-1.2853464747	-2.6384735559	0.9637225838
C	6.0	-2.0698344642	-2.5228226232	-0.2291333055
C	6.0	-3.1888927519	-3.3574623549	-0.4237668033
C	6.0	-3.4996442423	-4.3066219217	0.5830537830
C	6.0	-2.7614262431	-4.3888839328	1.7512768170
H	1.0	-3.0370470550	-5.0928443064	2.5305471777
H	1.0	-4.3607187471	-4.9493758576	0.4315484139

O	8.0	-1.6524339784	-1.5688660969	-1.0845952408
O	8.0	-0.2309059314	-1.8159534426	1.0336190888
O	8.0	-1.3336680536	-4.4542929590	4.1784414159
H	1.0	0.1353796835	-1.9772449120	2.8541960231
H	1.0	0.5199317011	-3.4090808546	5.4425205692
H	1.0	1.5540528586	-2.1321913717	4.8003489779
H	1.0	-1.3269004118	-1.7179720631	5.7313916823
H	1.0	0.0459927673	-1.5199301898	6.8171555726
H	1.0	1.8847996802	-0.2003445323	5.8062051943
H	1.0	0.9917488589	0.9370467968	6.8127548662
H	1.0	2.4779931921	2.1840331211	5.3995941899
H	1.0	0.8544683676	2.4856880180	4.7719395245
H	1.0	1.3705184838	1.0157106330	2.8797847116
O	8.0	4.2953435142	1.2615210595	4.0818229426
H	1.0	5.7255422474	0.1938371718	2.4044913994
H	1.0	6.3136795372	-0.9371603152	0.2691339023
C	6.0	-4.1292874781	-3.2676407509	-1.5909089743
N	7.0	-3.9660437137	-2.2055984900	-2.4253160918
H	1.0	-3.2080151621	-1.5643756445	-2.1983950212
O	8.0	-5.0284507966	-4.1171884179	-1.7672487867
C	6.0	-4.8713570361	-1.9054049412	-3.5263966503
C	6.0	-5.9613350155	-0.9032066596	-3.1130969904
O	8.0	-6.8168001981	-0.5580209999	-4.2132231242
H	1.0	-7.3537667472	-1.3370877511	-4.4346249437
H	1.0	-4.2951436439	-1.4922834204	-4.3605742363
H	1.0	-5.3292286908	-2.8407657950	-3.8580696587
H	1.0	-5.5028017793	0.0349634216	-2.7873642634
H	1.0	-6.5439533634	-1.3058755151	-2.2746676701
C	6.0	4.7540318244	-1.5909724304	-1.7777568984
N	7.0	3.8208728426	-1.7157898083	-2.7612525319
H	1.0	2.8777312757	-1.3968416523	-2.5362896739
C	6.0	4.1128935407	-2.2348534278	-4.0894538670
C	6.0	3.5116736682	-3.6302073531	-4.3187773530
H	1.0	3.7103277404	-1.5469335508	-4.8420526924
H	1.0	5.1988252167	-2.2714085992	-4.2063538889
O	8.0	5.9336821298	-1.9753855580	-1.9257136913
O	8.0	3.7434387542	-4.0887781052	-5.6591023231
H	1.0	4.6931368580	-4.2697780581	-5.7568815360
H	1.0	3.9112663959	-4.3410660206	-3.5841236137
H	1.0	2.4246479584	-3.5972148434	-4.1999850282
C	6.0	-0.2292167913	4.7798698303	-1.8210154283
N	7.0	0.5470236015	4.0189112402	-2.6389000768
O	8.0	-0.3975414088	6.0007146249	-2.0239724999
H	1.0	0.6298685705	3.0309086256	-2.4045185540
C	6.0	1.2805690556	4.5774817042	-3.7664580575
C	6.0	2.6723542490	5.0851688795	-3.3554608847
H	1.0	0.6996904577	5.4044634396	-4.1852088408
H	1.0	1.3845536667	3.8067379461	-4.5360943285
O	8.0	3.3819954906	5.6482477047	-4.4695327426
H	1.0	2.9467642280	6.4823484887	-4.7120889958
H	1.0	3.2866214975	4.2537148789	-2.9986234051
H	1.0	2.5765967057	5.8154760179	-2.5425137682

O	8.0	-0.1094457488	-0.3271486353	-2.8398918190
H	1.0	-0.5574212306	0.4746393620	-3.1673312237
H	1.0	-0.6523548946	-1.0846518154	-3.1250348807

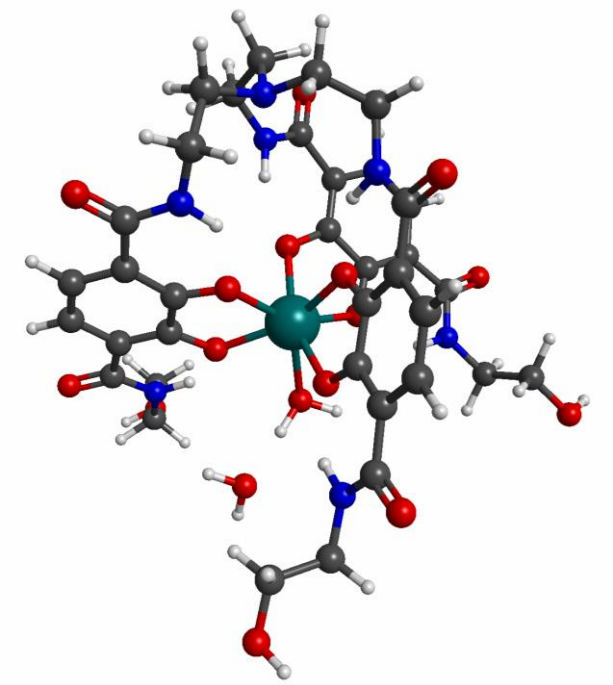
M11-L/DZVP/PCM: $E = -6523.122172$

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0108337779	-0.0847082318	-0.6572892787
O	8.0	1.9395160625	-0.7341606753	-1.2313732538
C	6.0	2.9145792411	-0.6484987878	-0.3559955978
C	6.0	4.1798929470	-1.2062851239	-0.4844402085
C	6.0	5.0903788588	-1.0252365908	0.5627331790
C	6.0	4.7543152877	-0.3332172251	1.6908069708
C	6.0	3.4888368573	0.2386643063	1.8397851070
C	6.0	2.5816530876	0.1027597602	0.7969111578
O	8.0	1.3907741327	0.6286756858	0.7732294083
C	6.0	3.1769679911	0.9118042667	3.1146677882
N	7.0	1.9219111476	1.3480588027	3.2727811356
C	6.0	1.4702014007	1.8282271103	4.5377176268
C	6.0	1.1605824268	0.7061903854	5.4961597385
N	7.0	0.0296597222	-0.0745887594	5.0707334242
C	6.0	-1.2088806213	0.5177580888	5.5014044555
C	6.0	-2.3425046870	0.2209645887	4.5521136981
N	7.0	-2.1683962617	0.8538050487	3.2849507914
C	6.0	-2.3871313954	2.1671512166	3.1449211756
C	6.0	-1.9704771450	2.7769347043	1.8673319676
C	6.0	-1.4121581913	2.0608612311	0.8156046457
C	6.0	-0.9246995467	2.7305751739	-0.3314893257
C	6.0	-1.0569061888	4.1071272713	-0.4464655113
C	6.0	-1.6768531992	4.8025042364	0.5976058501
C	6.0	-2.0996424849	4.1608442948	1.7269060498
H	1.0	-2.5429240641	4.7157091128	2.5506721241
H	1.0	-1.7771541062	5.8806083991	0.4954475987
O	8.0	-0.3685696877	1.9306704757	-1.2128922793
O	8.0	-1.2812094442	0.7653668052	0.7787898935
O	8.0	-2.8967023530	2.8333467420	4.0374691728
H	1.0	-1.6553854719	0.3824738710	2.5465553287
H	1.0	-3.2866497114	0.5545519990	4.9957687490
H	1.0	-2.4322778602	-0.8598143994	4.3787081288
H	1.0	-1.0900421294	1.6075939931	5.5466349525
H	1.0	-1.4824990305	0.1973421398	6.5276067046
C	6.0	0.1381928643	-1.4393756105	5.5128236707
C	6.0	0.9303794516	-2.2893018793	4.5520723985
N	7.0	0.2741238367	-2.4357880537	3.2927721390
C	6.0	-0.8105671098	-3.2124222622	3.1844563488
C	6.0	-1.5660393365	-3.1264464580	1.9212231096
C	6.0	-1.1861877008	-2.3359008637	0.8442583175
C	6.0	-2.0251365748	-2.2167531573	-0.2894580788
C	6.0	-3.2177575250	-2.9252187013	-0.3568643495

C	6.0	-3.5642435147	-3.7395901637	0.7262185043
C	6.0	-2.7651653202	-3.8367165669	1.8289322807
H	1.0	-3.0538393111	-4.4552131288	2.6758372056
H	1.0	-4.5049522278	-4.2818957258	0.6687671497
O	8.0	-1.5642061459	-1.3932311619	-1.2027257816
O	8.0	-0.0835623054	-1.6456027217	0.7721633149
O	8.0	-1.1683026065	-3.9488064073	4.0948643475
H	1.0	0.4509956404	-1.7727042198	2.5444159623
H	1.0	1.0946186230	-3.2791594556	4.9920963976
H	1.0	1.9195230595	-1.8514247089	4.3657556579
H	1.0	-0.8659322034	-1.8746967625	5.5886950699
H	1.0	0.5777569664	-1.5088636168	6.5287085816
H	1.0	2.0449950874	0.0578046527	5.5462757552
H	1.0	1.0190632018	1.1104793634	6.5196164486
H	1.0	2.2370213092	2.4782955139	4.9715705099
H	1.0	0.5813869258	2.4495805941	4.3652442985
H	1.0	1.2521030027	1.1247307475	2.5432685730
O	8.0	4.0241345358	1.0525162663	3.9883031957
H	1.0	5.4615918894	-0.2232815546	2.5100827291
H	1.0	6.0761069391	-1.4708968859	0.4570451857
C	6.0	-4.1749309403	-2.8522851262	-1.4775325495
N	7.0	-3.8313579425	-2.0611206896	-2.5008359982
H	1.0	-2.9780538976	-1.5229828373	-2.4012238075
O	8.0	-5.2188161626	-3.4893946671	-1.4758082185
C	6.0	-4.6988697271	-1.8653145352	-3.6128678780
C	6.0	-5.6900591217	-0.7541043914	-3.3740508826
O	8.0	-6.5272297771	-0.5529909444	-4.4719595319
H	1.0	-7.1191297108	-1.3079459942	-4.5366710422
H	1.0	-4.1016531488	-1.6420033726	-4.5029106864
H	1.0	-5.2329627616	-2.8026760311	-3.8070744949
H	1.0	-5.1586297852	0.1903749750	-3.2161899429
H	1.0	-6.2596704029	-0.9605452892	-2.4546471047
C	6.0	4.6326575276	-1.9914540024	-1.6486574495
N	7.0	3.7636908988	-2.1079071512	-2.6605010070
H	1.0	2.8451598991	-1.6958717121	-2.5384383792
C	6.0	4.0804973461	-2.8600590560	-3.8269386253
C	6.0	3.6943548605	-4.3110939443	-3.6880584200
H	1.0	3.5721195471	-2.4211319053	-4.6918053328
H	1.0	5.1589373679	-2.7824925688	-4.0089129770
O	8.0	5.7474773316	-2.4912797306	-1.6963347536
O	8.0	3.9994842692	-5.0496315901	-4.8319255004
H	1.0	4.9566280184	-5.1181057220	-4.8921803343
H	1.0	4.1713400603	-4.7321676147	-2.7891057547
H	1.0	2.6117674487	-4.3970709226	-3.5459638420
C	6.0	-0.5437003439	4.9067335131	-1.5750255131
N	7.0	0.2090901399	4.2557925879	-2.4704136178
O	8.0	-0.7844705979	6.1001126021	-1.6794624667
H	1.0	0.3843008385	3.2715177128	-2.3057398028
C	6.0	0.8461591676	4.9335847510	-3.5487892717
C	6.0	2.1864973730	5.4971189290	-3.1489032219
H	1.0	0.1910779970	5.7410048211	-3.8958120980
H	1.0	0.9770053888	4.2373760815	-4.3834660040

O	8.0	2.8489840877	6.0927712175	-4.2227689230
H	1.0	2.3803309417	6.8989033336	-4.4565072183
H	1.0	2.8364619645	4.6878989477	-2.7995010356
H	1.0	2.0591220769	6.1944663717	-2.3065432038
O	8.0	-0.0574833160	0.0958633303	-2.9558304931
H	1.0	-0.5979406750	0.8470200903	-3.2258932892
H	1.0	-0.3416232524	-0.6414375433	-3.5065655575

12. [Zr(TRENTAM)(H_2O)$_2$]$^{2-}$ (B3LYP/DZVP/PCM optimized geometry)



B3LYP/DZVP/PCM: E = –6599.847191

ATOM	CHARGE	X	Y	Z
ZR	40.0	0.0690307295	0.2082665995	-0.3288814056
O	8.0	1.9264553893	-0.7235852919	-1.0789187167
C	6.0	2.9874794113	-0.7115647154	-0.2595323642
C	6.0	4.1944744535	-1.4142351258	-0.4621056153
C	6.0	5.2175489234	-1.2896492942	0.5133439486
C	6.0	5.0385878199	-0.5370007276	1.6604263921
C	6.0	3.8256632905	0.1561970785	1.9000348004
C	6.0	2.8274085212	0.1023410373	0.9112390973
O	8.0	1.6672019374	0.7683485051	0.9724235542
C	6.0	3.6492364892	0.8114499910	3.2407624346
N	7.0	2.3863169875	1.1848676645	3.5776861221
C	6.0	2.0147041893	1.6199563497	4.9184514806
C	6.0	1.5156962847	0.4687621755	5.8088875769
N	7.0	0.2127958250	-0.0842481185	5.3960220330

C	6.0	-0.8999566501	0.7323295089	5.9132791213
C	6.0	-2.1907517751	0.6217854515	5.0857191204
N	7.0	-2.0880612849	1.2453729450	3.7732268858
C	6.0	-2.4701452992	2.5278386047	3.5369622911
C	6.0	-2.1550270423	3.0881271838	2.1798844105
C	6.0	-1.5115370148	2.3618597843	1.1570997220
C	6.0	-1.1149604333	3.0177571633	-0.0520413080
C	6.0	-1.4243709848	4.3737527621	-0.2696627652
C	6.0	-2.1152371229	5.0729266332	0.7530218364
C	6.0	-2.4596481577	4.4520825723	1.9410809458
H	1.0	-2.9557384620	5.0079252377	2.7305284168
H	1.0	-2.3496796962	6.1197935283	0.5861023385
O	8.0	-0.4311686641	2.2394502142	-0.9072365637
O	8.0	-1.1984145853	1.0636918173	1.2219488177
O	8.0	-3.0363923410	3.2258535840	4.4087271186
H	1.0	-1.5898403027	0.7686002949	3.0203275042
H	1.0	-2.9994165364	1.1129796540	5.6310869105
H	1.0	-2.4744105529	-0.4265738965	4.9482615680
H	1.0	-0.5960685318	1.7827470336	5.9120011993
H	1.0	-1.1287395246	0.4730695116	6.9639055168
C	6.0	0.0741083158	-1.4947286020	5.8029367364
C	6.0	0.7494351259	-2.4868246755	4.8428733864
N	7.0	0.1179021582	-2.5386769114	3.5316907246
C	6.0	-0.7977500200	-3.4766447764	3.1751684865
C	6.0	-1.4353299359	-3.3159160275	1.8246498980
C	6.0	-1.0716999634	-2.3205067377	0.8934587571
C	6.0	-1.8051951634	-2.1764799850	-0.3311406205
C	6.0	-2.8467475504	-3.0662780296	-0.6530657885
C	6.0	-3.1720101739	-4.0802736359	0.2845602752
C	6.0	-2.4987119136	-4.1903556962	1.4886316618
H	1.0	-2.7728850898	-4.9584993967	2.2057037988
H	1.0	-3.9802651342	-4.7615522335	0.0384269888
O	8.0	-1.4251515758	-1.1324383813	-1.0923785745
O	8.0	-0.0802801574	-1.4439255517	1.0687036050
O	8.0	-1.1150322536	-4.4258021872	3.9279840748
H	1.0	0.2969165904	-1.7977715942	2.8532741773
H	1.0	0.7027656712	-3.4848210512	5.2839485701
H	1.0	1.8060077755	-2.2323358553	4.7074964790
H	1.0	-0.9890664377	-1.7461365135	5.8442679104
H	1.0	0.4741638480	-1.6567591572	6.8206964292
H	1.0	2.2658414972	-0.3262325375	5.7716639924
H	1.0	1.4848589162	0.8201906025	6.8567319327
H	1.0	2.8929759653	2.0681877359	5.3879460880
H	1.0	1.2498878572	2.3977989185	4.8280186315
H	1.0	1.6583401912	1.0242155307	2.8839094444
O	8.0	4.6164762238	0.9525910587	4.0208918738
H	1.0	5.8153639747	-0.4854001897	2.4172589815
H	1.0	6.1431582338	-1.8325255263	0.3474778630
C	6.0	-3.6649004889	-3.0042532044	-1.9110853940
N	7.0	-3.3821628604	-2.0015060127	-2.7849325454
H	1.0	-2.6611581403	-1.3350537282	-2.5101327141
O	8.0	-4.5601591901	-3.8472839521	-2.1395420763

C	6.0	-4.1285860102	-1.7879444021	-4.0169971015
C	6.0	-5.3118923066	-0.8310418227	-3.8080905107
O	8.0	-6.0201316353	-0.5729935966	-5.0311815165
H	1.0	-6.4801788469	-1.3876515396	-5.2935876729
H	1.0	-3.4528079535	-1.3676973491	-4.7672225926
H	1.0	-4.4903317624	-2.7542784497	-4.3790645727
H	1.0	-4.9427417785	0.1396909339	-3.4677346435
H	1.0	-5.9868795460	-1.2320283041	-3.0416648861
C	6.0	4.4668151578	-2.3217228639	-1.6230620410
N	7.0	3.4467962881	-2.5096465143	-2.5047281647
H	1.0	2.5741312157	-2.0261642242	-2.2946666213
C	6.0	3.5425860393	-3.4091448818	-3.6455769384
C	6.0	2.9846725192	-4.8067693836	-3.3310105191
H	1.0	2.9955482915	-2.9783015193	-4.4902275819
H	1.0	4.5950386070	-3.4884623990	-3.9300642384
O	8.0	5.5754003732	-2.8800853363	-1.7675786676
O	8.0	3.0889583240	-5.6855723862	-4.4613312884
H	1.0	4.0293501951	-5.8867019160	-4.6009041840
H	1.0	3.4981667347	-5.2263230646	-2.4566273889
H	1.0	1.9176742311	-4.7445072577	-3.0986848586
C	6.0	-1.0419545460	5.1425318470	-1.5007663345
N	7.0	-0.2870093769	4.4855285915	-2.4229559468
O	8.0	-1.4053924446	6.3265370551	-1.6648009649
H	1.0	-0.0349580280	3.5211979872	-2.2038054129
C	6.0	0.2237963916	5.1194919954	-3.6302001220
C	6.0	1.6069754229	5.7527163527	-3.4069184128
H	1.0	-0.4849204530	5.8896560344	-3.9470605309
H	1.0	0.2903761227	4.3692164380	-4.4238662123
O	8.0	2.1124847736	6.3652228327	-4.6027622986
H	1.0	1.5629480008	7.1416961740	-4.8021253504
H	1.0	2.3342695356	4.9822881959	-3.1362458955
H	1.0	1.5557615728	6.4784616389	-2.5854647672
O	8.0	0.2049376958	0.4793825690	-2.6881804093
H	1.0	-0.6489935654	0.7575374801	-3.1177641823
H	1.0	0.5066169538	-0.3235329532	-3.1463602383
O	8.0	-2.2057092418	1.2055261260	-3.7449765223
H	1.0	-2.2414622879	1.5676085056	-4.6478676533
H	1.0	-2.6026619089	1.8913491343	-3.1809396647

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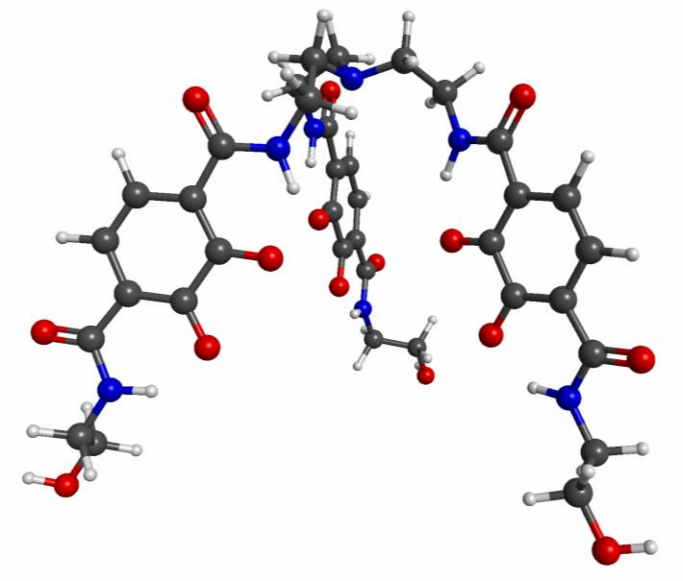
13. TRENTAM^{6-}



B3LYP/DZVP/PCM: $E = -2906.660459$, $G_{298.15} = 415.328$

ATOM	CHARGE	X	Y	Z
O	8.0	4.0126914718	-0.8553302193	-1.3633709617
C	6.0	4.6224444392	-1.1171902307	-0.2421207360
C	6.0	5.8734379767	-1.8069626418	-0.1582769272
C	6.0	6.4769912932	-2.0697038719	1.1141861800
C	6.0	5.8853281390	-1.6494161184	2.2799746922
C	6.0	4.6428872670	-0.9363608534	2.2652060787
C	6.0	3.9772736698	-0.6600798724	1.0295840434
O	8.0	2.8444913797	-0.0245258296	0.9432929321
C	6.0	4.1196771522	-0.4839566217	3.5796979110
N	7.0	2.9732894585	0.2538438125	3.5655326811
C	6.0	2.4093572380	0.8458026166	4.7681652013
C	6.0	1.4471573159	-0.0719514643	5.5466795236
N	7.0	0.0622882685	-0.1008301876	5.0389128541
C	6.0	-0.6746866090	1.0904388090	5.5031814272
C	6.0	-1.9343294597	1.4240387038	4.6803064968
N	7.0	-1.6908804248	2.2056902272	3.4769586574
C	6.0	-1.7247843328	3.5695566234	3.4730580721
C	6.0	-1.6275526085	4.2402972240	2.1505703772
C	6.0	-1.5524797520	3.5180729495	0.9175714192
C	6.0	-1.4555521161	4.2982126180	-0.3565520365
C	6.0	-1.4330788417	5.7272138571	-0.2799990806
C	6.0	-1.5271582238	6.3896509382	0.9875650555
C	6.0	-1.6205878060	5.6732267632	2.1545013186
H	1.0	-1.6966543315	6.1785770767	3.1134457626
H	1.0	-1.5225046680	7.4764972163	0.9949150492
O	8.0	-1.4001597657	3.6274776006	-1.4720272918
O	8.0	-1.5668916981	2.2210987799	0.8315999235
O	8.0	-1.8242355780	4.2170530950	4.5538323264
H	1.0	-1.6510145983	1.7887344819	2.5366029905

H	1.0	-2.6178481174	1.9883096254	5.3221403835
H	1.0	-2.4453898378	0.5023022817	4.3845107273
H	1.0	-0.0164835909	1.9613119182	5.4567433384
H	1.0	-0.9619045021	0.9722631949	6.5664991495
C	6.0	-0.6167855846	-1.3275103193	5.4968165427
C	6.0	-0.3449450392	-2.5734122119	4.6352519210
N	7.0	-1.1605186220	-2.6585920410	3.4305660194
C	6.0	-2.4735833097	-3.0239358428	3.4774424474
C	6.0	-3.1600460949	-3.2667769823	2.1835590805
C	6.0	-2.4766313369	-3.2586445183	0.9282422678
C	6.0	-3.2728201648	-3.5228127778	-0.3149878723
C	6.0	-4.6681737039	-3.8129533688	-0.1796732611
C	6.0	-5.2937457248	-3.7873791594	1.1092679112
C	6.0	-4.5743638996	-3.4977598320	2.2425085363
H	1.0	-5.0514838173	-3.4702893973	3.2185035352
H	1.0	-6.3625050825	-3.9804259841	1.1571345458
O	8.0	-2.6561701247	-3.4360248836	-1.4597752609
O	8.0	-1.2012224073	-3.0348924990	0.7921610374
O	8.0	-3.0632701177	-3.1584684442	4.5869460392
H	1.0	-0.7554849736	-2.6893449978	2.4850915692
H	1.0	-0.5295474174	-3.4582900551	5.2577335279
H	1.0	0.7043542122	-2.6020528794	4.3265535932
H	1.0	-1.6955147077	-1.1670785672	5.4954029519
H	1.0	-0.3395889739	-1.5522090751	6.5449225577
H	1.0	1.8595357258	-1.0831493749	5.5052901993
H	1.0	1.4582212275	0.2246427317	6.6141416202
H	1.0	3.2347343955	1.1078816114	5.4378938186
H	1.0	1.9045196485	1.7751686927	4.4854151744
H	1.0	2.5984054981	0.4223051053	2.6217383199
O	8.0	4.7102938514	-0.7371684830	4.6680338531
H	1.0	6.3487506998	-1.8416117697	3.2443739934
H	1.0	7.4228227206	-2.6053838630	1.1264604318
C	6.0	-5.5413295708	-4.1322768258	-1.3363838427
N	7.0	-4.9370520719	-4.1732171681	-2.5613512993
H	1.0	-3.9387244837	-3.9097405941	-2.5364416425
O	8.0	-6.7744040305	-4.3720438203	-1.2096724676
C	6.0	-5.6597199602	-4.3941592244	-3.8001540604
C	6.0	-6.1673619630	-3.0841187500	-4.4232638134
O	8.0	-6.8720224294	-3.3086960925	-5.6573173274
H	1.0	-7.6780958908	-3.8110423748	-5.4523197984
H	1.0	-5.0010434151	-4.8998037546	-4.5154230161
H	1.0	-6.5116247358	-5.0522666815	-3.6000320438
H	1.0	-5.3246617410	-2.4341327371	-4.6756022520
H	1.0	-6.8039701291	-2.5542617164	-3.7031417882
C	6.0	6.6227487434	-2.2609831742	-1.3555936575
N	7.0	6.0798809435	-1.9446184997	-2.5689182550
H	1.0	5.1830703419	-1.4363027664	-2.5021283301
C	6.0	6.7102883869	-2.2704822454	-3.8337289124
C	6.0	6.1676423531	-3.5734111451	-4.4420340118
H	1.0	6.5472646264	-1.4505852450	-4.5433237176
H	1.0	7.7885683365	-2.3699534774	-3.6716576296
O	8.0	7.7196813030	-2.8820492751	-1.2805763452

O	8.0	6.8014844586	-3.8894181823	-5.6939890634
H	1.0	7.7352414521	-4.0891496941	-5.5139236920
H	1.0	6.2875089437	-4.3960803843	-3.7253966834
H	1.0	5.1020833689	-3.4712599337	-4.6668748076
C	6.0	-1.3193881364	6.5938879099	-1.4789044101
N	7.0	-1.2611961073	5.9572883407	-2.6860916592
O	8.0	-1.2870714930	7.8537135658	-1.4110933489
H	1.0	-1.2759097149	4.9267671089	-2.6117786149
C	6.0	-1.1212788062	6.6609697986	-3.9468503975
C	6.0	0.3483887871	6.8874922113	-4.3345753515
H	1.0	-1.6270386901	7.6295406020	-3.8674625082
H	1.0	-1.6153260249	6.0839412053	-4.7366069532
O	8.0	0.4777518604	7.5684091381	-5.5957173245
H	1.0	0.0949586338	8.4560489170	-5.4967086034
H	1.0	0.8564467502	5.9274235284	-4.4644082436
H	1.0	0.8616886604	7.4402574603	-3.5375784861

M11-L/DZVP/PCM: E = –2906.541518

ATOM	CHARGE	X	Y	Z
O	8.0	3.9088621869	-0.8321193014	-1.4624502085
C	6.0	4.4887647822	-1.0817093227	-0.3573982720
C	6.0	5.7202831582	-1.7674415786	-0.2434665134
C	6.0	6.2997967752	-2.0209535473	1.0185518900
C	6.0	5.7027292103	-1.5964634883	2.1604250656
C	6.0	4.4820534500	-0.8889938265	2.1189125843
C	6.0	3.8366533290	-0.6205112394	0.8900980455
O	8.0	2.7297302255	-0.0051700361	0.7925768696
C	6.0	3.9564114720	-0.4333861029	3.4045550216
N	7.0	2.8396599813	0.3105771096	3.3774210882
C	6.0	2.3260429616	0.9012301228	4.5656341213
C	6.0	1.4365427328	-0.0188141549	5.3689016308
N	7.0	0.0656513837	-0.0441010425	4.9204049347
C	6.0	-0.6407171875	1.0830265783	5.4784588597
C	6.0	-1.9041017143	1.4363842998	4.7327076006
N	7.0	-1.6834381521	2.1711256595	3.5354881835
C	6.0	-1.7077959658	3.5132243526	3.5258057057
C	6.0	-1.6226924054	4.1631364619	2.2182118097
C	6.0	-1.5527574270	3.4399073249	1.0055824831
C	6.0	-1.4421522796	4.2020530514	-0.2581748383
C	6.0	-1.4210761760	5.6147380690	-0.1840026258
C	6.0	-1.5230249059	6.2763124507	1.0606638544
C	6.0	-1.6206299638	5.5749643979	2.2170526140
H	1.0	-1.7074942348	6.0839558749	3.1760976445
H	1.0	-1.5192973031	7.3655025323	1.0603306118
O	8.0	-1.3825046746	3.5355185358	-1.3397507489
O	8.0	-1.5779663984	2.1748016240	0.9233921373
O	8.0	-1.7882299798	4.1494960663	4.5828256683
H	1.0	-1.6581390983	1.7377206280	2.6127831791

H	1.0	-2.5438590422	2.0299250819	5.3966497113
H	1.0	-2.4597990480	0.5231995163	4.4804482110
H	1.0	0.0109480610	1.9659023230	5.4606558655
H	1.0	-0.8750784890	0.9007878666	6.5509459740
C	6.0	-0.5619464394	-1.2656760036	5.3585399133
C	6.0	-0.3350697070	-2.4316200584	4.4312751915
N	7.0	-1.1436270849	-2.3893327298	3.2554311125
C	6.0	-2.4297765886	-2.7790021185	3.3223553212
C	6.0	-3.1146344181	-3.0420967430	2.0596812409
C	6.0	-2.4339592025	-3.1541640794	0.8259845854
C	6.0	-3.2260059746	-3.5311139824	-0.3694736511
C	6.0	-4.6226829413	-3.6963700464	-0.2230998386
C	6.0	-5.2417501119	-3.5362260302	1.0361724099
C	6.0	-4.5137692480	-3.2268472358	2.1374158672
H	1.0	-4.9866253996	-3.1182863682	3.1127469525
H	1.0	-6.3218748029	-3.6687771961	1.0908596778
O	8.0	-2.5999926203	-3.6686614655	-1.4652949744
O	8.0	-1.1874557414	-2.9683095634	0.6666105309
O	8.0	-2.9862481636	-2.9132693753	4.4171500076
H	1.0	-0.7362355571	-2.4973404401	2.3258091869
H	1.0	-0.5307272562	-3.3576559492	4.9928271679
H	1.0	0.7152208995	-2.4640969207	4.1159120181
H	1.0	-1.6435260191	-1.1173269059	5.4368098328
H	1.0	-0.2198499964	-1.5336093831	6.3818232939
H	1.0	1.8586601104	-1.0285559181	5.2955623007
H	1.0	1.4841909582	0.2517161557	6.4470713807
H	1.0	3.1655376394	1.2160006514	5.1983162860
H	1.0	1.7745129527	1.8075502113	4.2858628993
H	1.0	2.4639578934	0.4904047446	2.4466112473
O	8.0	4.5160288970	-0.6826433410	4.4786212848
H	1.0	6.1498607879	-1.7829809309	3.1362999395
H	1.0	7.2455706149	-2.5615564883	1.0422751150
C	6.0	-5.5031604948	-4.0404020420	-1.3353839878
N	7.0	-4.9063364706	-4.3086719373	-2.5110605082
H	1.0	-3.8980743467	-4.1391802385	-2.5220815928
O	8.0	-6.7298778888	-4.1165701352	-1.2197903578
C	6.0	-5.6618377237	-4.5395824518	-3.6899804131
C	6.0	-6.0664018100	-3.2585705282	-4.3747662423
O	8.0	-6.8212758480	-3.4835848584	-5.5300302247
H	1.0	-7.6609715485	-3.8671243490	-5.2606990394
H	1.0	-5.0780624053	-5.1554481527	-4.3848723245
H	1.0	-6.5628731606	-5.1113530251	-3.4316898159
H	1.0	-5.1747648177	-2.7088791393	-4.6954922787
H	1.0	-6.6012842262	-2.6157761079	-3.6578949332
C	6.0	6.4771244320	-2.2348866163	-1.4008330037
N	7.0	5.9532144687	-1.9624714337	-2.6083261329
H	1.0	5.0760368110	-1.4378450400	-2.5847531279
C	6.0	6.6324016475	-2.3004238323	-3.8070425364
C	6.0	6.3219072046	-3.7018414478	-4.2671336502
H	1.0	6.3564428075	-1.5897456544	-4.5955352122
H	1.0	7.7167940173	-2.2079634500	-3.6521933195
O	8.0	7.5544141400	-2.8310906515	-1.3047695490

O	8.0	7.0065161379	-4.0428869625	-5.4381536539
H	1.0	7.9443673226	-4.0761499807	-5.2288316006
H	1.0	6.5366559282	-4.4080341549	-3.4500940560
H	1.0	5.2552070781	-3.7925062423	-4.4987784108
C	6.0	-1.2961076672	6.4667225947	-1.3628624513
N	7.0	-1.2424169560	5.8375868538	-2.5498972263
O	8.0	-1.2540730810	7.6995992343	-1.3061511549
H	1.0	-1.2464594678	4.8164426016	-2.4934254506
C	6.0	-1.0552898427	6.5525500932	-3.7609914048
C	6.0	0.3965048434	6.8487949637	-4.0395512996
H	1.0	-1.6118859491	7.4985632855	-3.7122867805
H	1.0	-1.4737534875	5.9740611323	-4.5933859877
O	8.0	0.5809741538	7.5407376119	-5.2409893504
H	1.0	0.1570998930	8.3994063514	-5.1527282991
H	1.0	0.9556431697	5.9121809688	-4.1401898270
H	1.0	0.8282980317	7.3932433041	-3.1849709736

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