Supporting information

Enantiomeric recognition of D- and L-lactate by CEST with the aid of a paramagnetic shift reagent

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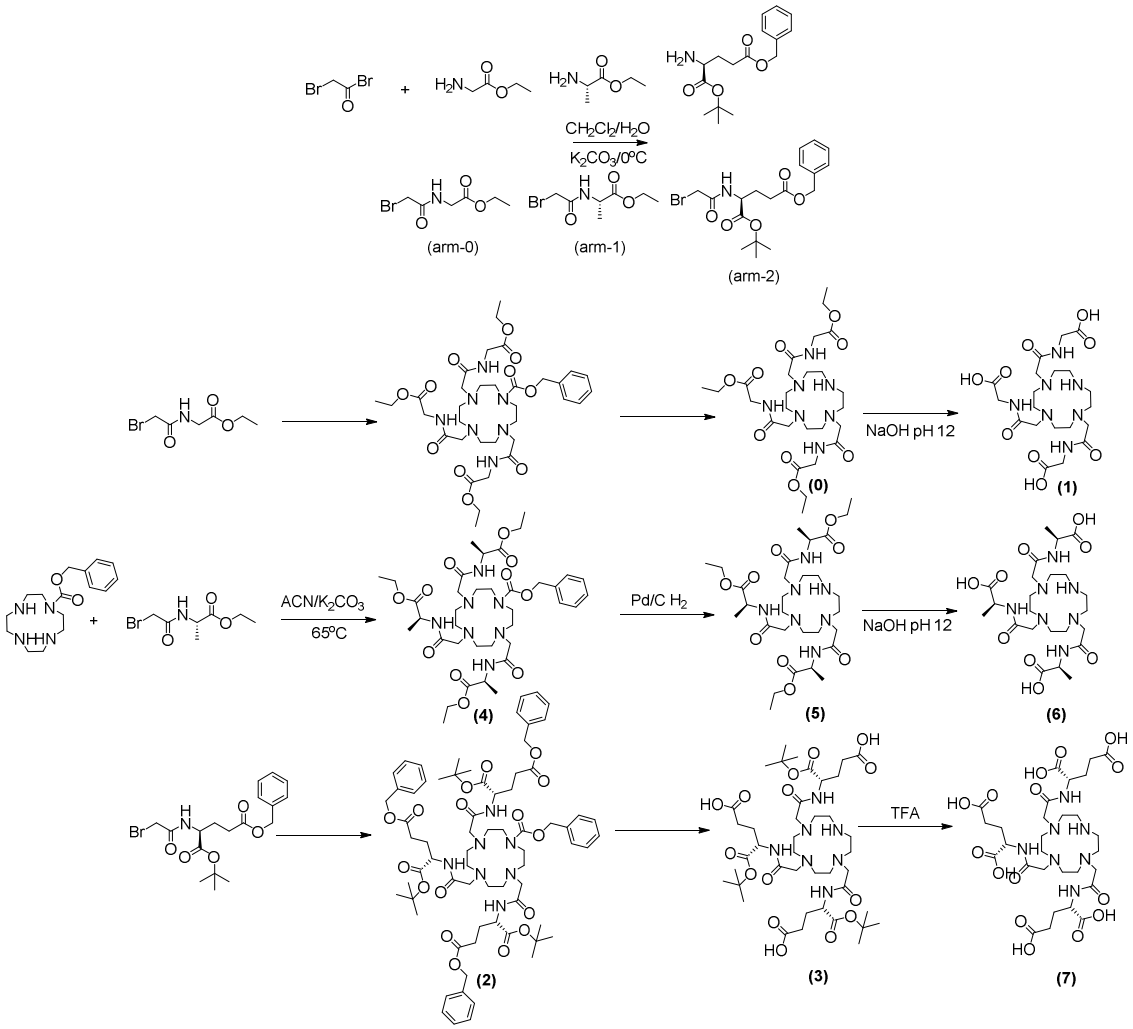
1. General

All reagents and solvents were purchased from commercial sources and used as received without other purification unless stated in the work. ^{1}H, ^{13}C and CEST Z-spectra NMR have been recorded on a Bruker AVANCE III 400 NMR spectrometer. Temperature unit controller Model # 2416 was used to control the temperature. Hydrogenation reactions were carried out using a Parr hydrogenation apparatus. Preparative HPLC was performed on a Waters Delta prep HPLC system equipped with a Waters 2996 photodiode array detector and a Phenomenex Luna C18 column (5 mm, 30 mm × 250 mm). The final concentration of the complexes were checked by Evan's method[1].

2. Synthesis and characterization



Scheme S1. Synthetic pathways used to obtain the final ligands studied in this work.

N-alkyl- bromoacetamides. Bromoacetyl bromide (1.1 equiv) was dissolved in dichloromethane (50 mL) and added dropwise to a cooled solution (0^{o}C) on a round flask

containing the amine (1 equiv) and potassium carbonate (5 equiv) in water. The biphasic mixture contains water (50 mL) and dichloromethane (100 mL). The resulting solution was allowed to warm to room temperature and stirred for 8 hours. The organic layer was washed with brine (100 mL) for three times and dried over Na_2SO_4. The organic phase solvents were removed under vacuum.

N-(2-bromoacetyl) L-glycine ethyl ester (arm-0): The title compound was prepared in an analogous manner to that described above and was obtained as a white solid. (Yield 95%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.28 (3H, t, CH_3), 3.91 (2H, s, $BrCH_2$), 4.06 (2H, d, $NHCH_2$), 4.23 (2H, q, CH_2CH_3), ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.1 (CH_2CH_3), 28.4 ($BrCH_2CO$), 39.7 ($NHCH_2CO$), 61.0 (CH_2CH_3), 169.5 (CH_2COO), 177.8 (CH_2CONH).

N-(2-bromoacetyl) L- alanine ethyl ester (arm-1): The title compound was prepared in an analogous manner to that described for arm-0 and was obtained as a white solid. (yield 96%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.29 (3H, t, CH_2CH_3), 1.48 (3H, d, $CHCH_3$), 4.19 (2H, s, $BrCH_2CO$), 4.21 (2H, q, CH_2CH_3), 4.35 (1H, q, NHCHCO), 8.03 (1H, s, NH). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.1 (CH_2CH_3), 17.3 ($CHCH_3$), 28.7 ($BrCH_2$), 51.1 ($NHCHCO$), 61.3 (CH_2CH_3), 171.5 ($CHCO$), 177.5 (CH_2CO).

N-(2-bromoacetyl) L-glutamic acid γ-benzyl ester α-tert-butyl ester (arm-2): The title compound was prepared in an analogous manner to that described for arm 0 and was obtained as a colorless oil. (Yield 98%) ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.47 (9H, s, CH_3), 2.03-2.22 (2H, m, $CHCH_2CH_2$), 2.45 (2H, m, CH_2CH_2CO), 3.82 (2H, m, $NHCH_2CH$). 3.85 (2H, s, $BrCH_2CO$), 4.51 (1H, m, CH_2CHCH_2), 5.12 (2H, s, OCH_2Ph), 7.35 (5H, m, Ph). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 27.2 ($CHCH_2CH_2$), 27.9 (CH_3), 28.8 (CH_2CH_2CO), 30.2 ($NHCHCH_2$), 52.6 ($BrCH_2$), 66.7 (OCH_2Ph), 82.8 ($C(CH_3)_3$), 128.6-135.8 (Ph), 165.7 ($CHCOO$), 170.2 ($CHCOO$), 172.4 ($BrCH_2CO$).

1,4,7,10 –tetraazacyclododecane-1,4,7-tris(2-acetamidoglycine) (1): Compound 0 was prepared using a previously reported method[2] with the yield of 79%. The ligand 0 (1 g, 1.6 mmol) was dissolved in water and a concentrated solution of 1N NaOH was used to change the pH to 12. The resulting solution was stirred for 12 hours and neutralized with a 1N HCl solution. The final solution was lyophilized and the solid was used in the next steps without further purification.

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido- L-glutamic acid γ-benzyl ester α-tert-butyl ester 10-benzycarbamate (2): 1-benzyloxycarbonyl-1,4,7,10- tetraazacyclododecane

trihydrochloride (1 g, 2.4 mmol) and bromo-N-(2-acetamido- L-glutamic acid γ-benzyl ester α-tert-butyl ester (3.04 g, 7.32 mmol) were dissolved in anhydrous CH_3CN in the presence of of K_2CO_3 (2.66 g, 19 mmol). The resulting solution was stirred at 65°C for 24 hours under N_2 condition. The organic phase was filtered and solvents removed under vacuum. The residue was purified by chromatography using a Al_2O_3 column eluted with 2%methanol/98% dichloromethane to afford the title compound as a white solid (2.1 g, 66%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.43 (27H, s, $C(C\underline{H}_3)_3$), 2.35 (12H, m, $CHC\underline{H}_2C\underline{H}_2CO$), 2.5-3.0(22H, m, $C\underline{H}_2$ on cyclen and $NC\underline{H}_2CO$), 3.85 (2H, s, $COC\underline{H}_2Ph$), 4.48 (3H, t, $NHC\underline{H}CH_2$), 5.09 (6H, s, $OC\underline{H}_2Ph$), 7.30-7.40 (20H, m, Ph). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 27.5 ($CH\underline{C}H_2CH_2$), 27.9 ($C(\underline{C}H_3)_3$), 30.57 ($CH_2\underline{C}H_2CO$), 30.59 ($CO\underline{C}H_2$), 49-55 (ring $\underline{C}H_2$), 57.8 (CH), 58.9 ($N\underline{C}H_2CO$), 66.4 ($O\underline{C}H_2Ph$), 82.3 ($\underline{C}(CH_3)_3$), 129-138 (Ph), 156.6 ($N\underline{C}OCH_2$), 170.0 ($CH_2\underline{C}ONH$), 171.1 ($CH\underline{C}OO$), 172.4 ($O\underline{C}OCH_2$).

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido- L-glutamic acid α-tert-butyl ester) (3): compound 2 (2.1 g, 1.6 mmol) was dissolved in ethanol and transferred to a flask with 20% palladium on carbon (wt %). The mixture was shaken on a Parr hydrogenator under a hydrogen pressure of 50 psi for 10 hours at room temperature. The resulting solution was filtered and solvent was removed under vacuum to afford the title compound as a colorless solid (1.4 g, 96%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.41 (27H, m, $C(C\underline{H}_3)_3$), 2.17-2.65 (28H, m, ring CH_2, $CHC\underline{H}_2C\underline{H}_2CO$), 3.25 (6H, s, $NC\underline{H}_2CO$), 4.55 (3H, t, $NHC\underline{H}CH_2$), 8.03 (3H, s, $N\underline{H}$). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 27.0 ($CH\underline{C}H_2CH_2$), 27.4 ($C(\underline{C}H_3)_3$), 31.1 ($CH_2\underline{C}H_2CO$), 41-55(ring $\underline{C}H_2$), 57.8 (CH), 59.9 ($N\underline{C}H_2CO$), 84.0 ($\underline{C}(CH_3)_3$), 164.8 ($CH_2\underline{C}ONH$), 171.3 ($O\underline{C}OCH_2$), 177.7 ($\underline{C}OO$).

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L-alanine ethyl ester 10-benzycarbamate (4): 1-benzyloxycarbonyl-1,4,7,10- tetraazacyclododecane trihydrochloride (1 g, 2.4 mmol) and N-(2-bromoacetyl) - L- alanine ethyl ester (1.75 g, 7.3 mmol) were dissolved in anhydrous CH_3CN in the presence of 8 equivalences of $NaHCO_3$ (1.61 g, 19 mmol). The resulting solution was stirred at 65°C for 24 hours under N_2 condition and then the organic phase was filtered and solvents removed under vacuum. The residue was purified by chromatography using a Al_2O_3 column eluted with 2%methanol/98% dichloromethane to afford the title compound as a colorless oil (1.0 g, 53%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.21-1.33 (18H, m, $CHC\underline{H}_3$, $CH_2C\underline{H}_3$), 2.16-3.28 (16H, m, ring $C\underline{H}_2$), 3.25 (6H, s, $NC\underline{H}_2CO$), 4.12-4.48 (9H, m, $C\underline{H}$, $C\underline{H}_2CH_3$), 5.04 (2H, s, $PhC\underline{H}_2O$), 7.28-7.53 (8H, m, Ph, $N\underline{H}$). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 14.3 ($CH_2\underline{C}H_3$), 18.2 ($CH\underline{C}H_3$), 44-55 (ring $\underline{C}H_2$ $\underline{C}H$), 59.5($N\underline{C}H_2CO$), 61.2 ($\underline{C}H_2CH_3$), 67.5 ($Ph\underline{C}H_2O$), 127-136 (Ph), 156.2 ($N\underline{C}OO$), 170.8 ($CH_2\underline{C}O$), 173.1 ($CH\underline{C}OO$).

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L-alanine ethyl ester (5): compound 4 (1.0 g, 1.2 mmol) was dissolved in ethanol (50 ml). 20% palladium on carbon (wt %) was then added. The reaction mixture was shaken on a Parr hydrogenator under a hydrogen pressure of 50 psi for 10 hours at room temperature. The resulting mixture was filtered and

solvents removed under vacuum to afford the title compound as a colorless oil (0.56 g, 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.12 -1.38 (18H, m, $CHC\underline{H}_3$, $CH_2C\underline{H}_3$), 2.46-2.96 (16H, m, ring $C\underline{H}_2$), 3.25 (6H, s, $NC\underline{H}_2CO$), 4.11-4.46 (9H, m, $C\underline{H}$, $C\underline{H}_2CH_3$), 7.93 (3H, s, $N\underline{H}$). ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 17.4 ($CH_2\underline{C}H_3$), 17.7 ($CH\underline{C}H_3$), 44-55 (ring $\underline{C}H_2$ $\underline{C}H$), 57.2 ($N\underline{C}H_2CO$), 59.5 ($\underline{C}H_2CH_3$), 171.0 ($N\underline{C}OO$), 172.0 ($CH_2\underline{C}O$), 173.2 ($CH\underline{C}OO$).

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L-alanine (6): compound 5 (0.56 g, 0.86 mmol) was dissolved in H_2O. Slowly change the pH to 12 using 1N NaOH solution and leave the reaction for 16 hours at room temperature. The residue was then lyophilized to afford title compound as a white solid (310 mg, 63%). ^{1}H NMR (400 MHz, D_2O): δ (ppm) 1.36 (9H, d, $C\underline{H}CH_3$), 2.46-2.65 (16H, m, ring $C\underline{H}_2$), 3.25 (6H, s, $NC\underline{H}_2CO$), 4.19 (3H, q, $C\underline{H}CH_3$), 8.03 (3H, s, $N\underline{H}$). ^{13}C NMR (100 MHz, D_2O): δ (ppm) 17.5 ($CH\underline{C}H_3$), 45.2-55.1 (ring $\underline{C}H_2$, $\underline{C}H$), 58.1 ($N\underline{C}H_2CO$), 172.8 ($CH_2\underline{C}ONH$), 180.3 ($\underline{C}OO$).

1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L- glutamic acid (7): compound 3 (1.4 g, 1.5 mmol) was reacted directly with 4 mL TFA for 8 hours. Solvent was then removed under vacuum and the final compound was obtained as a yellow oil (900 mg, 79%). ^{1}H NMR (400 MHz, D_2O): δ (ppm) 2.17 (6H, m, $CHC\underline{H}_2CH_2$), 2.40- 2.60 (m, cyclen ring CH_2 plus $C\underline{H}_2COO^-$), 3.25 (6H, s, $NHC\underline{H}_2$), 4.45 (3H, t, $NHC\underline{H}$). ^{13}C NMR (100 MHz, D_2O): δ (ppm) 28 ($CH\underline{C}H_2$), 31.9 ($CHCH_2\underline{C}H_2$), 45.2-65.2 (cyclen rings CH_2, $N\underline{C}H_2$ and $\underline{C}H$), 170-183 ($CH\underline{C}OO^-$, $CH_2\underline{C}OO^-$ and $\underline{C}ONH$).

General procedure for the preparation of Yb^{3+} complexes.

Yb (III)- 1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido- L-Glutamic acid α-tert-butyl ester) (Yb1): The ligand was dissolved in acetonitrile or H_2O and 0.95 equivalents of $YbCl_3$ were added. Concentrated solutions of 1N NaOH and 1N HCl were used to adjust the pH to 5.5~6.0. Xylenol Orange tests were performed until no free metal was detected. Samples were filtered using 2 um membrane filter for further experiment. Stock solutions were prepared with miliQ Water. m/z (ESI-MS^+) : 904 $(M+H)^+$.

Yb (III)- 1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L-alanine ethyl ester (Yb2): complex was synthesized in an analogous manner to that described for Yb 1 using ligand 5. The title compound was obtained as a colorless solid. m/z (ESI-MS^+) :734 $(M+H)^+$.

Yb (III)- 1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L-alanine (Yb3): complex was synthesized in an analogous manner to that described for Yb 1 using ligand 6. The title compound was obtained as a colorless solid. m/z (ESI-MS^+) :790 $(M+H)^+$.

Yb (III)- 1,4,7,10- tetraazacyclododecane- 1,4,7 –tris(2-acetamido) L- glutamic acid (Yb4): complex was synthesized in an analogous manner to that described for Yb 1 using ligand 7. The title compound was obtained as a colorless solid .m/z (ESI-MS^+) :846 $(M+H)^+$.

3. ^{1}H NMR spectra of free Yb^{3+} complexes.

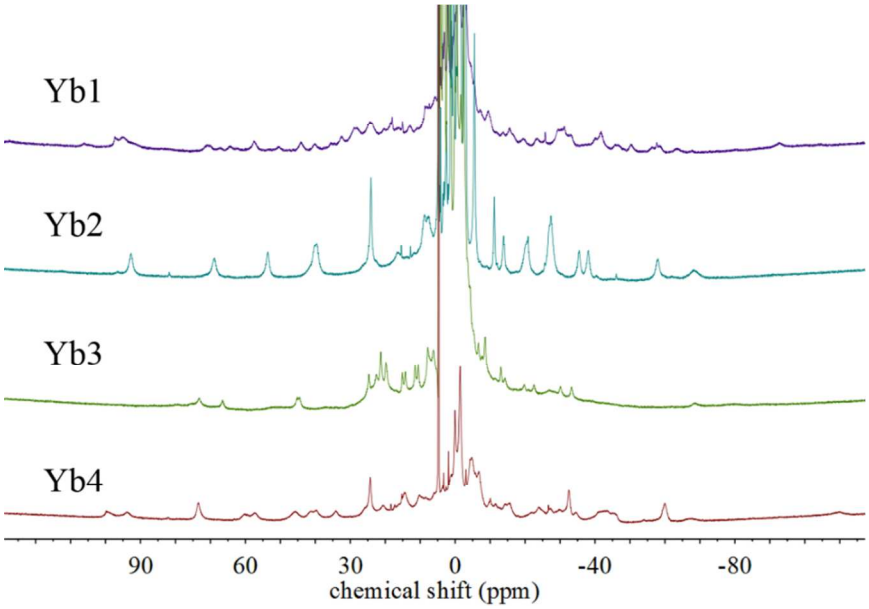


Figure S1. Proton NMR of $Yb_{1\text{-}4}$ complexes (50 mM) in the absence of lactate. Samples were dissolved in D_2O.

4. H_4 proton chemical shift of Yb complexes with D and L lactate.

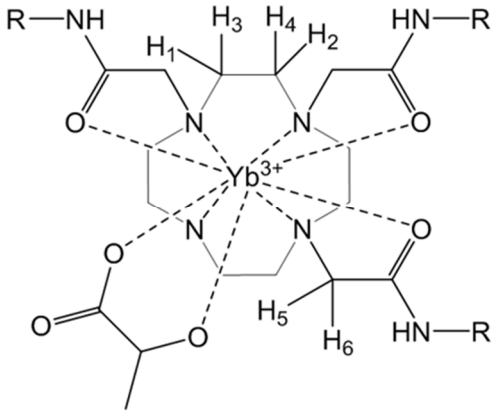


Figure S2. Schematic representation of the Yb-lac complex with the proton number assignments ($H_{1\text{-}6}$).

Table S1. Chemical shifts of all four ethylene proton resonances in the five Yb_x complexes with D- and L-lactate. The most highly shifted downfield resonance is assigned to the axial H_4 proton. All NMR spectra were recorded at 25°C in D_2O at 9.4 T. pD = 6.5

	L-lactate (ppm)				D-lactate (ppm)			
Yb0	101.3/100.5	77.2/75.4	67.1/66.3	53.6/52.1	101.3/100.5	77.2/75.4	67.1/66.3	53.6/52.1
Yb1	84.7	68.9	42.1	41.0	82.9	67.8	43.7	39.2
Yb2	85.3	65.2	47.6	41.0	85.8	67.1	50.0	43.7
Yb3	98.1	75.7	65.0	52.8	96.9	73.2	64.3	50.5
Yb4	97.4	74.3	62.6	50.4	95.8	72.1	61.5	48.1

5. Solid state X-ray crystal structure analysis of Yb_3 dimer

A colorless crystal was obtained by slow evaporation of diethyl ether into a vial containing a concentrated solution of Yb_3 complex and L-lactate (1:1) dissolved in water and methanol (4:1).

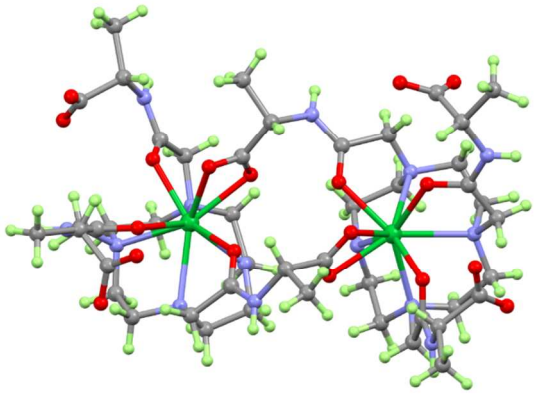


Figure S3. ORTEP representation of Yb_3 dimer. One of the carboxylates on the side arms would coordinate to another Yb_3 complex metal ion to form a dimer.

Note: the crystal growth attempt yielding crystals of the Yb_3 dimer was adjusted to pH 7.4.

The crystal structure presented is based on data that does not meet the standards set forth by the crystallographic community (as judged with the online checkCIF as a guide). However, a rough model of the data does provide identification evidence of the Yb_3 dimer. This rough model (using orthorhombic space group C*222*) has the following unit cell parameters based on single crystal X-ray diffraction data collected at T = 100 K:

a = 19.329 (5) Å, b = 46.225 (12) Å, c = 19.127 (5) Å, V = 17090 (8) $Å^3$

6. 2D COSY NMR of Yb_3 + L or D lactate

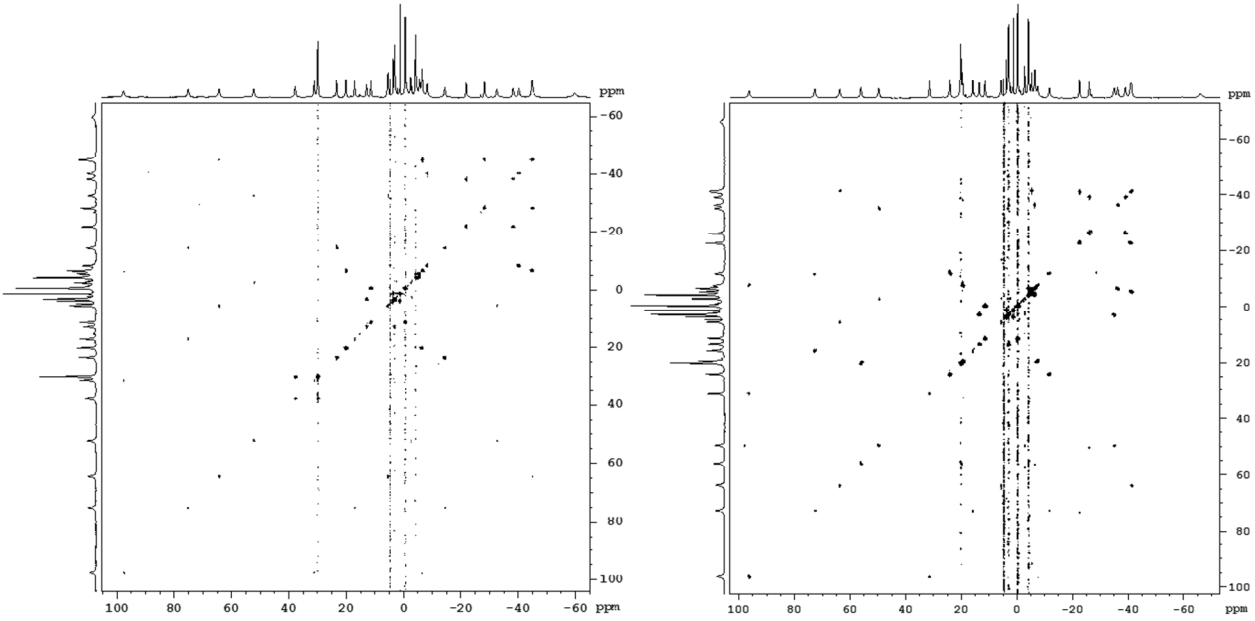
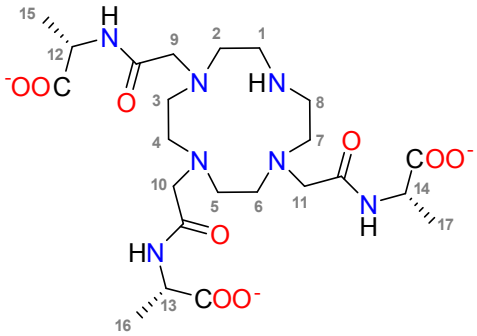


Figure S4. 2D COSY NMR of Yb_3 with L-lactate (left) or D-lactate (right). The samples contained equimolar Yb_3:lactate concentrations in D_2O.

7. DFT computational details

Table S2. Comparison of the experimental and calculated (using Eq 1) ^{1}H NMR shifts (ppm) of L-lactate•Yb_3 and D-lactate•Yb_3 and axial and rhombic contributions to the observed pseudocontact shifts.[a]



	L-lactate•Yb_3				D-lactate•Yb_3			
	Experimental	Calculated	δ_i^{pse}(axial)	δ_i^{pse}(rhomb)	Experimental	Calculated	δ_i^{pse}(axial)	δ_i^{pse}(rhomb)
H_{1ax}	75.17	75.21	-13.98	-58.13	72.72	72.07	-17.45	-51.52
H_{1eq}	17.07	20.53	-2.21	-15.22	18.85	19.08	2.92	-18.90

H_{2ax}	-14.45	-14.45	-23.00	40.56	-11.78	-10.90	30.00	-15.99
H_{2eq}	23.39	24.89	-13.06	-8.73	24.14	26.16	-1.36	-21.70
H_{3ax}	91.71	88.27	-19.56	-71.80	96.35	92.41	-25.30	-64.00
H_{3eq}	31.19	32.42	-4.12	-25.20	31.43	33.25	-14.78	-15.37
H_{4ax}	-6.48	-6.94	27.73	-17.69	-7.51	-6.95	-12.69	22.74
H_{4eq}	20.14	20.72	3.70	-21.32	19.55	19.92	-3.84	-12.98
H_{5ax}	64.37	62.26	-20.18	-38.98	63.72	59.10	-6.63	-49.37
H_{5eq}	5.39	7.54	-6.91	-2.47	5.69	6.31	12.02	-15.23
H_{6ax}	-44.94	-41.50	-21.02	65.62	-40.90	-39.0	34.47	7.67
H_{6eq}	-6.48	-3.90	-11.96	18.96	-6.55	-3.66	5.89	0.88
H_{7ax}	52.27	49.47	-11.61	-34.77	49.68	45.49	-21.23	-21.16
H_{7eq}	-2.46	-0.48	1.63	1.95	-2.80	-1.03	-12.34	16.47
H_{8ax}	-32.52	-31.89	38.41	-3.42	-35.01	-33.38	-18.38	54.87
H_{8eq}	5.39	8.46	11.18	-16.54	3.04	5.91	-9.93	7.12
H_{9ax}	-40.26	-45.71	-16.84	65.65	-36.23	-40.06	7.32	35.84
H_{9eq}	-8.23	-6.87	0.12	28.46	-5.53	-3.76	-10.08	16.93
H_{10ax}	-38.28	-42.26	38.41	-3.42	-41.24	-45.05	18.74	29.40
H_{10eq}	-21.86	-19.93	7.59	15.44	-26.04	-21.19	22.93	1.37
H_{11ax}	-44.94	-48.20	-21.02	65.62	-39.08	-41.28	8.78	35.60
H_{11eq}	-28.26	-25.48	0.12	28.46	-22.51	-22.73	-6.91	32.74
H_{12}	-5.60	-4.32	8.29	0.21	-6.55	-4.42	-10.24	18.83
H_{13}	11.39	10.90	-3.82	4.56	11.48	10.90	6.24	-12.96
H_{14}	12.91	11.93	4.56	-12.31	13.52	13.05	-9.63	0.75
H_{15}	-4.21	*c*	*c*	*c*	-4.15	*c*	*c*	*C*
H_{16}	-0.57	*c*	*c*	*c*	-0.30	*c*	*c*	*C*
H_{17}	3.12	*c*	*c*	*c*	3.04	*c*	*c*	*C*
$CH_{lact.}$	37.84	33.73	-14.32	-15.32	56.09	57.80	-8.42	-45.28
$CH_{3lact.}$	29.94	28.80	-7.55	-19.94	20.20	22.54	-5.45	-15.79
NH	-59.68	-62.15	51.46	14.73	-65.91	-68.19	49.58	22.66
$[\chi_{zz} - 1/3(\chi_{xx} + \chi_{yy} + \chi_{zz})]^b$		1130 ± 48				1279 ± 57		
$(\chi_{xx} - \chi_{yy})^b$		-3825 ± 86				-3501 ± 90		

[a] The diamagnetic shifts were estimated to be 4.10 and 1.31 ppm for lactate CH and methyl protons, respectively, 1.32 ppm for the methyl protons of the ligand, 4.18 ppm for protons H12, H13 and H14, 4.04 ppm for amine NH protons and 3.1 ppm for the remaining protons. [b] In ppm×Å^3. [c] Not included in the analysis.

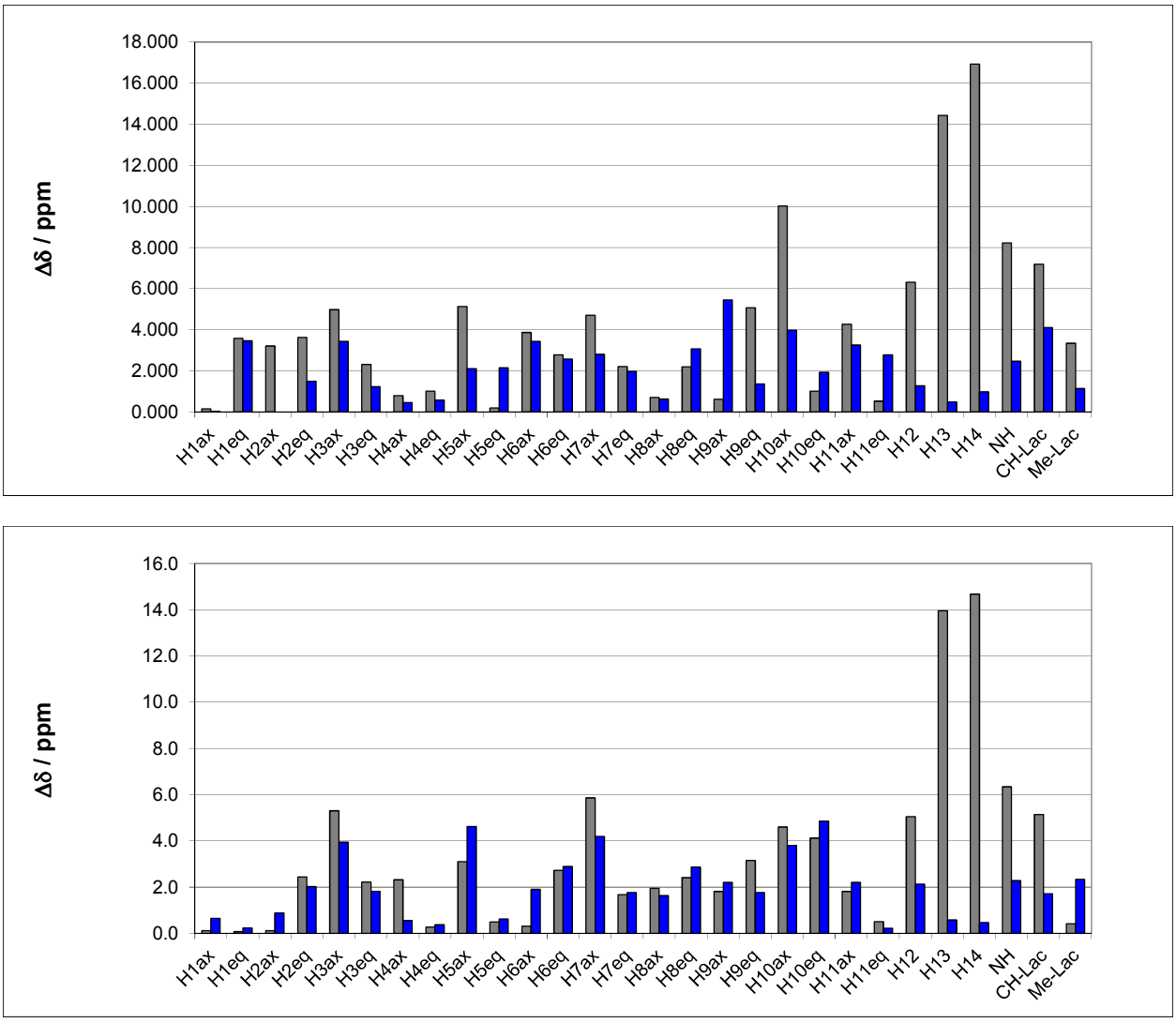


Figure S5. Absolute differences (ppm) between the experimental and calculated pseudocontact shifts obtained for the *S*-Λ(δδδδ) (blue bars) and *S*-Δ(λλλλ) (grey bars) isomers of L-lactate•Yb_3 (top) and D-lactate•Yb_3 (bottom).

Computational Details

Geometry optimizations were performed using the hybrid meta-GGA approximation to DFT with the TPSSh exchange-correlation functional,[3] and the Gaussian 09 package (Revision E.01).[4] The large-core relativistic effective core potential (LCRECP) of Dolg *et al.* and the related [5s4p3d]-GTO valence basis set were used for Yb,[5] together with the standard 6-311G(d,p) basis set for all remaining atoms atoms. The LCRECP approach includes 46+$4f^{13}$ electrons of Yb(III) in the core, and thus calculations were conducted on a pseudo-singlet state configuration. No symmetry constraints have been imposed during the optimizations. The default values for the integration grid (75 radial shells and 302 angular points) and the SCF energy convergence criteria (10^{-8}) were used in all calculations. The stationary points found on the potential energy

surfaces were confirmed to represent local energy minima using frequency analysis (0 imaginary frequencies). Solvent effects (water) were included by using the integral equation formalism variant of the polarizable continuum model (IEFPCM).[6]

Optimized Cartesian Coordinates obtained with DFT calculations

Λ(δδδδ), D-lactate•Yb_0, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.026748	-0.594166	-0.214257
2	8	2.262815	-0.604988	0.517192
3	8	0.207793	1.713855	0.107810
4	8	-2.196819	-0.149619	0.455128
5	8	0.071194	-0.120452	2.160109
6	8	-0.165845	-2.435877	1.097975
7	8	-0.021928	-3.547786	3.045537
8	7	1.787911	0.290984	-2.036917
9	7	-1.164454	0.801528	-2.118331
10	7	-1.733187	-2.060582	-1.452353
11	7	1.137038	-2.506722	-1.481515
12	7	4.449217	-0.026045	0.410251
13	1	5.229696	0.453354	-0.052058
14	7	-0.361853	3.864017	-0.320979
15	1	-0.904481	4.563394	-0.842087
16	7	-4.376376	-0.732678	0.663527
17	1	-5.158411	-1.365760	0.463423
18	6	1.173338	1.355503	-2.876443
19	1	1.193341	2.287568	-2.310168
20	1	1.763894	1.525623	-3.786081
21	6	-0.253697	1.010198	-3.280434
22	1	-0.262482	0.094703	-3.873954
23	1	-0.644118	1.809653	-3.924280
24	6	-2.393004	0.092964	-2.583668
25	1	-3.193310	0.301573	-1.874129
26	1	-2.720050	0.486066	-3.554829
27	6	-2.173457	-1.410268	-2.717346
28	1	-1.410790	-1.606708	-3.471487
29	1	-3.102377	-1.872562	-3.077315
30	6	-1.142427	-3.400679	-1.741691
31	1	-1.056341	-3.917302	-0.784529
32	1	-1.802611	-3.984724	-2.395508
33	6	0.239958	-3.288323	-2.364368
34	1	0.202067	-2.793525	-3.337565
35	1	0.635154	-4.296121	-2.537534
36	6	2.408568	-2.142856	-2.148840
37	1	3.185076	-2.066288	-1.388234
38	1	2.725012	-2.921022	-2.853431
39	6	2.245318	-0.830571	-2.908080

40	1	1.500175	-0.962522	-3.694782
41	1	3.188904	-0.563517	-3.401877
42	6	2.926527	0.848290	-1.273812
43	1	3.820916	0.965628	-1.897617
44	1	2.636757	1.834775	-0.903359
45	6	3.212230	0.002654	-0.045725
46	6	4.912721	-0.700553	1.616222
47	1	4.391730	-0.317660	2.498179
48	6	-1.534328	2.099492	-1.508243
49	1	-1.736167	2.865093	-2.266807
50	1	-2.444307	1.948318	-0.923388
51	6	-0.480563	2.567259	-0.519183
52	6	0.504932	4.526090	0.646200
53	1	0.265297	4.204640	1.663423
54	6	-2.871478	-2.232585	-0.521456
55	1	-3.767600	-2.600709	-1.035462
56	1	-2.574397	-2.968865	0.229659
57	6	-3.147397	-0.945703	0.233144
58	6	-4.827390	0.384828	1.483174
59	1	-4.294471	0.403669	2.438052
60	6	0.023337	-2.515630	2.376024
61	6	0.371132	-1.193158	3.085434
62	1	0.537368	0.686961	2.416083
63	1	1.344106	-3.080703	-0.664640
64	6	-6.355170	0.208239	1.732693
65	8	-6.891021	1.103817	2.419080
66	8	-6.879072	-0.817379	1.215415
67	6	0.281381	6.062347	0.505524
68	8	-0.560879	6.412819	-0.367455
69	8	0.962275	6.774333	1.272476
70	6	6.443373	-0.441888	1.749677
71	8	6.959472	0.265980	0.840581
72	8	6.988874	-0.965406	2.743895
73	6	-0.378018	-1.007032	4.397807
74	1	-0.061842	-0.087429	4.897236
75	1	-1.455527	-0.960284	4.219445
76	1	-0.166728	-1.853929	5.052877
77	1	1.452840	-1.205819	3.259783
78	1	-4.643259	1.336042	0.976440
79	1	1.554045	4.285972	0.453725
80	1	4.722302	-1.775545	1.553441

E(RTPSSh) =-2225.2975105 Hartree
Zero-point correction = 0.641500
Thermal correction to Energy = 0.685764
Thermal correction to Enthalpy = 0.686708
Thermal correction to Gibbs Free Energy = 0.560812
Sum of electronic and zero-point Energies = -2224.656010
Sum of electronic and thermal Energies = -2224.611746
Sum of electronic and thermal Enthalpies = -2224.610802
Sum of electronic and thermal Free Energies = -2224.736698

Δ(λλλλ), D-lactate•Yb_0, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.050999	-0.597326	-0.207319
2	8	2.282463	-0.653283	0.521259
3	8	0.220783	1.710183	0.138279
4	8	-2.175459	-0.142724	0.461553
5	8	0.036357	-0.128578	2.169487
6	8	-0.208507	-2.439047	1.093406
7	8	-0.634740	-3.500527	3.027679
8	7	1.826191	0.284261	-2.013301
9	7	-1.120517	0.824269	-2.117329
10	7	-1.724074	-2.033266	-1.477260
11	7	1.141929	-2.515505	-1.478884
12	7	4.472928	-0.085355	0.441400
13	1	5.260338	0.392697	-0.010171
14	7	-0.300622	3.869484	-0.306269
15	1	-0.819728	4.577450	-0.839760
16	7	-4.371392	-0.677997	0.617695
17	1	-5.164599	-1.289153	0.393519
18	6	1.229565	1.361981	-2.848578
19	1	1.252691	2.288303	-2.273014
20	1	1.830335	1.535129	-3.750921
21	6	-0.196458	1.033502	-3.268977
22	1	-0.207380	0.122775	-3.869648
23	1	-0.573294	1.841429	-3.910283
24	6	-2.349725	0.130000	-2.600816
25	1	-3.155032	0.337355	-1.896140
26	1	-2.665398	0.535106	-3.570748
27	6	-2.138442	-1.372734	-2.745265
28	1	-1.364776	-1.568035	-3.488417
29	1	-3.064302	-1.826098	-3.124017
30	6	-1.147372	-3.380058	-1.762953
31	1	-1.077525	-3.899487	-0.805989
32	1	-1.807745	-3.954496	-2.425138
33	6	0.242003	-3.282738	-2.371916
34	1	0.218581	-2.783176	-3.343071
35	1	0.626482	-4.294407	-2.545984
36	6	2.419083	-2.158378	-2.140851
37	1	3.195312	-2.098619	-1.378718
38	1	2.727132	-2.933449	-2.852482
39	6	2.273588	-0.837524	-2.889698
40	1	1.530284	-0.955057	-3.680405
41	1	3.222315	-0.578529	-3.377887
42	6	2.967455	0.822871	-1.240911
43	1	3.864948	0.938930	-1.860552
44	1	2.685730	1.807941	-0.860366
45	6	3.239317	-0.042063	-0.023160
46	6	4.923847	-0.783219	1.638849

47	1	4.409403	-0.402245	2.525527
48	6	-1.486962	2.122243	-1.505544
49	1	-1.674186	2.892800	-2.262826
50	1	-2.404862	1.976582	-0.931627
51	6	-0.440848	2.574805	-0.502619
52	6	0.565046	4.518493	0.670780
53	1	0.301041	4.210167	1.686022
54	6	-2.880390	-2.192348	-0.566731
55	1	-3.776922	-2.529548	-1.100813
56	1	-2.616752	-2.950343	0.175081
57	6	-3.140477	-0.912593	0.205988
58	6	-4.810748	0.434646	1.450326
59	1	-4.291891	0.425186	2.413057
60	6	-0.433146	-2.481108	2.367607
61	6	-0.484195	-1.119395	3.086775
62	1	-0.266874	0.755456	2.416666
63	1	1.344073	-3.099542	-0.667764
64	6	0.292292	-1.110336	4.396670
65	1	0.181181	-0.148796	4.904770
66	1	1.354187	-1.291891	4.211636
67	1	-0.091668	-1.898885	5.046087
68	1	-1.542385	-0.900256	3.269870
69	6	-6.345536	0.286521	1.673870
70	8	-6.871753	1.179242	2.371166
71	8	-6.883486	-0.716224	1.127108
72	6	0.379585	6.058358	0.515326
73	8	-0.438674	6.421583	-0.375140
74	8	1.063001	6.760144	1.289305
75	6	6.458584	-0.552379	1.776476
76	8	6.986251	0.163576	0.880347
77	8	6.995864	-1.102321	2.760938
78	1	1.611262	4.252372	0.497835
79	1	-4.598651	1.390215	0.963108
80	1	4.714484	-1.853744	1.562544

E(RTPSSh) = -2225.2975108 Hartree
Zero-point correction = 0.641595
Thermal correction to Energy = 0.685796
Thermal correction to Enthalpy = 0.686740
Thermal correction to Gibbs Free Energy = 0.561253
Sum of electronic and zero-point Energies = -2224.655916
Sum of electronic and thermal Energies = -2224.611715
Sum of electronic and thermal Enthalpies = -2224.610771
Sum of electronic and thermal Free Energies = -2224.736258

Λ(δδδδ), D-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	70	0.055355	-0.702379	-0.304536
2	8	2.275003	-0.573219	0.469889
3	8	0.185582	1.631037	-0.252441
4	8	-2.193837	-0.216434	0.265284
5	8	0.032126	0.052046	1.999677
6	8	-0.127134	-2.376974	1.220031
7	8	0.043388	-3.249705	3.283752
8	7	1.840499	-0.009982	-2.177852
9	7	-1.117796	0.434024	-2.380832
10	7	-1.647279	-2.342596	-1.371882
11	7	1.229894	-2.728306	-1.293333
12	7	4.447322	0.071528	0.354470
13	1	5.195680	0.602082	-0.108370
14	7	-0.530837	3.703669	-0.838484
15	1	-1.189730	4.305649	-1.351023
16	7	-4.339897	-0.880968	0.615018
17	1	-5.050900	-1.623399	0.595498
18	6	1.224553	0.933425	-3.152015
19	1	1.211808	1.925663	-2.698659
20	1	1.833854	1.008565	-4.062147
21	6	-0.185556	0.511614	-3.541513
22	1	-0.164908	-0.470699	-4.016299
23	1	-0.574774	1.217048	-4.287729
24	6	-2.323845	-0.354821	-2.772450
25	1	-3.138525	-0.079151	-2.103863
26	1	-2.642300	-0.092075	-3.789273
27	6	-2.074334	-1.858161	-2.715770
28	1	-1.295531	-2.129577	-3.429265
29	1	-2.987845	-2.379629	-3.030690
30	6	-1.026569	-3.695956	-1.487213
31	1	-0.953325	-4.093467	-0.473829
32	1	-1.661794	-4.366594	-2.079732
33	6	0.367950	-3.632199	-2.090146
34	1	0.343347	-3.262799	-3.117848
35	1	0.785675	-4.645010	-2.128267
36	6	2.508675	-2.424106	-1.977065
37	1	3.267567	-2.235884	-1.218227
38	1	2.854023	-3.277420	-2.572799
39	6	2.331861	-1.221116	-2.896918
40	1	1.598393	-1.466528	-3.667200
41	1	3.276148	-0.997733	-3.410318
42	6	2.953173	0.659675	-1.471989
43	1	3.859137	0.710667	-2.088151
44	1	2.639931	1.680995	-1.241464
45	6	3.224708	-0.009228	-0.135753
46	6	4.883778	-0.337822	1.691976
47	1	4.166055	0.038669	2.427371
48	6	-1.523566	1.789732	-1.947167
49	1	-1.681661	2.459701	-2.800631
50	1	-2.467914	1.699645	-1.405922
51	6	-0.538439	2.390327	-0.955396
52	6	0.143838	4.495655	0.194157

53	1	-0.028424	4.024971	1.167020
54	6	-2.799526	-2.425695	-0.447162
55	1	-3.681422	-2.861702	-0.931650
56	1	-2.507071	-3.070871	0.385331
57	6	-3.112224	-1.072491	0.166417
58	6	-4.814458	0.226078	1.449914
59	1	-4.094236	0.391369	2.257572
60	6	0.051879	-2.300583	2.499344
61	6	0.332206	-0.891989	3.055055
62	1	0.467442	0.898487	2.169060
63	1	1.427611	-3.191084	-0.406447
64	6	-5.006020	1.527233	0.666191
65	6	1.649783	4.628694	-0.047597
66	6	5.002236	-1.858939	1.828939
67	1	-5.460358	2.264645	1.330092
68	1	-4.052776	1.917685	0.303231
69	1	-5.671956	1.365650	-0.186711
70	6	-6.163807	-0.253444	2.084304
71	8	-6.698614	0.549546	2.878609
72	8	-6.573746	-1.391806	1.719930
73	1	1.842724	5.044558	-1.040917
74	1	2.059887	5.308371	0.701377
75	1	2.153360	3.662999	0.036460
76	6	-0.555981	5.897033	0.190578
77	8	-1.442292	6.069001	-0.693632
78	8	-0.152742	6.700710	1.057697
79	1	4.031661	-2.344841	1.705139
80	1	5.695039	-2.255353	1.080507
81	1	5.393282	-2.088030	2.821790
82	6	6.261611	0.361821	1.937852
83	8	6.730574	1.016997	0.964410
84	8	6.758721	0.185801	3.071092
85	6	-0.470096	-0.579344	4.311083
86	1	-0.200234	0.403005	4.707518
87	1	-1.541218	-0.590329	4.092880
88	1	-0.257503	-1.335747	5.068542
89	1	1.406374	-0.845939	3.265525

E(RTPSSh) = -2343.2838577
Zero-point correction = 0.724926
Thermal correction to Energy = 0.773606
Thermal correction to Enthalpy = 0.774551
Thermal correction to Gibbs Free Energy = 0.639431
Sum of electronic and zero-point Energies = -2342.558932
Sum of electronic and thermal Energies = -2342.510251
Sum of electronic and thermal Enthalpies = -2342.509307
Sum of electronic and thermal Free Energies = -2342.644426

Δ(λλλλ), D-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	-0.049411	-0.688915	-0.290027
2	8	-2.270819	-0.574785	0.416363
3	8	-0.134771	1.634469	-0.036456
4	8	2.156760	-0.313408	0.521659
5	8	-0.015788	-0.211218	2.144791
6	8	0.044012	-2.567200	1.002175
7	8	-0.259765	-3.707383	2.916062
8	7	-1.711005	0.212210	-2.169238
9	7	1.273438	0.623210	-2.172158
10	7	1.705117	-2.227795	-1.425167
11	7	-1.178707	-2.582777	-1.547832
12	7	-4.425514	0.119925	0.244927
13	1	-5.184902	0.527937	-0.314113
14	7	0.535533	3.758084	-0.470111
15	1	1.056601	4.426752	-1.051157
16	7	4.337614	-0.933096	0.701919
17	1	5.116154	-1.532002	0.395426
18	6	-1.025355	1.228324	-3.017182
19	1	-1.027842	2.177134	-2.479252
20	1	-1.579320	1.393264	-3.950210
21	6	0.399917	0.817863	-3.365899
22	1	0.392394	-0.120575	-3.922901
23	1	0.835348	1.577440	-4.028707
24	6	2.494004	-0.133604	-2.577283
25	1	3.273483	0.065375	-1.841563
26	1	2.871286	0.227880	-3.542471
27	6	2.230198	-1.630420	-2.684780
28	1	1.498470	-1.821478	-3.470337
29	1	3.158093	-2.135023	-2.984293
30	6	1.077744	-3.552341	-1.716783
31	1	0.937984	-4.050451	-0.756829
32	1	1.740871	-4.166385	-2.338970
33	6	-0.277608	-3.401629	-2.391599
34	1	-0.189692	-2.920519	-3.368402
35	1	-0.698698	-4.398469	-2.567422
36	6	-2.424600	-2.193644	-2.246392
37	1	-3.209093	-2.069824	-1.499730
38	1	-2.757768	-2.976746	-2.937616
39	6	-2.198192	-0.905844	-3.029299
40	1	-1.443835	-1.082746	-3.798276
41	1	-3.120395	-0.609906	-3.545760
42	6	-2.838312	0.838492	-1.444232
43	1	-3.717437	0.969035	-2.086638
44	1	-2.515965	1.825498	-1.103805
45	6	-3.181587	0.056342	-0.187380
46	6	-4.977966	-0.516077	1.442747
47	1	-4.635847	-1.554555	1.480315
48	6	-4.564578	0.208530	2.727696

49	1	-3.481245	0.183366	2.866035
50	1	-5.046142	-0.282488	3.575108
51	1	-4.890376	1.252549	2.696639
52	6	1.668034	1.929249	-1.596967
53	1	1.907362	2.663460	-2.375511
54	1	2.563224	1.774869	-0.990260
55	6	0.604742	2.453572	-0.647726
56	6	-0.387399	4.480611	0.408795
57	1	-1.400381	4.100083	0.246177
58	6	-0.019543	4.336099	1.888819
59	1	-0.091608	3.296267	2.215757
60	1	-0.707370	4.944996	2.477961
61	1	1.000159	4.692328	2.063325
62	6	2.793469	-2.419833	-0.439597
63	1	3.692883	-2.842036	-0.903441
64	1	2.429038	-3.118485	0.318161
65	6	3.099873	-1.127665	0.295468
66	6	4.874073	0.234348	1.406671
67	1	4.480968	1.141133	0.938115
68	6	4.525901	0.236469	2.897878
69	1	3.449654	0.332144	3.057621
70	1	5.029146	1.082599	3.368809
71	1	4.872619	-0.686054	3.372467
72	6	-0.181297	-2.659576	2.273832
73	6	-0.413554	-1.316214	2.996426
74	1	0.939401	-0.069894	2.250938
75	1	-1.415427	-3.135227	-0.724224
76	6	6.424575	0.193970	1.189503
77	8	7.056429	1.168779	1.648277
78	8	6.869636	-0.824731	0.588346
79	6	-0.340823	5.977108	-0.046965
80	8	-1.132039	6.743428	0.543238
81	8	0.498525	6.253081	-0.950646
82	6	-6.532601	-0.506221	1.266222
83	8	-7.179155	-1.085117	2.165362
84	8	-6.968320	0.099577	0.246215
85	6	0.253545	-1.240364	4.361276
86	1	1.342225	-1.311407	4.268514
87	1	-0.000482	-0.304019	4.863156
88	1	-0.088397	-2.078044	4.970417
89	1	-1.495330	-1.201260	3.099897

E(RTPSSh) =-2343.2848806 Hartree
Zero-point correction = 0.726201
Thermal correction to Energy = 0.774341
Thermal correction to Enthalpy = 0.775285
Thermal correction to Gibbs Free Energy = 0.643051
Sum of electronic and zero-point Energies = -2342.558680
Sum of electronic and thermal Energies = -2342.510540
Sum of electronic and thermal Enthalpies = -2342.509596
Sum of electronic and thermal Free Energies = -2342.641830

Λ(λλλλ), D-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.078435	-0.866349	-0.208714
2	8	-2.073134	0.007343	0.200994
3	8	0.443509	1.379594	-0.805081
4	8	2.251759	-0.506780	0.687448
5	8	0.167015	0.521522	1.894546
6	8	-0.388156	-2.022747	1.691742
7	8	-1.015876	-2.253244	3.836669
8	7	-1.933101	-2.294811	-1.142992
9	7	-0.526385	-0.208702	-2.701509
10	7	2.116441	-1.287811	-1.871561
11	7	0.702670	-3.330552	-0.414393
12	7	-4.232153	-0.340575	0.813386
13	1	-5.023684	-0.978242	0.970968
14	7	-0.409775	3.273792	-1.719306
15	1	-1.085997	3.737779	-2.339281
16	7	4.393462	0.218552	0.483062
17	1	5.178867	0.538934	-0.099875
18	6	-2.511095	-1.687688	-2.377203
19	1	-3.151772	-0.857080	-2.074724
20	1	-3.155269	-2.410875	-2.892400
21	6	-1.443472	-1.189676	-3.338519
22	1	-0.836791	-2.024365	-3.693704
23	1	-1.928554	-0.751428	-4.220562
24	6	0.709327	-0.059579	-3.525771
25	1	1.166317	0.898921	-3.273429
26	1	0.449830	-0.016574	-4.591162
27	6	1.704503	-1.185438	-3.295296
28	1	1.261477	-2.141154	-3.579146
29	1	2.577528	-1.034019	-3.943306
30	6	2.720317	-2.627936	-1.611436
31	1	3.282175	-2.562660	-0.676383
32	1	3.431956	-2.886786	-2.405576
33	6	1.660034	-3.708276	-1.475061
34	1	1.110289	-3.837927	-2.409480
35	1	2.145343	-4.666260	-1.255678
36	6	-0.507706	-4.190399	-0.381886
37	1	-0.907198	-4.130019	0.630400
38	1	-0.256942	-5.236962	-0.590930
39	6	-1.536281	-3.706787	-1.395494
40	1	-1.118365	-3.753185	-2.403505
41	1	-2.415285	-4.363657	-1.382964
42	6	-2.943384	-2.211881	-0.067146
43	1	-2.579548	-2.765557	0.801881
44	1	-3.908379	-2.631439	-0.377031
45	6	-3.075770	-0.751143	0.335330
46	6	-4.540798	0.973537	1.384786

47	1	-3.764399	1.236155	2.109727
48	6	-4.636826	2.073863	0.322933
49	1	-3.673272	2.247045	-0.161134
50	1	-4.960051	2.994642	0.811682
51	1	-5.374483	1.805071	-0.439092
52	6	-1.159551	1.120399	-2.575471
53	1	-2.146340	1.011243	-2.120462
54	1	-1.280927	1.611401	-3.548929
55	6	-0.309969	1.963287	-1.633640
56	6	0.191361	4.259667	-0.816407
57	1	0.029455	3.934857	0.215711
58	6	1.691903	4.441266	-1.064164
59	1	2.242410	3.521557	-0.853379
60	1	2.056714	5.234983	-0.409987
61	1	1.874469	4.733386	-2.102711
62	6	3.112202	-0.250331	-1.534666
63	1	2.742983	0.722883	-1.867368
64	1	4.079865	-0.437367	-2.015902
65	6	3.249553	-0.185070	-0.023449
66	6	4.697721	0.468314	1.895199
67	1	3.906979	1.092397	2.322804
68	6	4.823149	-0.826820	2.703474
69	1	3.877447	-1.372612	2.728858
70	1	5.116710	-0.569785	3.722516
71	1	5.593018	-1.472270	2.270239
72	6	-0.637351	-1.574264	2.882160
73	6	-0.468965	-0.051750	3.058346
74	1	1.131883	0.449096	2.002607
75	1	1.162328	-3.436487	0.489794
76	6	6.035057	1.281933	1.913063
77	8	6.428140	1.644214	3.042081
78	8	6.578528	1.472676	0.788192
79	6	-0.590433	5.595703	-1.045613
80	8	-0.248584	6.550294	-0.315240
81	8	-1.473099	5.571276	-1.949932
82	6	-5.896099	0.805169	2.150537
83	8	-6.289638	1.813711	2.774171
84	8	-6.452686	-0.324670	2.046180
85	6	0.263611	0.320760	4.340200
86	1	1.290109	-0.060501	4.325445
87	1	0.289980	1.405406	4.466452
88	1	-0.253144	-0.126755	5.190293
89	1	-1.474737	0.376750	3.068856

E(RTPSSh) = -2343.2824274 Hartree
Zero-point correction = 0.725412
Thermal correction to Energy = 0.773786
Thermal correction to Enthalpy = 0.774731
Thermal correction to Gibbs Free Energy = 0.640668
Sum of electronic and zero-point Energies = -2342.557015
Sum of electronic and thermal Energies = -2342.508641
Sum of electronic and thermal Enthalpies = -2342.507697

Sum of electronic and thermal Free Energies = -2342.641759

Δ(δδδδ), D-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	-0.073687	-0.849155	-0.204323
2	8	2.078310	-0.054557	0.370470
3	8	-0.346756	1.435438	-0.677568
4	8	-2.291431	-0.437740	0.577764
5	8	-0.266004	0.401048	1.991998
6	8	0.228017	-2.137451	1.642106
7	8	0.685749	-2.546721	3.803370
8	7	1.942384	-2.277835	-1.103613
9	7	0.689718	-0.061394	-2.608239
10	7	-2.021003	-1.108222	-2.009760
11	7	-0.749786	-3.274485	-0.599989
12	7	4.226426	-0.485580	0.979201
13	1	5.047427	-1.104456	0.943460
14	7	0.568757	3.361095	-1.453830
15	1	1.131304	3.861162	-2.153414
16	7	-4.405359	0.339050	0.274244
17	1	-5.213260	0.484459	-0.344898
18	6	2.613008	-1.615580	-2.260792
19	1	3.256737	-0.823888	-1.872104
20	1	3.266787	-2.326798	-2.780179
21	6	1.617638	-1.030217	-3.249282
22	1	1.012515	-1.826431	-3.685293
23	1	2.163995	-0.556116	-4.074934
24	6	-0.485959	0.172947	-3.498376
25	1	-0.932142	1.128978	-3.217906
26	1	-0.157170	0.270531	-4.540844
27	6	-1.523409	-0.933018	-3.398359
28	1	-1.095762	-1.883098	-3.721496
29	1	-2.352994	-0.712191	-4.082658
30	6	-2.672913	-2.443396	-1.867213
31	1	-3.286350	-2.418302	-0.962881
32	1	-3.343443	-2.633196	-2.714865
33	6	-1.648571	-3.558511	-1.738138
34	1	-1.043615	-3.642885	-2.642842
35	1	-2.167962	-4.515283	-1.610758
36	6	0.430123	-4.174626	-0.548369
37	1	0.766865	-4.191552	0.488003
38	1	0.162174	-5.197167	-0.839092
39	6	1.531809	-3.661715	-1.465330
40	1	1.177548	-3.639121	-2.498470
41	1	2.393768	-4.340197	-1.436674
42	6	2.884093	-2.287245	0.038255

43	1	2.437842	-2.853664	0.858690
44	1	3.845779	-2.742195	-0.228333
45	6	3.056610	-0.846426	0.492772
46	6	4.653462	0.864023	1.359093
47	1	4.324919	1.563591	0.584376
48	6	1.347796	1.240279	-2.366466
49	1	2.298057	1.077895	-1.854380
50	1	1.545536	1.779954	-3.300939
51	6	0.456022	2.049544	-1.435098
52	6	-0.198177	4.319061	-0.653179
53	1	-1.258897	4.057246	-0.715221
54	6	-3.011032	-0.064348	-1.677403
55	1	-2.601180	0.914926	-1.937476
56	1	-3.951244	-0.200227	-2.226113
57	6	-3.238978	-0.067285	-0.176922
58	6	-4.839181	0.402431	1.672067
59	1	-4.462661	-0.478951	2.197773
60	6	0.392370	-1.788191	2.879228
61	6	0.234474	-0.281831	3.162616
62	1	-1.238793	0.357460	2.002329
63	1	-1.267737	-3.421485	0.266254
64	6	-4.349405	1.675625	2.371234
65	6	0.237607	4.336451	0.815611
66	6	4.099116	1.311154	2.713963
67	1	-4.743653	1.688715	3.388718
68	1	-3.258347	1.721305	2.414111
69	1	-4.713415	2.561913	1.843421
70	6	-6.403366	0.355177	1.645390
71	8	-6.957417	0.270453	2.761663
72	8	-6.935461	0.431930	0.501878
73	1	1.303195	4.573427	0.892895
74	1	-0.329399	5.111126	1.335090
75	1	0.054096	3.372163	1.294795
76	6	0.008868	5.715791	-1.326305
77	8	0.815048	5.747376	-2.299233
78	8	-0.637949	6.657285	-0.819264
79	1	3.011945	1.411234	2.684025
80	1	4.369034	0.593808	3.494566
81	1	4.538387	2.279115	2.961573
82	6	6.219364	0.833476	1.368363
83	8	6.750963	-0.291760	1.147604
84	8	6.776597	1.926270	1.604929
85	6	-0.618933	0.003491	4.391369
86	1	-0.636252	1.074161	4.607408
87	1	-1.646117	-0.345343	4.241509
88	1	-0.200691	-0.528159	5.247189
89	1	1.241373	0.115065	3.313980

E(RTPSSh) = -2343.2813551 Hartree
Zero-point correction = 0.725710
Thermal correction to Energy = 0.773966
Thermal correction to Enthalpy = 0.774910

```
Thermal correction to Gibbs Free Energy = 0.641985
Sum of electronic and zero-point Energies = -2342.555645
Sum of electronic and thermal Energies = -2342.507389
Sum of electronic and thermal Enthalpies = -2342.506445
Sum of electronic and thermal Free Energies = -2342.639370
```

Λ(δδδδ), L-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.079345	-0.701331	-0.295414
2	8	2.302191	-0.600605	0.462209
3	8	0.171877	1.633967	-0.218715
4	8	-2.172762	-0.221232	0.293305
5	8	0.021078	0.039370	2.010417
6	8	-0.131706	-2.385198	1.214080
7	8	-0.453743	-3.237036	3.268281
8	7	1.857922	0.003803	-2.166999
9	7	-1.100012	0.448486	-2.373901
10	7	-1.633264	-2.328749	-1.384103
11	7	1.243953	-2.725084	-1.296483
12	7	4.473698	0.048156	0.353610
13	1	5.219746	0.588351	-0.101321
14	7	-0.520197	3.710721	-0.819026
15	1	-1.166517	4.316891	-1.342710
16	7	-4.334773	-0.860927	0.586504
17	1	-5.055674	-1.592997	0.541535
18	6	1.243834	0.954737	-3.134309
19	1	1.228207	1.942669	-2.671425
20	1	1.855627	1.039269	-4.041967
21	6	-0.164211	0.534171	-3.531144
22	1	-0.141199	-0.444860	-4.012350
23	1	-0.551919	1.243971	-4.273977
24	6	-2.303199	-0.338987	-2.775724
25	1	-3.120442	-0.071590	-2.106441
26	1	-2.620501	-0.067577	-3.790623
27	6	-2.049250	-1.841077	-2.729436
28	1	-1.263052	-2.105215	-3.437409
29	1	-2.958168	-2.363911	-3.055288
30	6	-1.016753	-3.684283	-1.497344
31	1	-0.948373	-4.082088	-0.483799
32	1	-1.652029	-4.352441	-2.092682
33	6	0.379944	-3.625330	-2.095689
34	1	0.360021	-3.255488	-3.123310
35	1	0.793853	-4.639664	-2.133065
36	6	2.520349	-2.416803	-1.984211
37	1	3.283808	-2.239190	-1.227759
38	1	2.859442	-3.265356	-2.590239
39	6	2.345085	-1.204949	-2.893542

40	1	1.610227	-1.442302	-3.665013
41	1	3.289603	-0.980938	-3.406288
42	6	2.972138	0.667118	-1.457571
43	1	3.875025	0.729818	-2.077229
44	1	2.656614	1.684010	-1.210763
45	6	3.249169	-0.023941	-0.134001
46	6	4.913971	-0.386497	1.681829
47	1	4.197045	-0.026283	2.426051
48	6	-1.510786	1.801610	-1.937425
49	1	-1.663221	2.475283	-2.788950
50	1	-2.459637	1.708716	-1.404383
51	6	-0.535353	2.397483	-0.934423
52	6	0.145876	4.500140	0.221200
53	1	-0.048380	4.036195	1.193238
54	6	-2.796102	-2.409693	-0.472371
55	1	-3.677930	-2.826902	-0.973127
56	1	-2.524198	-3.073076	0.352608
57	6	-3.101594	-1.062626	0.159004
58	6	-4.810627	0.238137	1.431263
59	1	-4.101909	0.383088	2.252760
60	6	-0.324473	-2.291617	2.490437
61	6	-0.433781	-0.859921	3.048251
62	1	-0.315260	0.932999	2.160416
63	1	1.447138	-3.193590	-0.413765
64	6	-4.975992	1.553490	0.665377
65	6	1.657112	4.615546	0.005416
66	6	5.035799	-1.909960	1.787722
67	6	0.360443	-0.660133	4.332091
68	1	0.209593	0.348099	4.726577
69	1	1.427149	-0.812310	4.148267
70	1	0.024825	-1.384153	5.076645
71	1	-1.498742	-0.673186	3.227934
72	1	-5.433267	2.284926	1.333844
73	1	-4.013072	1.939941	0.324186
74	1	-5.629862	1.412540	-0.200322
75	6	-6.175006	-0.236923	2.036357
76	8	-6.711933	0.557484	2.837633
77	8	-6.592462	-1.363113	1.643916
78	1	1.872005	5.024143	-0.986423
79	1	2.060507	5.295142	0.758072
80	1	2.148867	3.645173	0.103766
81	6	-0.538439	5.909075	0.198994
82	8	-1.411820	6.084238	-0.697417
83	8	-0.137496	6.714435	1.065548
84	1	4.065980	-2.395242	1.655746
85	1	5.727928	-2.289503	1.029939
86	1	5.429240	-2.158744	2.774857
87	6	6.291370	0.309929	1.938598
88	8	6.758174	0.984055	0.977136
89	8	6.790894	0.112572	3.067345

E(RTPSSh) = -2343.2837707 Hartree

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Zero-point correction = 0.724919
Thermal correction to Energy = 0.773611
Thermal correction to Enthalpy = 0.774556
Thermal correction to Gibbs Free Energy = 0.639201
Sum of electronic and zero-point Energies = -2342.558852
Sum of electronic and thermal Energies = -2342.510159
Sum of electronic and thermal Enthalpies = -2342.509215
Sum of electronic and thermal Free Energies = -2342.644570
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Δ(λλλλ), L-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	-0.044260	-0.677521	-0.272061
2	8	-2.290379	-0.608653	0.412503
3	8	-0.121073	1.636099	0.059421
4	8	2.189012	-0.312747	0.449515
5	8	-0.049413	-0.242031	2.123332
6	8	0.077949	-2.547152	1.007433
7	8	0.306385	-3.674759	2.937452
8	7	-1.738724	0.269890	-2.129463
9	7	1.235006	0.682347	-2.160837
10	7	1.694675	-2.192216	-1.493283
11	7	-1.191050	-2.547557	-1.563793
12	7	-4.456447	0.055651	0.261461
13	1	-5.218711	0.471643	-0.286421
14	7	0.489904	3.773407	-0.400666
15	1	0.984520	4.449546	-0.997281
16	7	4.368732	-0.936182	0.611832
17	1	5.144123	-1.533855	0.299505
18	6	-1.071932	1.311720	-2.957486
19	1	-1.069333	2.244008	-2.390898
20	1	-1.640000	1.503186	-3.877171
21	6	0.349019	0.918298	-3.336932
22	1	0.337957	0.002264	-3.929596
23	1	0.775636	1.703411	-3.975454
24	6	2.446417	-0.064605	-2.609492
25	1	3.242193	0.114977	-1.886815
26	1	2.802589	0.320962	-3.573488
27	6	2.178160	-1.558640	-2.750993
28	1	1.422048	-1.727477	-3.518328
29	1	3.096552	-2.052879	-3.094868
30	6	1.064358	-3.511898	-1.792993
31	1	0.946613	-4.025775	-0.837956
32	1	1.714330	-4.116371	-2.438398
33	6	-0.304684	-3.353990	-2.435525
34	1	-0.237391	-2.858839	-3.406882
35	1	-0.728442	-4.348571	-2.617295
36	6	-2.439791	-2.141736	-2.250051

37	1	-3.224326	-2.038899	-1.501035
38	1	-2.771273	-2.909172	-2.959536
39	6	-2.220511	-0.836309	-3.006946
40	1	-1.467562	-0.995584	-3.781132
41	1	-3.146180	-0.537458	-3.516099
42	6	-2.868280	0.868712	-1.386333
43	1	-3.745835	1.022056	-2.026213
44	1	-2.548251	1.842701	-1.007822
45	6	-3.207847	0.032457	-0.165447
46	6	-5.002974	-0.656514	1.418269
47	1	-4.624398	-1.682921	1.410574
48	6	-4.630239	0.016802	2.743196
49	1	-3.548475	0.019551	2.894421
50	1	-5.105123	-0.530976	3.559169
51	1	-4.990937	1.049727	2.758926
52	6	1.638830	1.968252	-1.547066
53	1	1.876449	2.725134	-2.304014
54	1	2.535793	1.789146	-0.950097
55	6	0.585805	2.470692	-0.573850
56	6	-0.439883	4.486582	0.479046
57	1	-1.446635	4.085602	0.326637
58	6	-0.062066	4.367757	1.958014
59	1	-0.132258	3.334070	2.303726
60	1	-0.748356	4.985026	2.539995
61	1	0.957957	4.727800	2.121395
62	6	2.814705	-2.401048	-0.548172
63	1	3.703867	-2.798431	-1.052488
64	1	2.486812	-3.129005	0.198110
65	6	3.125910	-1.121915	0.208072
66	6	4.899251	0.216364	1.343792
67	1	4.524852	1.133388	0.878998
68	6	4.512112	0.201948	2.825462
69	1	3.431258	0.294871	2.953571
70	1	5.002558	1.041582	3.320920
71	1	4.845922	-0.726706	3.297712
72	6	0.227404	-2.630621	2.290240
73	6	0.356788	-1.290382	3.037579
74	1	0.352626	0.597655	2.382448
75	1	-1.428693	-3.117823	-0.752499
76	6	6.453380	0.170627	1.163116
77	8	7.079785	1.133006	1.656108
78	8	6.908604	-0.837283	0.551685
79	6	-0.425875	5.978800	0.004879
80	8	-1.219809	6.738428	0.599300
81	8	0.392860	6.256840	-0.916863
82	6	-6.554250	-0.692781	1.220555
83	8	-7.189653	-1.346908	2.075392
84	8	-7.000700	-0.045120	0.231480
85	6	-0.457512	-1.242582	4.322991
86	1	-0.291192	-0.299792	4.850790
87	1	-1.523641	-1.343297	4.105126
88	1	-0.152299	-2.067408	4.969230

89	1	1.421852	-1.161720	3.260391

E(RTPSSh) = -2343.284795 Hartree
Zero-point correction = 0.725903
Thermal correction to Energy = 0.774254
Thermal correction to Enthalpy = 0.775198
Thermal correction to Gibbs Free Energy = 0.642092
Sum of electronic and zero-point Energies = -2342.558892
Sum of electronic and thermal Energies = -2342.510541
Sum of electronic and thermal Enthalpies = -2342.509597
Sum of electronic and thermal Free Energies = -2342.642703

Λ(λλλλ), L-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	0.159420	-0.887098	-0.148587
2	8	-2.073195	-0.099249	0.076691
3	8	0.350310	1.330905	-0.908106
4	8	2.317576	-0.401347	0.696805
5	8	0.048716	0.692322	1.735706
6	8	-0.274577	-1.839357	1.856947
7	8	-0.421343	-1.895492	4.097492
8	7	-1.761169	-2.520583	-0.952321
9	7	-0.453441	-0.493203	-2.687325
10	7	2.230717	-1.342949	-1.801725
11	7	0.917352	-3.312548	-0.144421
12	7	-4.167321	-0.522343	0.847837
13	1	-4.893891	-1.193430	1.127073
14	7	-0.708829	3.054373	-1.938324
15	1	-1.434348	3.394264	-2.583196
16	7	4.394399	0.481452	0.438504
17	1	5.139821	0.835494	-0.174097
18	6	-2.348967	-2.067249	-2.246989
19	1	-3.050987	-1.259233	-2.033805
20	1	-2.930629	-2.876496	-2.705672
21	6	-1.294093	-1.590744	-3.235132
22	1	-0.628573	-2.415645	-3.496491
23	1	-1.788009	-1.274171	-4.163135
24	6	0.765768	-0.321314	-3.529450
25	1	1.160588	0.678491	-3.339725
26	1	0.499063	-0.362597	-4.593382
27	6	1.830679	-1.362563	-3.230559
28	1	1.459134	-2.362204	-3.459666
29	1	2.697522	-1.191089	-3.881934
30	6	2.887628	-2.630925	-1.435672
31	1	3.454328	-2.467803	-0.515706
32	1	3.601180	-2.932196	-2.213178

33	6	1.866406	-3.731221	-1.198439
34	1	1.299328	-3.938043	-2.108521
35	1	2.384953	-4.657639	-0.925829
36	6	-0.235871	-4.237029	-0.003741
37	1	-0.636425	-4.089406	0.999235
38	1	0.078974	-5.283055	-0.098491
39	6	-1.292343	-3.928311	-1.055631
40	1	-0.875800	-4.064055	-2.055791
41	1	-2.134068	-4.625938	-0.961568
42	6	-2.784374	-2.386396	0.105832
43	1	-2.395254	-2.822177	1.029275
44	1	-3.720017	-2.893632	-0.160242
45	6	-3.006067	-0.902247	0.352259
46	6	-4.538136	0.822956	1.295414
47	1	-3.743069	1.211438	1.939366
48	6	-4.768640	1.792260	0.131793
49	1	-3.847240	1.973265	-0.426075
50	1	-5.130302	2.737855	0.539335
51	1	-5.525122	1.394480	-0.551487
52	6	-1.186631	0.789767	-2.682696
53	1	-2.180091	0.638143	-2.256727
54	1	-1.303023	1.196978	-3.694696
55	6	-0.452284	1.772625	-1.779573
56	6	-0.263563	4.150663	-1.073908
57	1	-0.397042	3.849313	-0.030378
58	6	1.201739	4.525152	-1.313860
59	1	1.867798	3.696182	-1.063360
60	1	1.447170	5.384147	-0.687104
61	1	1.358648	4.800549	-2.361100
62	6	3.169920	-0.235537	-1.537563
63	1	2.759726	0.689977	-1.949981
64	1	4.151404	-0.409909	-1.995819
65	6	3.285887	-0.053154	-0.033242
66	6	4.655698	0.884421	1.822423
67	1	3.782075	1.420902	2.204558
68	6	4.957321	-0.313110	2.729234
69	1	4.099384	-0.986294	2.793152
70	1	5.197472	0.057732	3.727210
71	1	5.817296	-0.871626	2.347541
72	6	-0.210281	-1.308184	3.037015
73	6	0.214494	0.170576	3.074338
74	1	0.623800	1.458354	1.604714
75	1	1.409857	-3.313764	0.748968
76	6	5.867066	1.873446	1.770540
77	8	6.183538	2.392179	2.862634
78	8	6.404797	2.029538	0.637717
79	6	-1.220668	5.353667	-1.367206
80	8	-1.017055	6.381624	-0.687026
81	8	-2.089653	5.161917	-2.265200
82	6	-5.833077	0.654512	2.159134
83	8	-6.273496	1.703340	2.677064
84	8	-6.301041	-0.517058	2.232698

85	6	-0.571291	0.992940	4.086264
86	1	-0.203512	2.021842	4.116868
87	1	-1.633201	1.004645	3.827586
88	1	-0.457148	0.547777	5.076223
89	1	1.282360	0.181465	3.320681

E(RTPSSh) = -2343.2814821 Hartree
Zero-point correction = 0.725316
Thermal correction to Energy = 0.773884
Thermal correction to Enthalpy = 0.774828
Thermal correction to Gibbs Free Energy = 0.640017
Sum of electronic and zero-point Energies = -2342.556166
Sum of electronic and thermal Energies = -2342.507598
Sum of electronic and thermal Enthalpies = -2342.506654
Sum of electronic and thermal Free Energies = -2342.641466

Δ(δδδδ), L-lactate•Yb_3, 0 imaginary frequencies

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	70	-0.100184	-0.807033	-0.224939
2	8	2.129000	-0.139280	0.288157
3	8	-0.207198	1.519464	-0.551811
4	8	-2.308370	-0.423292	0.567893
5	8	-0.103261	0.370170	1.941953
6	8	0.179134	-2.141275	1.585433
7	8	0.100465	-2.637734	3.775078
8	7	1.831072	-2.315415	-1.201861
9	7	0.681658	0.040999	-2.603216
10	7	-2.062810	-0.899067	-2.060015
11	7	-0.908282	-3.176834	-0.722012
12	7	4.217513	-0.742505	0.961197
13	1	4.992377	-1.416985	0.924802
14	7	0.772297	3.415840	-1.325871
15	1	1.316437	3.901053	-2.049954
16	7	-4.414836	0.396930	0.317854
17	1	-5.205776	0.624337	-0.297480
18	6	2.517569	-1.644124	-2.344598
19	1	3.216354	-0.911280	-1.937264
20	1	3.115144	-2.370192	-2.909480
21	6	1.543374	-0.957794	-3.290088
22	1	0.884024	-1.698639	-3.745069
23	1	2.105864	-0.487146	-4.107052
24	6	-0.476928	0.392133	-3.474625
25	1	-0.872858	1.350271	-3.131253
26	1	-0.141979	0.538544	-4.509456
27	6	-1.571322	-0.660951	-3.439465
28	1	-1.197860	-1.608797	-3.829596

29	1	-2.392805	-0.350385	-4.098291
30	6	-2.769403	-2.211534	-1.990869
31	1	-3.401036	-2.204963	-1.099191
32	1	-3.428891	-2.337655	-2.858770
33	6	-1.791906	-3.370085	-1.891535
34	1	-1.170575	-3.435002	-2.787075
35	1	-2.349187	-4.311339	-1.820961
36	6	0.220865	-4.140677	-0.693737
37	1	0.558522	-4.202405	0.340550
38	1	-0.101701	-5.140096	-1.009207
39	6	1.345788	-3.662925	-1.602388
40	1	0.989226	-3.591355	-2.632336
41	1	2.169515	-4.387893	-1.598614
42	6	2.780161	-2.413824	-0.071349
43	1	2.306619	-2.974544	0.737820
44	1	3.711079	-2.917465	-0.359902
45	6	3.040762	-1.000911	0.424212
46	6	4.723078	0.558246	1.406514
47	1	4.447483	1.313867	0.664787
48	6	1.421567	1.286746	-2.308714
49	1	2.363310	1.040470	-1.814398
50	1	1.643888	1.856712	-3.219413
51	6	0.597253	2.111211	-1.328821
52	6	0.077463	4.394615	-0.486137
53	1	-0.985354	4.138693	-0.455147
54	6	-3.003032	0.162716	-1.648261
55	1	-2.542393	1.138821	-1.820126
56	1	-3.943340	0.120575	-2.212283
57	6	-3.241378	0.025799	-0.153974
58	6	-4.877318	0.316900	1.705065
59	1	-4.569972	-0.645583	2.123833
60	6	-0.009272	-1.852443	2.834197
61	6	-0.457833	-0.407113	3.111457
62	1	-0.642901	1.171452	1.902631
63	1	-1.455196	-3.333620	0.124290
64	6	-4.325832	1.454914	2.569518
65	6	0.638845	4.438442	0.938970
66	6	4.180757	0.969414	2.778485
67	6	0.147262	0.181664	4.376836
68	1	-0.239772	1.187677	4.559314
69	1	1.235901	0.229596	4.297236
70	1	-0.112944	-0.454617	5.224516
71	1	-1.550954	-0.433997	3.187261
72	1	-4.746768	1.367963	3.572654
73	1	-3.236296	1.411786	2.636380
74	1	-4.612953	2.424097	2.151238
75	6	-6.440723	0.365931	1.648198
76	8	-7.023227	0.210287	2.742538
77	8	-6.944594	0.576436	0.508623
78	1	1.705210	4.682101	0.919764
79	1	0.113320	5.214861	1.497697
80	1	0.508418	3.480784	1.448408

81	6	0.243170	5.778229	-1.197330
82	8	1.000426	5.791700	-2.208813
83	8	-0.378695	6.727739	-0.674710
84	1	3.099213	1.116312	2.750384
85	1	4.414788	0.204994	3.525564
86	1	4.661353	1.904076	3.073387
87	6	6.283219	0.432541	1.433763
88	8	6.749863	-0.716518	1.190601
89	8	6.901825	1.482912	1.708936

E(RTPSSh) = -2343.2804807 Hartree
Zero-point correction = 0.725264
Thermal correction to Energy = 0.773767
Thermal correction to Enthalpy = 0.774712
Thermal correction to Gibbs Free Energy = 0.641352
Sum of electronic and zero-point Energies = -2342.555216
Sum of electronic and thermal Energies = -2342.506713
Sum of electronic and thermal Enthalpies = -2342.505769
Sum of electronic and thermal Free Energies = -2342.639129

References

(1) Djanashvili, K.; Peters, J. A. *Contrast Media Mol. Imaging* **2007**, *2*, 67.
(2) Wu, Y.; Soesbe, T. C.; Kiefer, G. E.; Zhao, P.; Sherry, A. D. *J. Am. Chem. Soc.* **2010**, *132*, 14002.
(3) Tao, J. M.; Perdew, J. P.; Staroverov, V. N.; Scuseria, G. E. *Phys. Rev. Lett.* **2003,** 91, 146401.
(4) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision B.01*, Gaussian, Inc.: Wallingford CT, 2009.
(5) Dolg, M.; Stoll, H.; Savin, A. *Theor. Chim. Acta* **1989,** 75, 173-194.
(6) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005,** 105, 2999-3093.