

Supplementary Information

Hydroxyquinoline-functionalised Aza-crown Macrocycles for Lanthanide Coordination

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1. General Considerations

Reagents: All measurements were carried out at atmospheric pressure with stirring unless otherwise stated. No special precautions were taken to exclude air or moisture during reactions, workups or purifications unless otherwise stated. All solvents were obtained from commercial sources and used without further purifications. The chelator **H₂KHQ (3)** was prepared following **Scheme 1**. 2-Bromomethyl-8-hydroxyquinoline (**2**) was prepared as previously described.^{1,2} Macropa was prepared as previously described.³

Instruments and characterisation: TLC was performed on Kieselgel 60 F 254 plates (Merck) and visualisation achieved under UV fluorescence (254 and 366 nm). Flash silica column chromatography was performed on a Biotage Isolera™ 4 System advanced automated flash purification unit using 10 g, 25 g, or 50 g Sfär Duo cartridges, unless otherwise told. Reverse-phase flash chromatography was performed using the same Biotage Isolera™ 4 System with Biotage® Sfär Ultra C18 cartridges (12 g). ¹H, ¹³C{¹H} and 2D NMR spectra were recorded on a Bruker AV-400, AV-500, or DRX-400 spectrometer. Chemical shifts are reported in ppm and spectra are referenced to D₂O at δ = 4.79 ppm (¹H); CD₃OD at δ = 3.31 (¹H) and 49.2 ppm (¹³C{¹H}); CDCl₃ at δ = 7.26 (¹H) and 77.2 (¹³C{¹H}); DMSO-d₆ at δ = 2.50 (¹H).⁴ ¹³C{¹H} were assigned where possible using 2D correlation spectroscopy such as HMBC and HSQC. Spectra were processed and analysed using *MestReNova* (Mestrelab Research S.L.). software. Signal multiplicities are indicated as: s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), dt (doublet of triplets), ddd (doublet of doublets of doublets), ddt (doublet of doublets of triplets), ddq (doublet of doublets of quartets), m (multiplet); defined as all multi-peak signals where overlap or complex coupling of signals makes definitive descriptions of peaks difficult. Numbering of magnetically inequivalent environments is recorded where full assignment was achieved.

Analytical HPLC was performed on an Agilent 1260 Infinity II HPLC using a ZORBAX Eclipse XDB-C18 column (4.6 × 150 mm, 5 μ m) in at 40 °C with a flowrate of 1 mL/min and UV-Vis spectroscopic detection at 254 nm. Mobile phase A of 2mM NH₄OAc in H₂O and mobile phase B of 5 % 2 mM NH₄OAc in H₂O in 95 % MeCN were used as shown below.

Gradient, min	A, %	B, %
0.00	95	5
5.00	95	5
25.00	5	95
27.00	5	95
28.00	95	5
30.00	95	5

Liquid chromatography – mass spectrometry (LC-MS) was performed on an Agilent InfinityLab LC/MSD XT unit on an Agilent Poroshell HPH C18 3.0x50 mm 2.7 μ m column in either an acidic or basic gradient at 40 °C with a flowrate of 0.8 mL/min and UV-Vis spectroscopic detection at 254 nm. Acidic methods include mobile phase A of 0.1 % HCOOH in H₂O and mobile phase B of 0.1 % HCOOH in 90:10 MeCN: H₂O. Basic methods include mobile phase A of 0.1 % NH₄OH in H₂O and mobile phase B of 0.1 % NH₄OH in 90:10 MeCN: H₂O. Gradients are as shown below.

Gradient, min	A, %	B, %
0.00	95	5
7.00	0	100
8.00	0	100
8.10	95	5
10.00	95	5

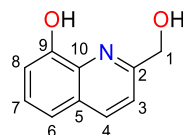
High resolution ES+ mass spectrometry analyses were conducted by Dr. Malgorzata Puchnarewicz at the Mass Spectrometry Service, Imperial College London on a Waters LCT Premier (ES-ToF)/Acquity i-Class spectrometer. UV-visible absorption spectra were measured using an Agilent Technologies Cary 60 Spectrophotometer operating with WinUV software. The sample was held in a quartz cuvette with a path length of 1 cm. Absorbance spectra were collected using 20 μ M solutions in H₂O, against a baseline of pure solvent in an optically matched cuvette with a scan rate of 300 nm min⁻¹ and a data interval of 0.5 nm. Extinction coefficients were calculated from the Beer Lambert Law ($A=\epsilon cl$) where A = the absorbance at a particular wavelength, ϵ is the extinction coefficient, c is the concentration, and l is the path length (width of the quartz cuvette, 1 cm). Phosphorescence spectra were recorded on an Agilent Technologies Carry Eclipse Fluorescence Spectrophotometer in phosphorescence mode, in quartz

cuvettes with a path length of 1 cm. Phosphorescence spectra were collected using 20 μM solutions in H_2O with the excitation and emission slits set at 10 or 20 nm, a gate time of 0.1 ms and delay time of 0.1 ms.

2. Synthesis

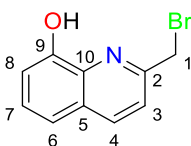
2.1. Experimental details

Synthesis of 1.¹



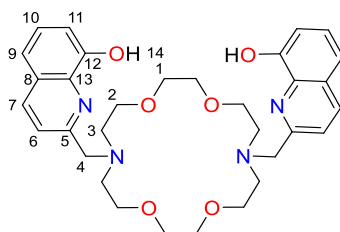
2-Formyl-8-hydroxyquinoline (1.00 g, 5.78 mmol) was dissolved in anhydrous MeOH (20 mL). NaBH_4 (0.29 g, 7.51 mmol, 1.3 eq.) was added slowly and the reaction stirred for 5 h at 20 $^\circ\text{C}$. The reaction mixture went from dark yellow to pale yellow. The solvent was removed *in vacuo* and H_2O (30 mL) was added. The resultant solution was neutralized using aqueous HCl (2 M) and then extracted with EtOAc (3 x 100 mL). The organic layer was dried over Na_2SO_4 , filtered and concentrated *in vacuo*. 2-Hydroxymethyl-8-hydroxyquinoline was isolated as a yellow solid (1.01 g, 5.78 mmol, 100 %) and characterised by ^1H NMR, matching literature.² **^1H NMR (400 MHz, CDCl_3) δ_{H} (ppm):** 8.15 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H, H_4), 7.45 (t, $^3J_{\text{HH}} = 8.0$ Hz, 1H, H_6), 7.41 – 7.31 (m, 2H, $\text{H}_{3,7}$), 7.21 (d, $^3J_{\text{HH}} = 7.5$ Hz, 1H, H_8), 4.97 (s, 2H, H_1).

Synthesis of 2.¹



Concentrated HBr (48 % in H_2O , 25 mL) was added dropwise to 2-hydroxymethyl-8-hydroxyquinoline (compound 1) (0.96 g, 5.49 mmol). The resulting orange solution was heated under reflux for 4 h and then cooled in an ice-water bath. Saturated Na_2CO_3 (aq.) was added until pH = 7. The product was extracted with DCM (3 x 100 mL) and the organic layer was dried over Na_2SO_4 , filtered, and concentrated *in vacuo*. The product was isolated by silica column chromatography (SiO_2 , hexane:EtOAc, 8:2) as a white solid (0.632 g, 2.67 mmol, 49 %). ^1H NMR data matched literature.^{1,2} **^1H NMR (400 MHz, CDCl_3) δ_{H} (ppm):** 8.10 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H, H_4), 7.52 (d, $^3J_{\text{HH}} = 8.5$ Hz, 1H, H_6), 7.48 – 7.39 (t, $^3J_{\text{HH}} = 8.0, 8.0$ Hz, 1H, H_7), 7.28 (d, $^3J_{\text{HH}} = 8.0$ Hz, 1H, H_3), 7.18 (d, $^3J_{\text{HH}} = 7.5$ Hz, 1H, H_8), 4.66 (d, $^3J_{\text{HH}} = 1.0$ Hz, 2H, H_1).

Synthesis of H_2KHQ .

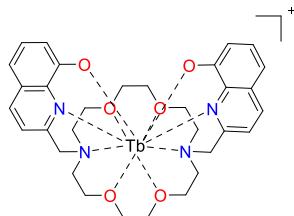


Under a N_2 atmosphere, 2-bromomethyl-8-hydroxyquinoline (compound 2) (0.59 g, 2.5 mmol, 2.1 eq.), K_{22} (0.30 g, 1.19 mmol) and Na_2CO_3 (0.76 g, 7.15 mmol, 6 eq.) were added to anhydrous MeCN (40 mL) and heated under reflux for 48 h. After 48 h, the reaction mixture was cooled to room temperature and filtered cold. The solvent was removed *in vacuo* isolating a yellow residue. The crude product was isolated by silica column chromatography (SiO_2 , DCM:MeOH + 0.1 % TEA, 8:2) as a yellow solid. The pure product was then isolated following reverse phase chromatography (C18, 0 – 100 % MeCN + 0.1 % FA in H_2O + 0.1 % FA) as a white solid (0.19 g, 0.33 mmol, 27%). **^1H NMR (400 MHz, CDCl_3) δ_{H} (ppm):** 8.07 (d, $^3J_{\text{HH}} = 8.5$ Hz, 2H, H_7), 7.66 (d, $^3J_{\text{HH}} = 8.5$ Hz, 2H, H_9), 7.40 (t, $^3J_{\text{HH}} = 8.0$ Hz, 2H, H_{10}), 7.28 (d, $^3J_{\text{HH}} = 8.5$ Hz, 2H, H_6), 7.14 (d, $^3J_{\text{HH}} = 7.5$ Hz, 2H, H_{11}), 4.02 (s, 4H, H_4), 3.67 (t, $^3J_{\text{HH}} = 6.0$ Hz, 8H, H_2), 3.62 (s, 8H, H_1), 2.93 (t, $^3J_{\text{HH}} = 6.0$ Hz, 8H, H_3). **$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ_{C} (ppm):** 158.9 (C_5), 152.2 (C_{12}),

137.5 (C₁₃), 136.4 (C₇), 127.6 (C₈), 127.3 (C₁₀), 122.1 (C₉), 117.7 (C₆), 110.06 (C₁₁), 70.9 (C₁), 70.1 (C₂), 62.0 (C₄), 54.6 (C₃).

HRMS (ES-TOF⁺): *m/z* calcd. for C₃₂H₄₁N₄O₆ ([M+H]⁺) at 577.3026; found as 577.3027. Analytical HPLC: T_R = 20.8 min.

Synthesis of [Tb-KHQ]⁺



H₂KHQ (0.010 g, 0.02 mmol) was dissolved in H₂O (pH 4 - 5) and TbCl₃•6H₂O (0.009 g, 0.022 mmol, 1.2 eq.) was added. The reaction was left at RT for 30 mins. The product was isolated by reverse phase chromatography (C18, 0 – 100 % MeCN+ 0.1 % NH₃ (aq.) in H₂O + 0.1 % NH₃ (aq.)). The product fractions were concentrated *in vacuo* to isolate yellow solid (0.0094 g, 0.013 mmol, 65 %). **¹H NMR (400 MHz, D₂O) δ_H (ppm):** 179.95, 114.27, 52.92, 13.34, 8.44, 7.31, 4.79, 3.73, 3.64, 3.38, 3.25, 2.88, 2.10, 1.95, 1.27, -0.34, -13.81, -45.14, -81.33, -95.67, -108.00, -121.37, -127.75, -203.83, -227.95. **HRMS(ES-TOF⁺):** *m/z* calcd. for C₃₂H₃₈N₄TbO₆ [M]⁺ at 733.2039; found as 733.2076.

2.2. Supplementary Data

¹H NMR: compound 1, CDCl₃

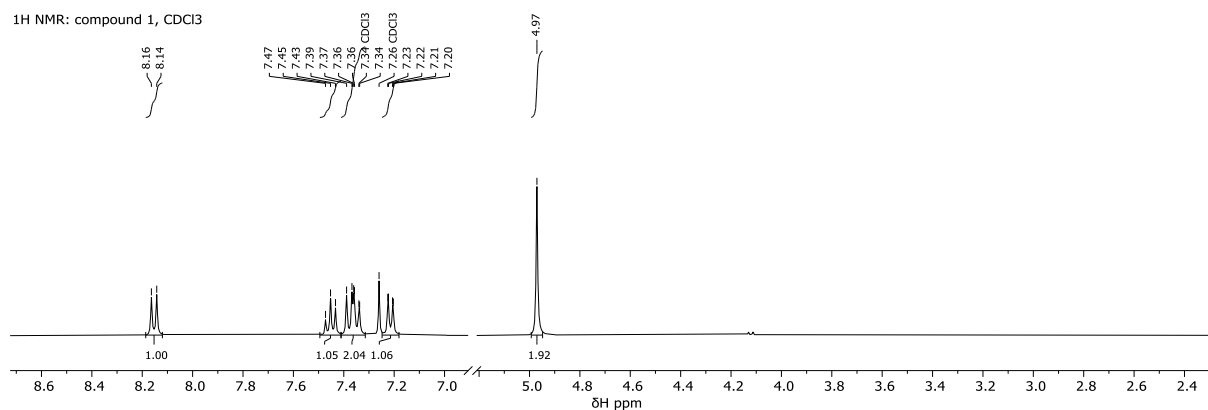


Figure S1. ¹H NMR spectrum of compound 1 (CDCl₃, 400 MHz, 298 K). Matches literature data. ²

¹H NMR: compound 2, CDCl₃

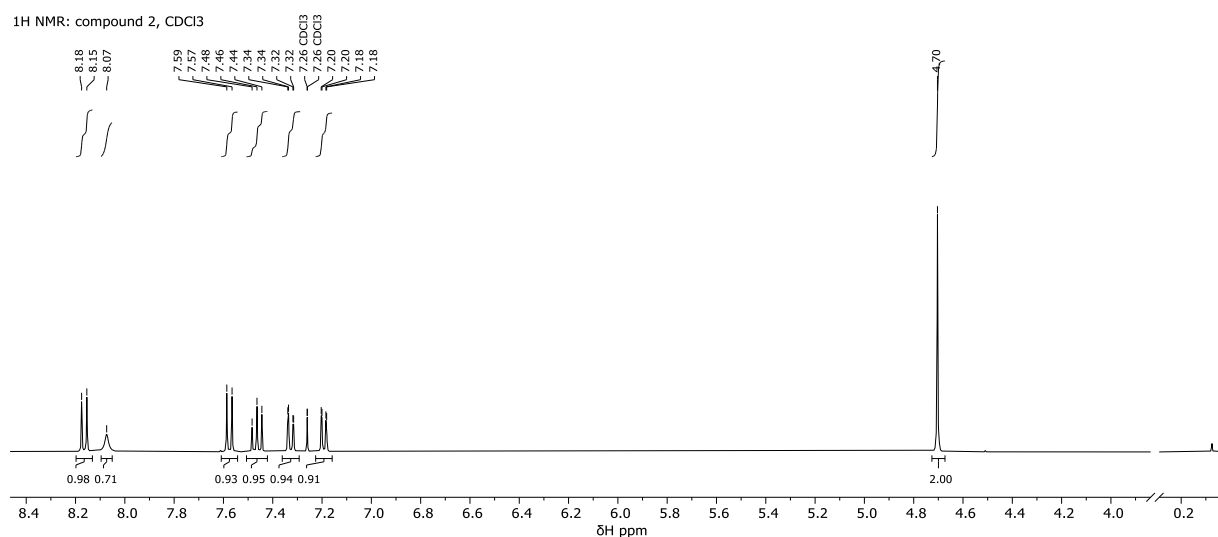


Figure S2. ¹H NMR spectrum of compound **2** (CDCl₃, 400 MHz, 298 K). Matches literature data. ²

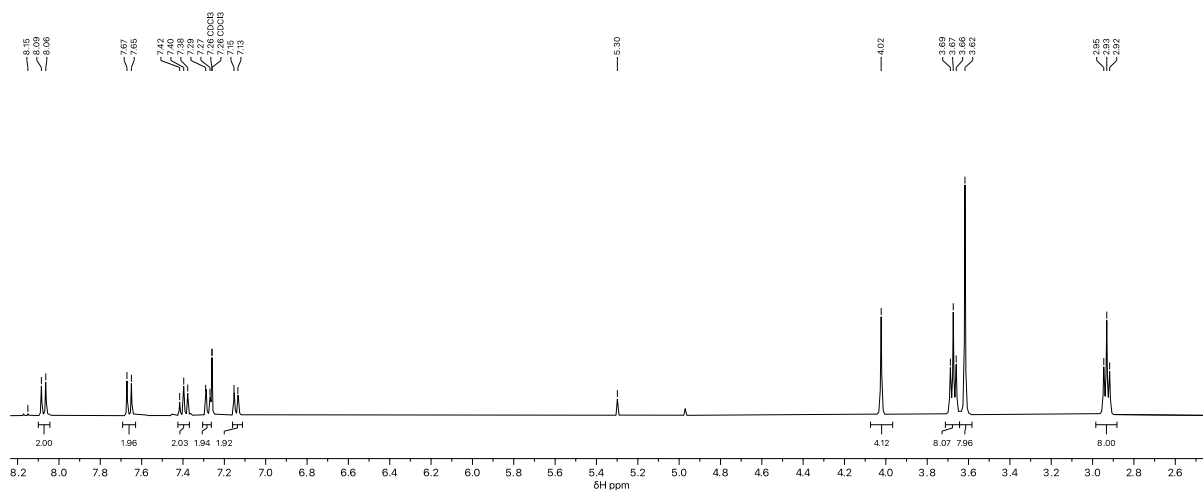


Figure S3. ¹H NMR spectrum of **H₂KHQ**. (CDCl₃, 400 MHz, 298 K). The peak at 5.30 ppm is residual DCM.

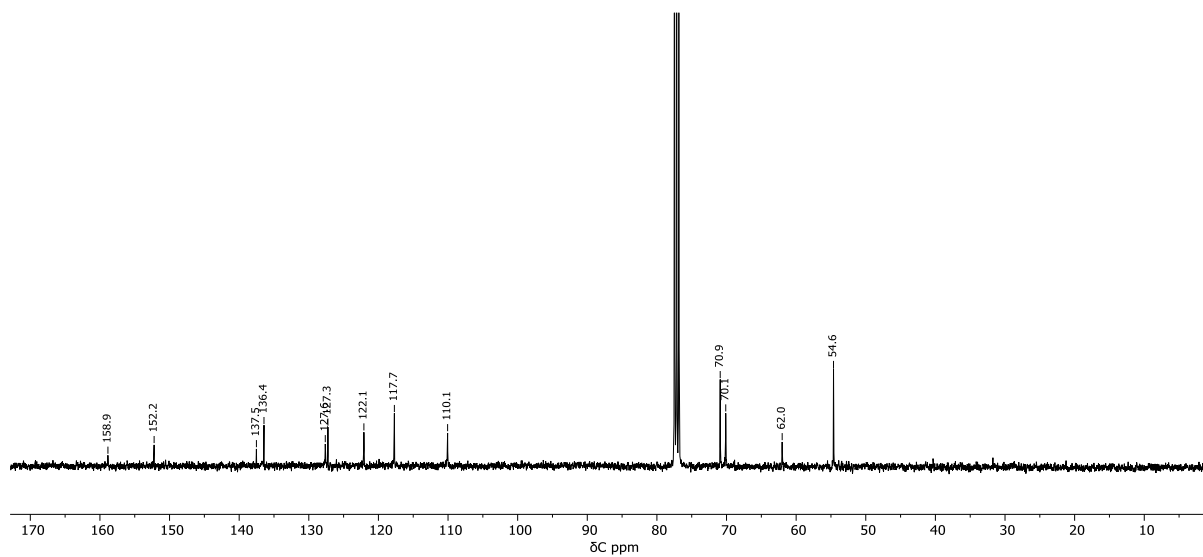


Figure S4. ¹³C{¹H} NMR spectrum of **H₂KHQ**. (CDCl₃, 101 MHz, 298 K)

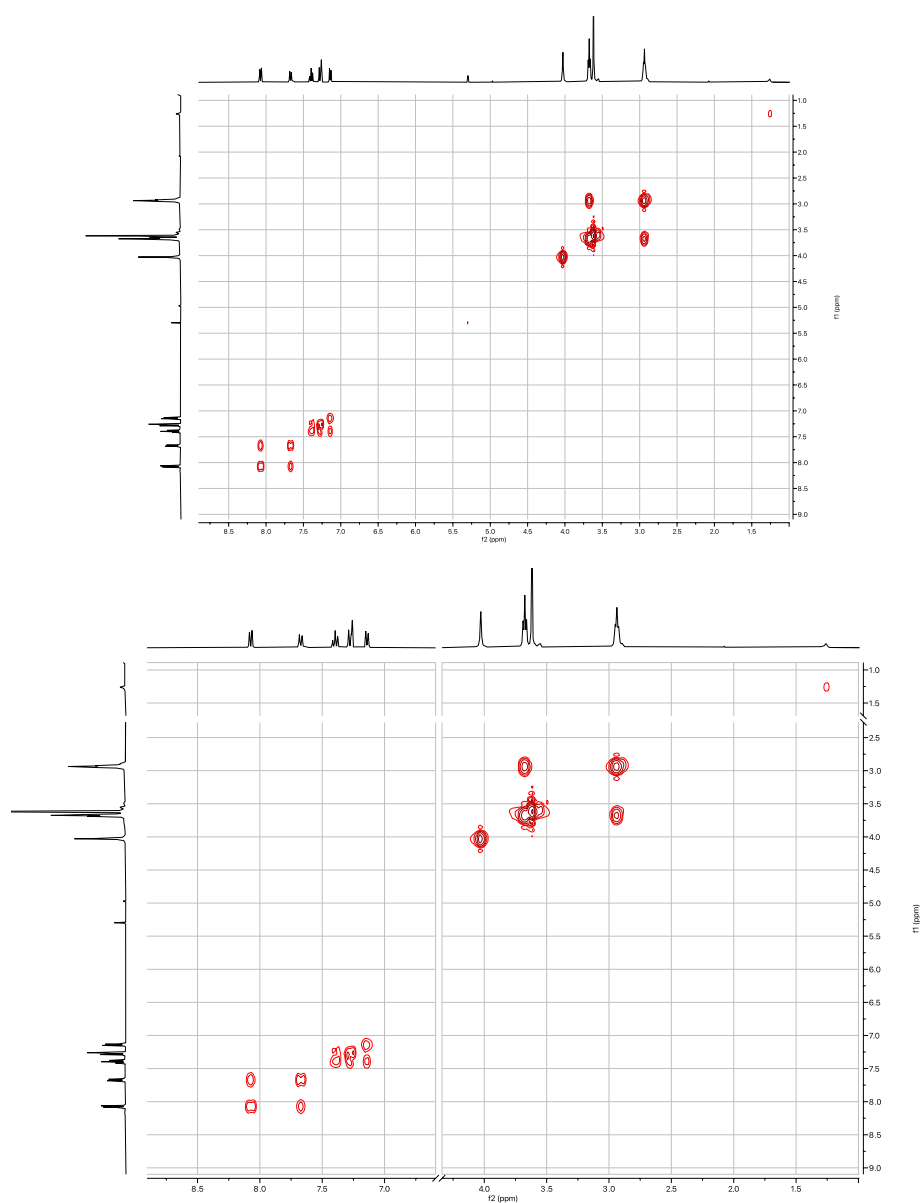


Figure S5. Full width (top) and expanded (bottom) ^1H - ^1H COSY NMR spectrum of H_2KHQ . (CDCl_3 , 298 K)

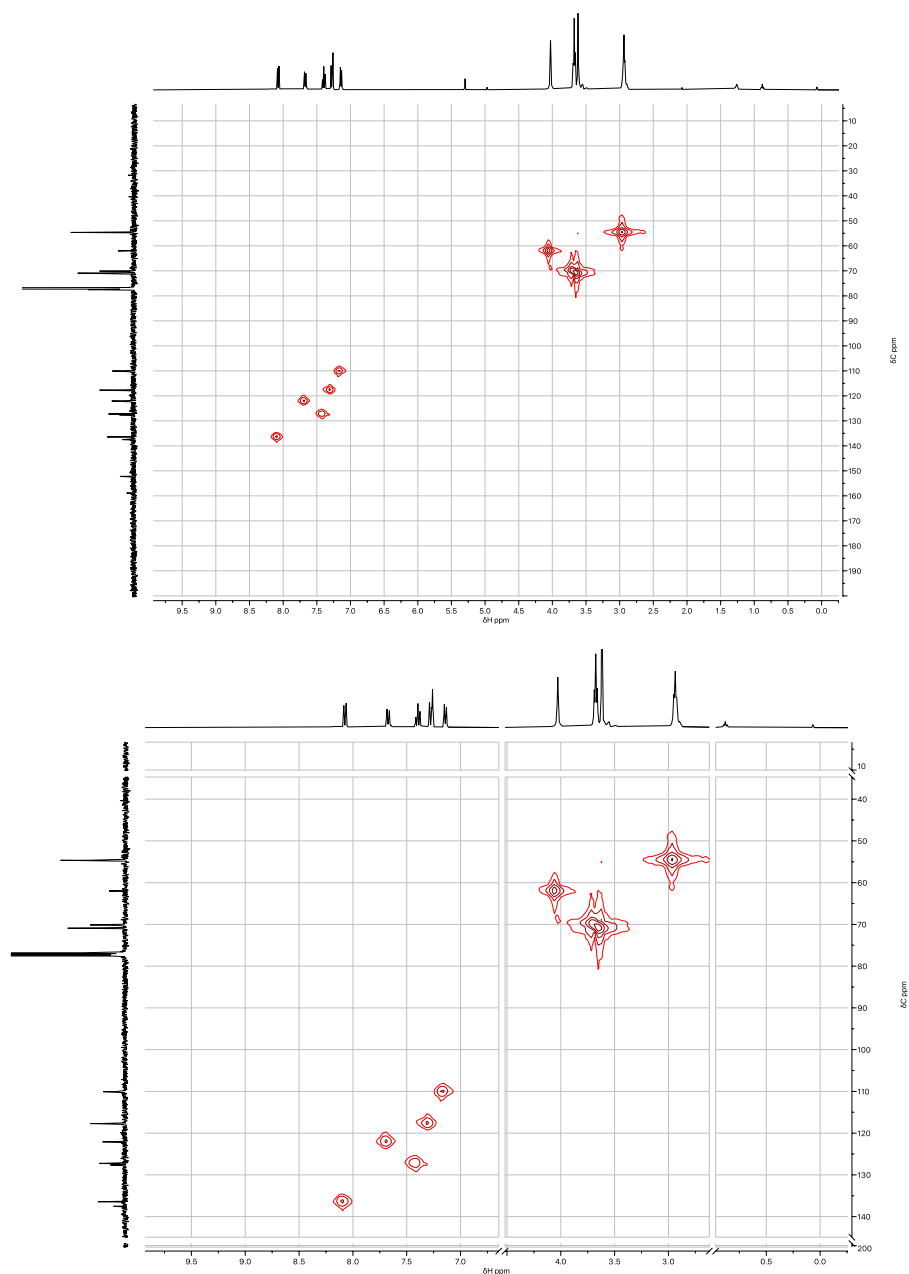


Figure S6. Full width (top) and expanded (bottom) ^1H - ^{13}C HMQC NMR spectrum of H_2KHQ . (CDCl_3 , 298 K).

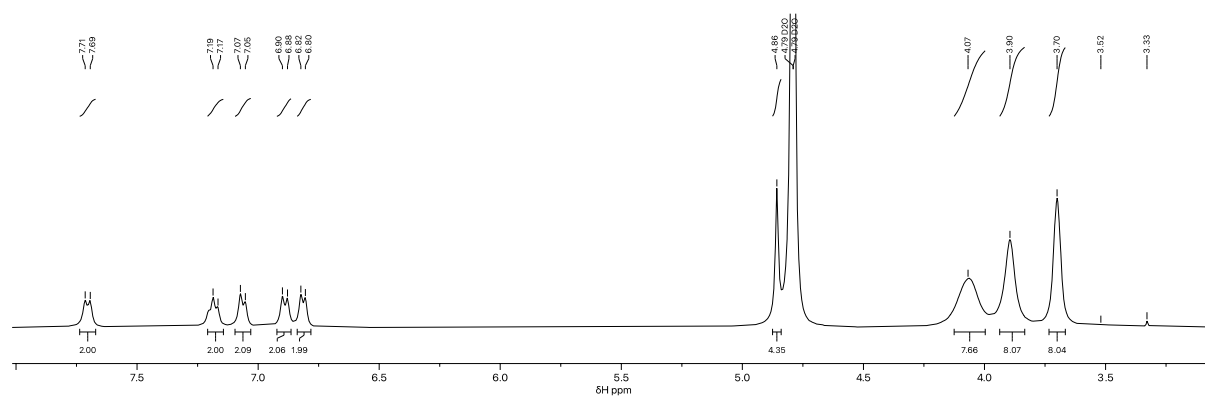


Figure S7. ^1H NMR spectrum of H_2KHQ . (D_2O , $\text{pD} = 5$, 400 MHz, 298 K).

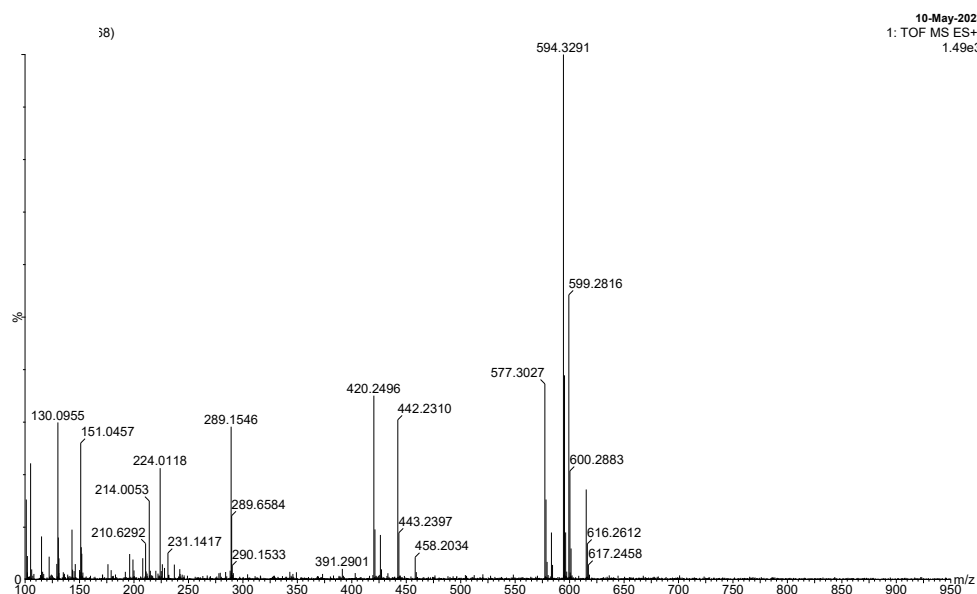


Figure S8. HRMS(ES-TOF+) of **H₂KHQ**. *m/z* calcd. for C₃₂H₄₁N₄O₆ ([M+H]⁺) at 577.3026; found as 577.3027.

3. X-ray Crystallography

3.1. Experimental Details

Single crystal X-ray data were collected using an Agilent Xcalibur PX Ultra A diffractometer, and the structures were refined using the OLEX2 and SHELX-2019 program systems.^{5–7} Details of the individual data collection are provided in the relevant CIFs. A summary of the fundamental crystal and refinement data are given in Table S1. Atomic coordinates, anisotropic displacement parameters and bond lengths and angles can be found in the .cif files, which have been deposited in the Cambridge Crystallographic Data Centre.

3.2. Supplementary Data

Table S1. Crystal Data, Data Collection and Refinement Parameters for the structures **[H₂KHQ](ClO₄)₂** and **[La-HKHQ](ClO₄)₂**. ^[a] Completeness to 0.84 Å resolution. ^[b] $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$; $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$.

	[H₂KHQ](ClO₄)₂	[La-HKHQ](ClO₄)₂
Formula	C ₃₂ H ₄₂ Cl ₂ N ₄ O ₁₄	C ₃₂ H ₃₉ Cl ₂ LaN ₄ O ₁₄
Solvent	—	—
Formula weight	777.59	913.48
Colour, habit	yellow platy	pale green platy
Temperature / K	173	173
Crystal system	monoclinic	monoclinic
Space group	P2 ₁ /c	P2 ₁ /c
<i>a</i> / Å	10.2238(4)	20.3932(4)
<i>b</i> / Å	14.4135(6)	11.4737(2)
<i>c</i> / Å	12.2816(5)	16.2053(4)
α / deg	90	90
β / deg	101.310(4)	109.809(3)
γ / deg	90	90
<i>V</i> / Å ³	1774.68(13)	3567.43(14)
<i>Z</i>	2	4
<i>D_c</i> / g cm ^{−3}	1.455	1.701
Radiation used	Cu K α	Cu K α
μ / mm ^{−1}	2.291	11.283
No. of unique reflns		

measured (R_{int})	11296 (0.0487)	21197 (0.0606)
obs, $ F_o > 4\sigma(F_o)$	2644	4382
Completeness (%) ^[a]	99.9	97.4
No. of variables	243	498
$R_1(\text{obs})$, $wR_2(\text{all})$ ^[b]	0.0488, 0.1413	0.0385, 0.0992
CCDC code	2435038	2435039

[H₂KHQ](ClO₄)₂

N–H and O–H hydrogen atoms were refined freely. The interatomic distances of O21–O7 (2.896 Å), and O21–N12 (2.886 Å) are indicative of a hydrogen bonding interaction (<3.5 Å).

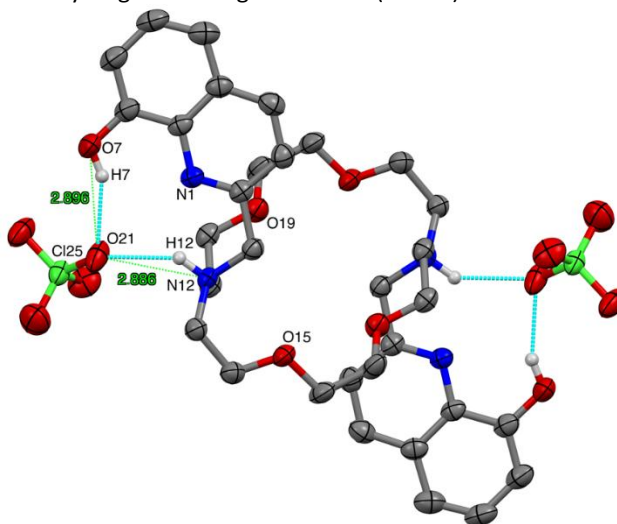


Figure S9. The structure of [H₂KHQ](ClO₄)₂ (50% probability ellipsoids). H atoms omitted for clarity. H-bonding contacts in teal and interatomic distances in green.

[La-HKHQ](ClO₄)₂

O–H hydrogen atoms were refined freely. The interatomic distances of O43–O8 (2.691 Å) are indicative of a hydrogen bonding interaction (<3.5 Å).

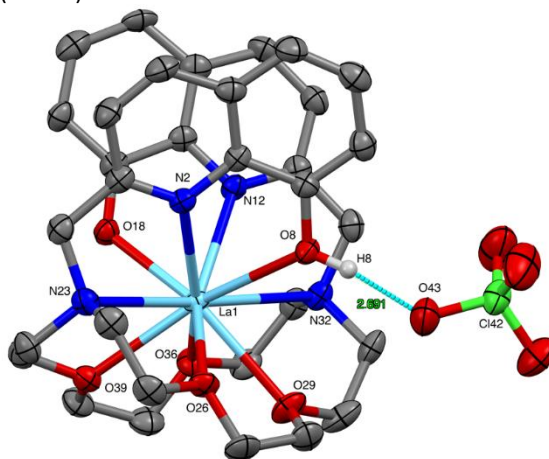


Figure S10. The structure of [La-HKHQ](ClO₄)₂ (50% probability ellipsoids). H atoms and second perchlorate anion omitted for clarity. H-bonding contacts in teal and interatomic distances in green.

4. NMR spectroscopy of Ln³⁺ complexes

4.1. Experimental Details

The NMR samples were prepared by mixing the **H₂KHQ** ligand and LnCl₃ stock solutions (LaCl₃•7H₂O, TbCl₃•6H₂O, LuCl₃•6H₂O) in a 1:1.2 molar ratio in D₂O. The pD was carefully adjusted with NaOD/DCl solutions. The ¹H NMR spectra were referenced to residual internal HDO solvent peak at 4.79 ppm, which was calculated according to the literature equation that accounts for the temperature dependence of the HDO chemical shift.⁴ The ¹³C{¹H} spectra were referenced indirectly to the corresponding ¹H spectra using the “absolute reference” function provided in *MestReNova* (Mestrelab Research S.L.).

[La-KHQ]⁺

¹H NMR (400 MHz, D₂O) δ_H (ppm): 7.64 (d, ³J_{HH} = 8.5 Hz, 2H, H_{HQ}), 6.99 (t, ³J_{HH} = 8.0 Hz, 2H, H_{HQ}), 6.92 (d, ³J_{HH} = 8.5 Hz, 2H, H_{HQ}), 6.59 (d, ³J_{HH} = 8.0 Hz, 2H, H_{HQ}), 6.47 (d, ³J_{HH} = 7.5 Hz, 2H, H_{HQ}), 4.88 (d, ³J_{HH} = 16.5 Hz, 2H, H_{CH2}), 4.35 (t, ³J_{HH} = 10.0 Hz, 2H, H_{CH2}), 4.24 – 4.11 (m, 4H, H_{CH2}), 4.04 (dd, ³J_{HH} = 16.5, 17.5 Hz, 6H, H_{CH2}), 3.94 (s, 4H, H_{CH2}), 3.71 – 3.64 (m, 2H, H_{CH2}), 3.54 (t, ³J_{HH} = 11.0 Hz, 2H, H_{CH2}), 3.15 (d, ³J_{HH} = 13.5 Hz, 2H, H_{CH2}), 2.94 (d, ³J_{HH} = 8.0 Hz, 2H, H_{CH2}), 2.69 (d, ³J_{HH} = 14.0 Hz, 2H, H_{CH2}). **¹³C{¹H} NMR (126 MHz, D₂O) δ_C (ppm):** 171.7, 162.9, 156.5, 141.8, 138.36, 129.1, 128.3, 120.0, 112.6, 111.6, 73.7, 71.9, 71.5, 65.6, 57.5, 55.9. **HRMS(ES-TOF⁺):** *m/z* calcd. for C₃₂H₃₈N₄LaO₆ [M]⁺ at 713.1855; found as 713.1829.

[Lu-KHQ]⁺

¹H NMR (400 MHz, D₂O, pD 9) δ_H (ppm): 8.48 (d, ³J_{HH} = 8.5 Hz, 2H, H_{HQ}), 7.58 – 7.51 (m, 4H, H_{HQ}), 7.30 (d, ³J_{HH} = 8.5 Hz, 2H, H_{HQ}), 6.94 (d, ³J_{HH} = 7.5 Hz, 2H, H_{HQ}), 4.68 – 4.05 (m, 8H, H_{CH2}), 3.85 (s, 2H, H_{CH2}), 3.78 (s, 2H, H_{CH2}), 3.60 (t, ³J_{HH} = 19.0 Hz, 6H, H_{CH2}), 3.30 (d, ³J_{HH} = 20.0 Hz, 4H, H_{CH2}), 3.07 (s, 2H, H_{CH2}), 2.79 (d, ³J_{HH} = 11.5 Hz, 2H, H_{CH2}), 2.59 (d, ³J_{HH} = 12.5 Hz, 2H, H_{CH2}). **HRMS(ES-TOF⁺):** *m/z* calcd. for C₃₂H₃₈N₄LuO₆ [M]⁺ at 749.2199; found as 749.2186.

4.2. Supplementary Data

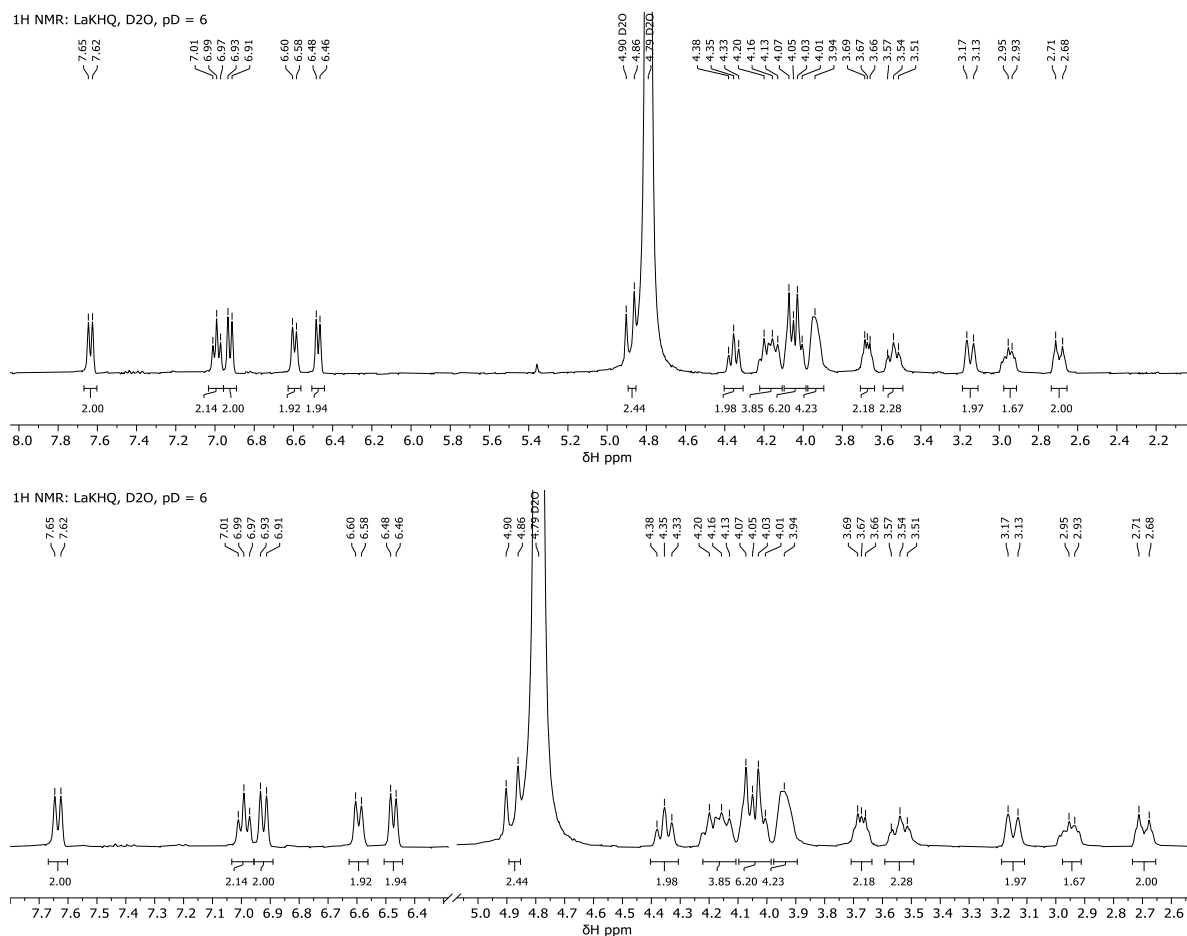
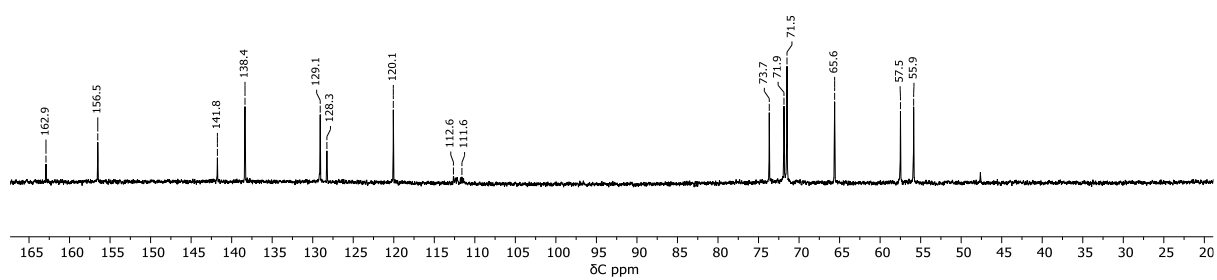


Figure S11. Full width (top) and expanded (bottom) ¹H NMR spectrum of [La-KHQ]⁺ D₂O, pD = 6, 400 MHz, 298 K).

$^{13}\text{C}\{^1\text{H}\}$ NMR of LaKHQ



$^{13}\text{C}\{^1\text{H}\}$ NMR of LaKHQ

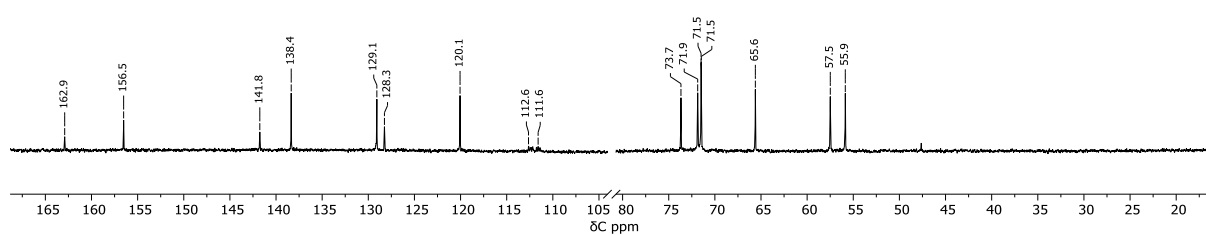


Figure S12. Full width (top) and expanded (bottom) $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{La-KHQ}]^+$ (D_2O , $\text{pD} = 6$, 126 MHz, 353 K).

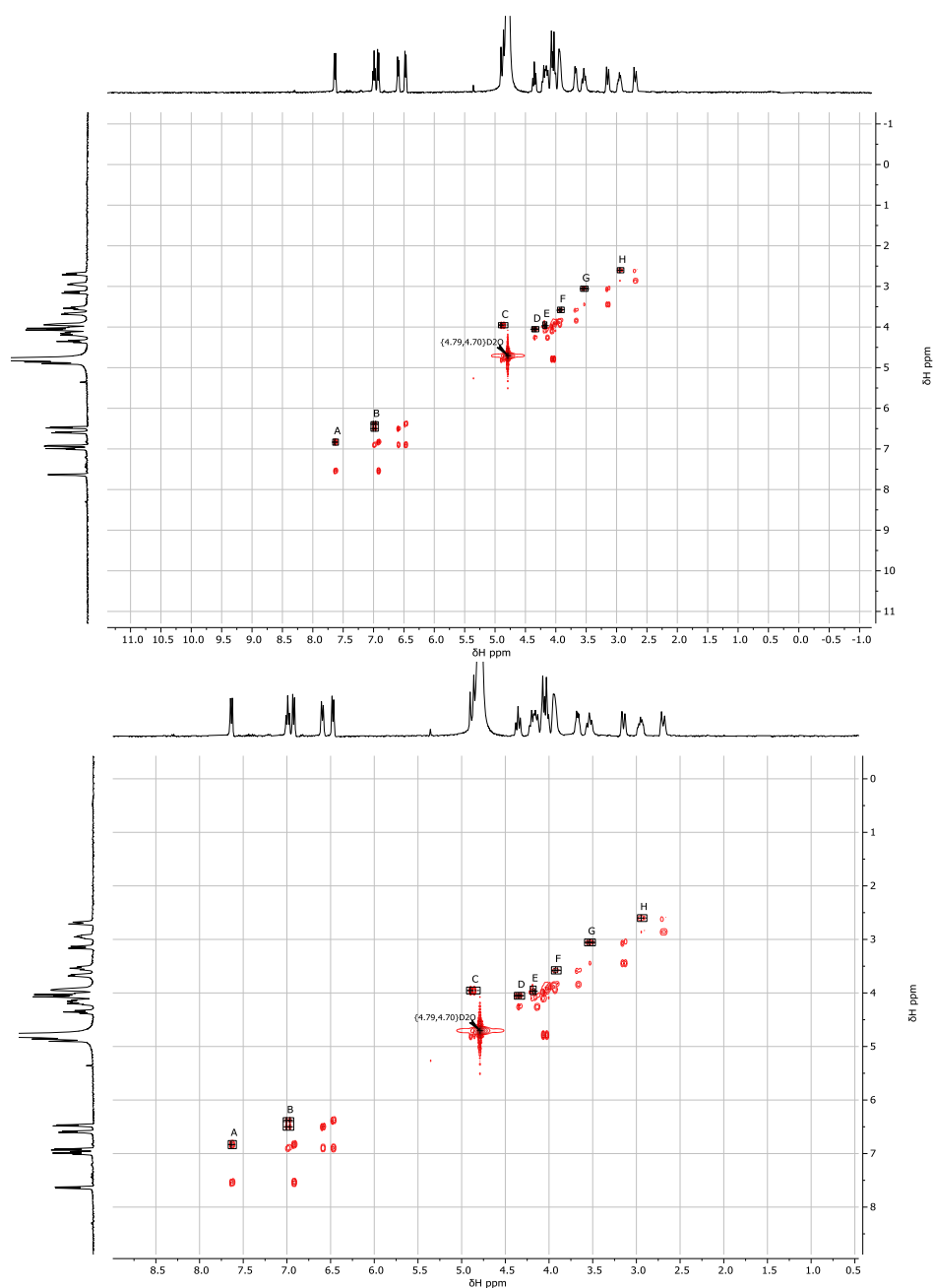


Figure S13. Full width (top) and expanded (bottom) ^1H - ^1H COSY NMR spectrum of $[\text{La-KHQ}]^+$ (D_2O , $\text{pD} = 6$, 298 K).

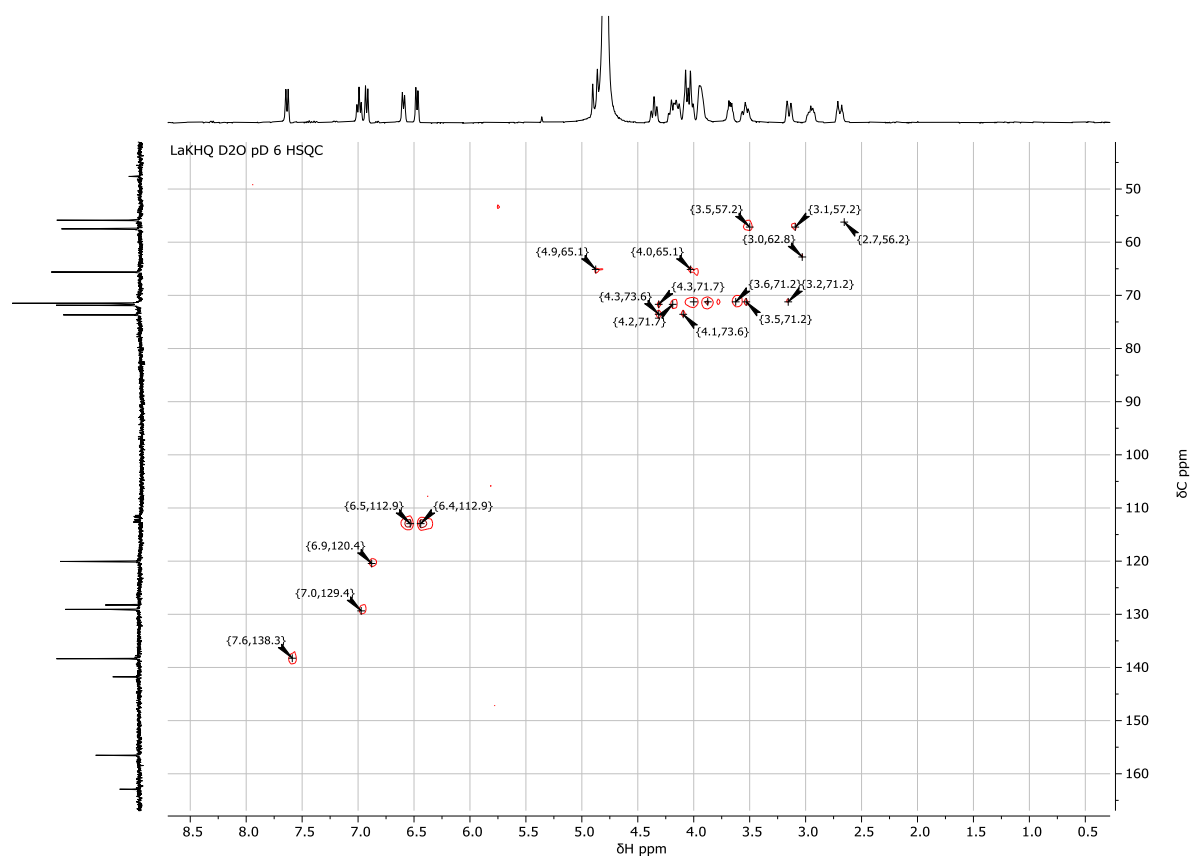


Figure S14. Full width ^1H - ^{13}C HSQC NMR spectrum of $[\text{La-KHQ}]^+$ (D_2O , pD = 6, 298 K).

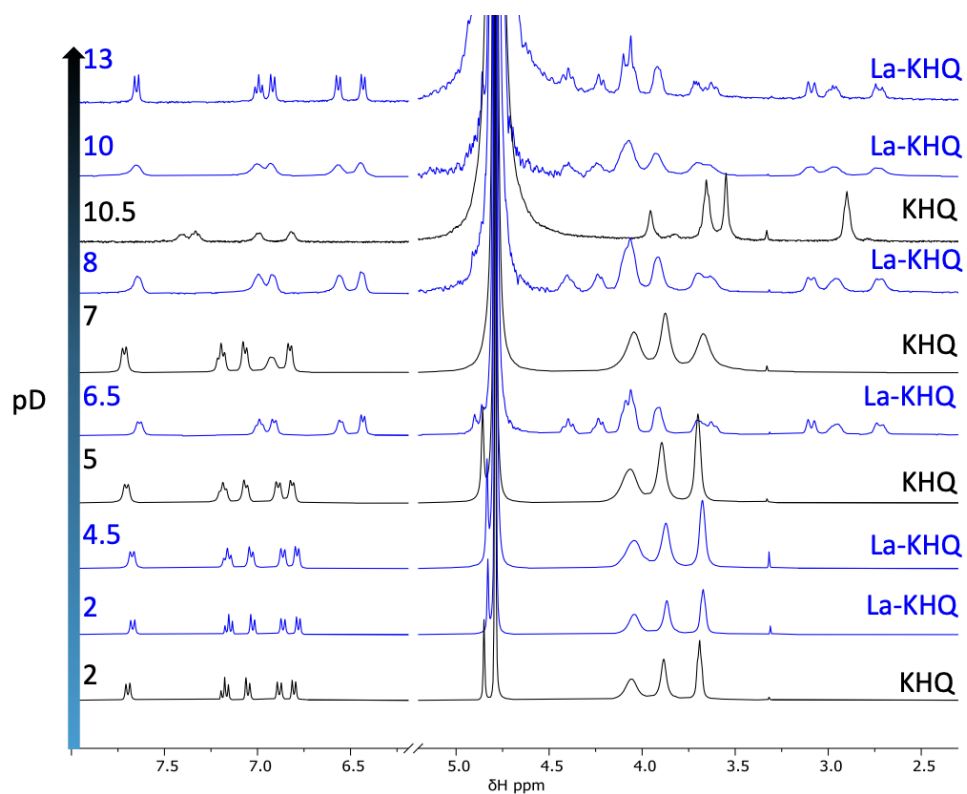


Figure S15. ^1H NMR spectroscopic pD-titration series of H_2KHQ (black spectra) and $[\text{La-KHQ}]^+$ (blue spectra) obtained from 0.014 M of the compounds in D_2O solutions. The pD range was 2 – 13 (bottom to top) and adjusted using DCl/NaOD . The signal at 4.79 ppm is the residual HDO resonance, overlapping with the bridging CH_2 signals. As the pD was increased, the peaks corresponding to free ligand disappeared.

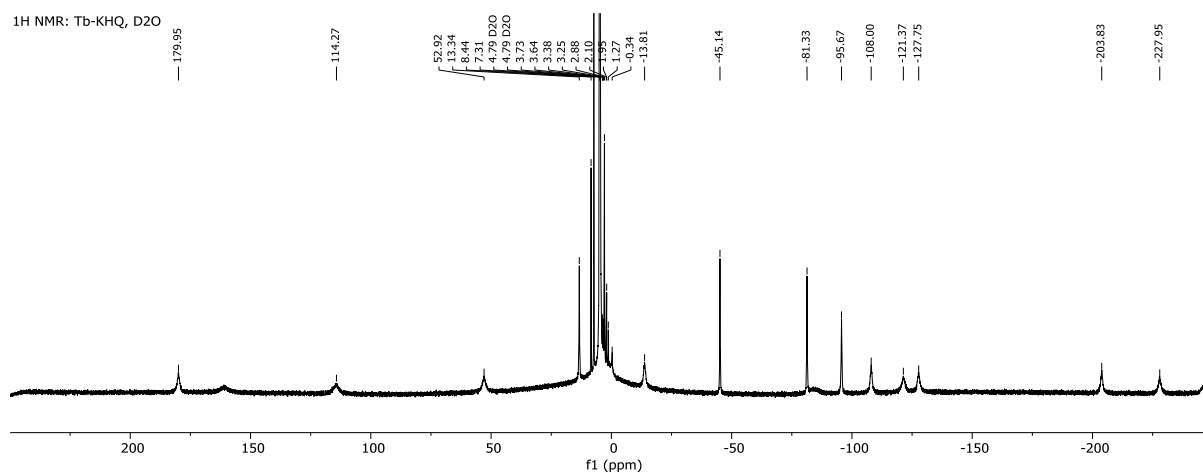


Figure S16. Full width ^1H NMR spectrum of $[\text{Tb-KHQ}]^+$ (D_2O , 400 MHz, 298 K).

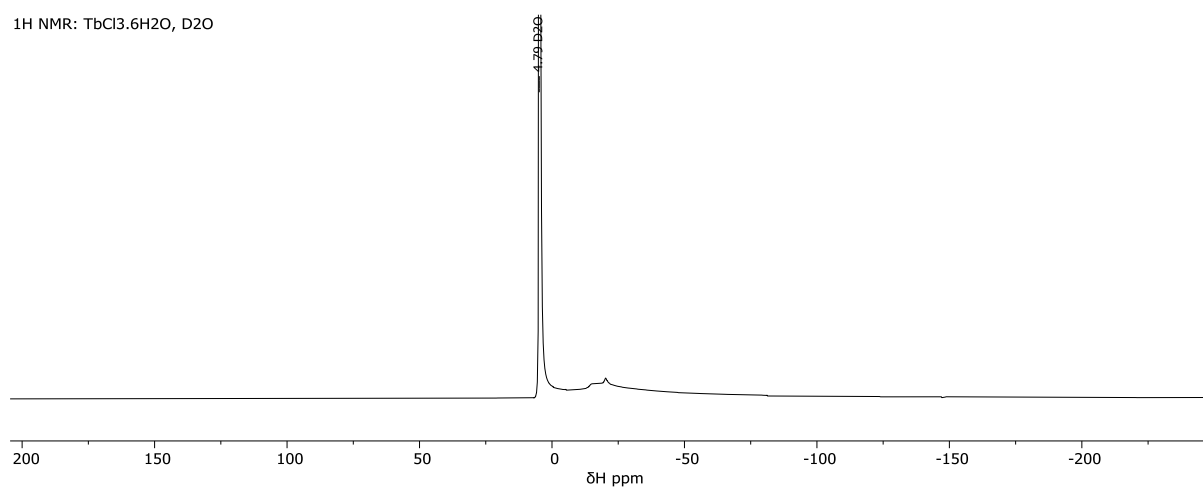
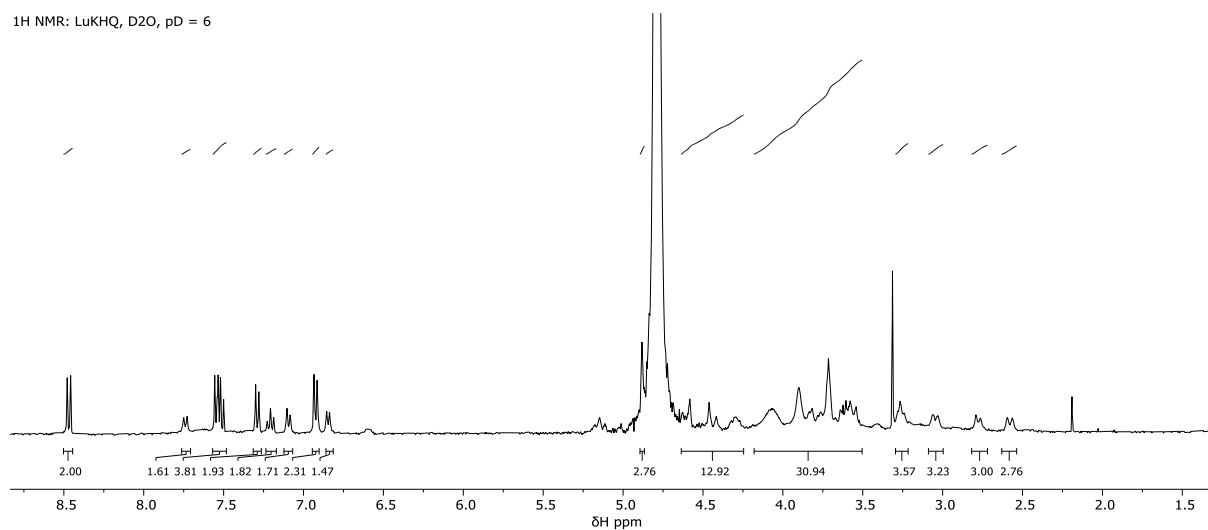


Figure S17. Full-width ^1H NMR spectrum of $\text{TbCl}_3 \cdot 6\text{H}_2\text{O}$ (D_2O , 400 MHz, 298 K).

¹H NMR: LuKHQ, D₂O, pD = 6



¹H NMR: LuKHQ, D₂O, pD = 6

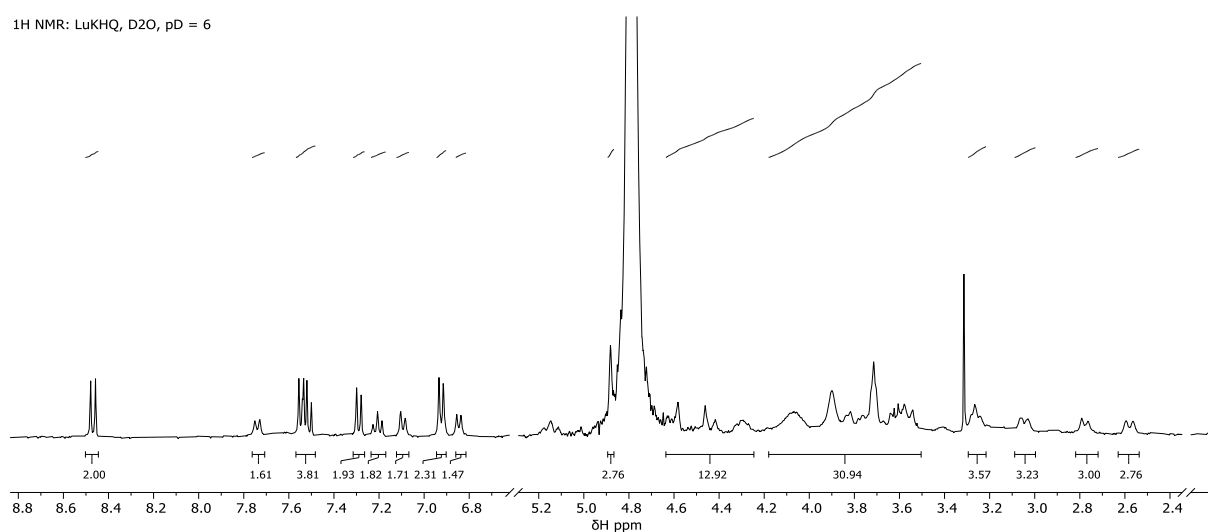


Figure S18. Full width (top) and expanded (bottom) ¹H NMR spectrum of [Lu-KHQ]⁺ (D₂O, pD = 6, 400 MHz, 298 K).

¹H NMR: LuKHQ, D₂O, pD = 9

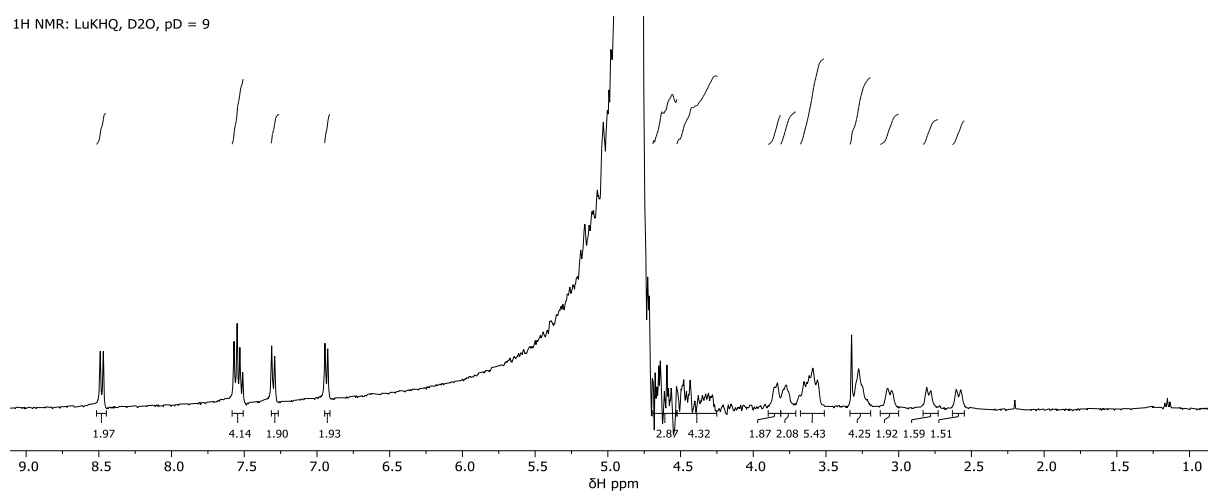


Figure S19. Full width ¹H NMR spectrum of [Lu-KHQ]⁺ (D₂O, pD = 9, 400 MHz, 298 K).

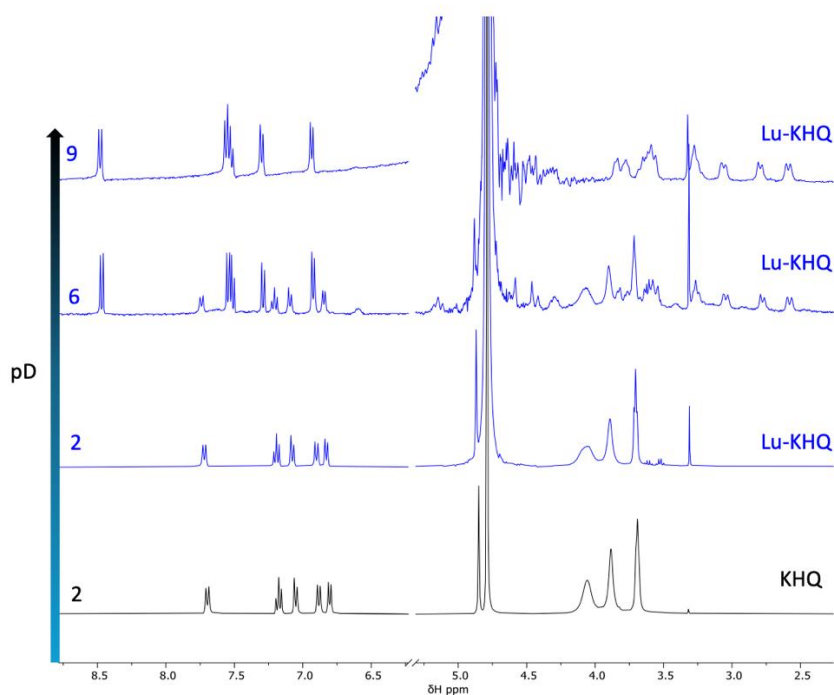


Figure S20. ^1H NMR pD-titration series of H_2KHQ (black spectra) and $[\text{Lu-KHQ}]^+$ (blue spectra) obtained from 0.014 M of the compounds in D_2O solutions. The pD range was 2 – 10 (bottom to top) and adjusted using DCl/NaOD . The signal at 4.79 ppm is the residual HDO resonance, overlapping with the bridging CH_2 signals. As the pD was increased, the peaks corresponding to free ligand disappeared.

5. LC-MS and HPLC experiments

5.1. Experimental Details

10 mM H_2KHQ stock solutions were prepared by dissolving the ligand in 20 mM NH_4OAc buffer (pH 6.5). 24 mM Ln^{3+} stock solutions were prepared by dissolving the chloride salts ($\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$, $\text{TbCl}_3 \cdot 6\text{H}_2\text{O}$, $\text{LuCl}_3 \cdot 6\text{H}_2\text{O}$) in 20 mM NH_4OAc buffer (pH 6.5). The reaction samples were prepared by mixing stock solutions of the H_2KHQ ligand and Ln^{3+} stock solutions in a 1:1.2 molar ratio in 20 mM NH_4OAc buffer (pH 6.5) to a final concentration of 1 mM. The samples were then left at room temperature or heated to 90 °C for 30 minutes.

5.2. Supplementary Data

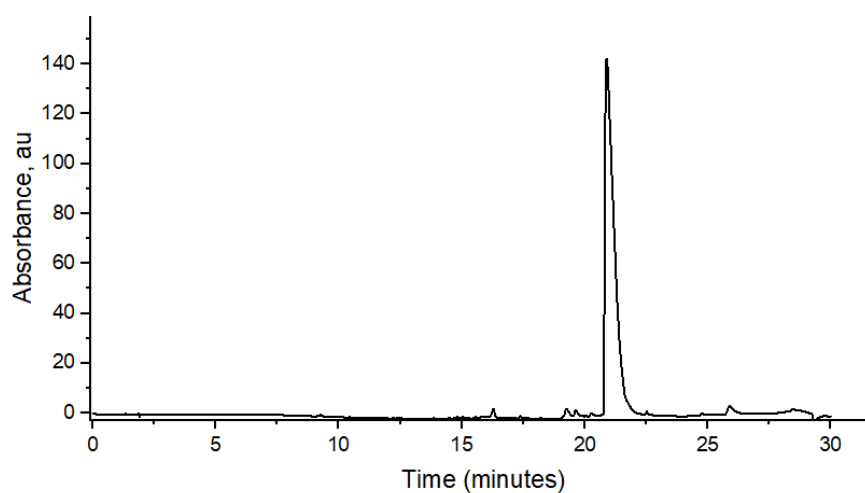


Figure S21. HPLC chromatogram of H_2KHQ (retention time= 20.9 min).

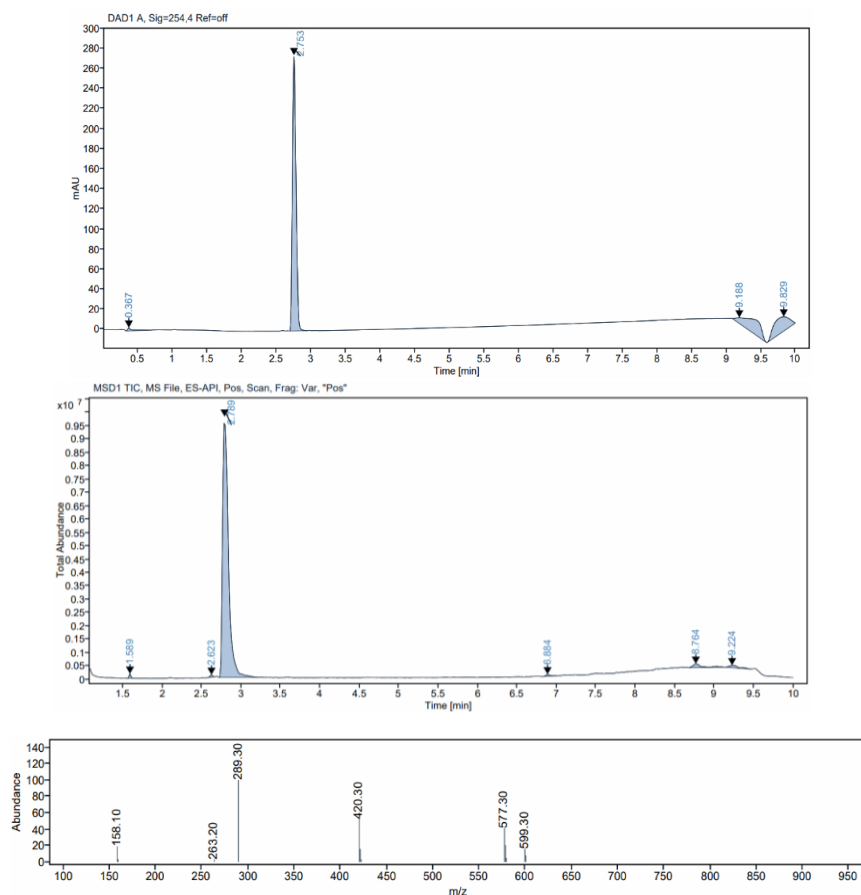


Figure S22. LC-MS of H_2KHQ . Measured in acidic methods. Retention time = 2.7 min with m/z calcd. for $\text{C}_{32}\text{H}_{41}\text{N}_4\text{O}_6$ ($[\text{M}+\text{H}]^+$) at 577.30; found as 577.30. m/z calcd. for $\text{C}_{32}\text{H}_{41}\text{N}_4\text{O}_6$ ($[\text{M}+\text{H}]^{2+}$) at 289.65; found as 289.30.

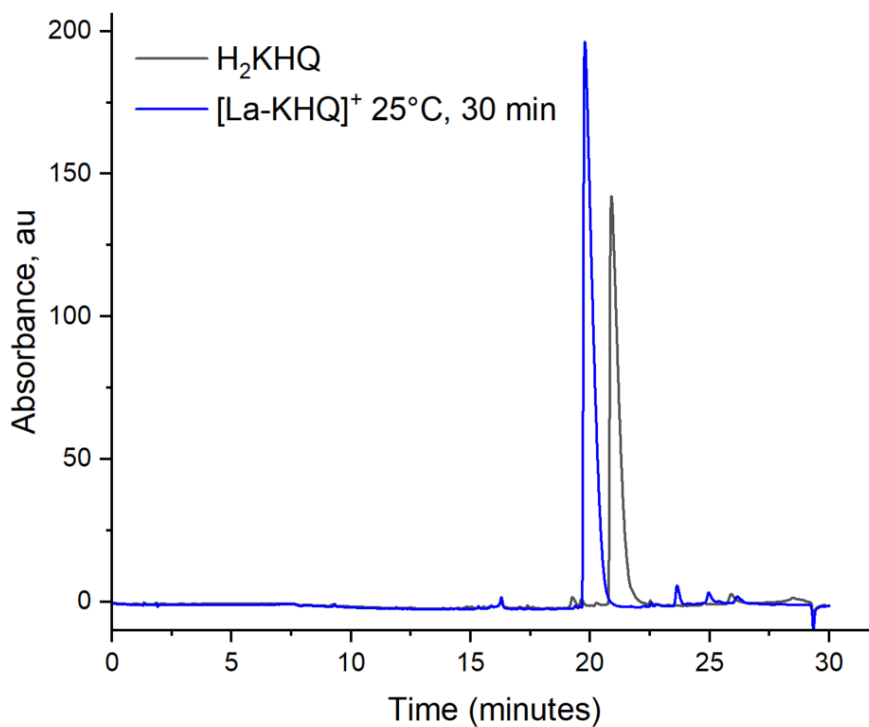


Figure S23. HPLC chromatogram of $[\text{La-KHQ}]^+$. $[\text{La-KHQ}]^+$ retention time = 19.9 min, H_2KHQ retention time = 20.9 min.

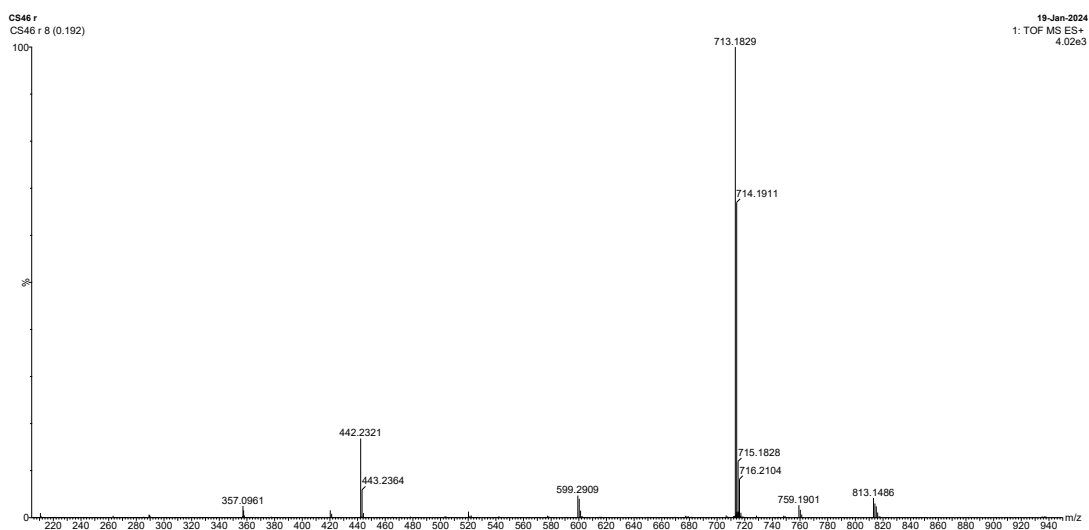


Figure S24. HRMS(ES-TOF+) of $[\text{La-KHQ}]^+$ m/z calcd. for $\text{C}_{32}\text{H}_{38}\text{N}_4\text{LaO}_6$ $[\text{M}]^+$ at 713.1849; found as 713.1829.

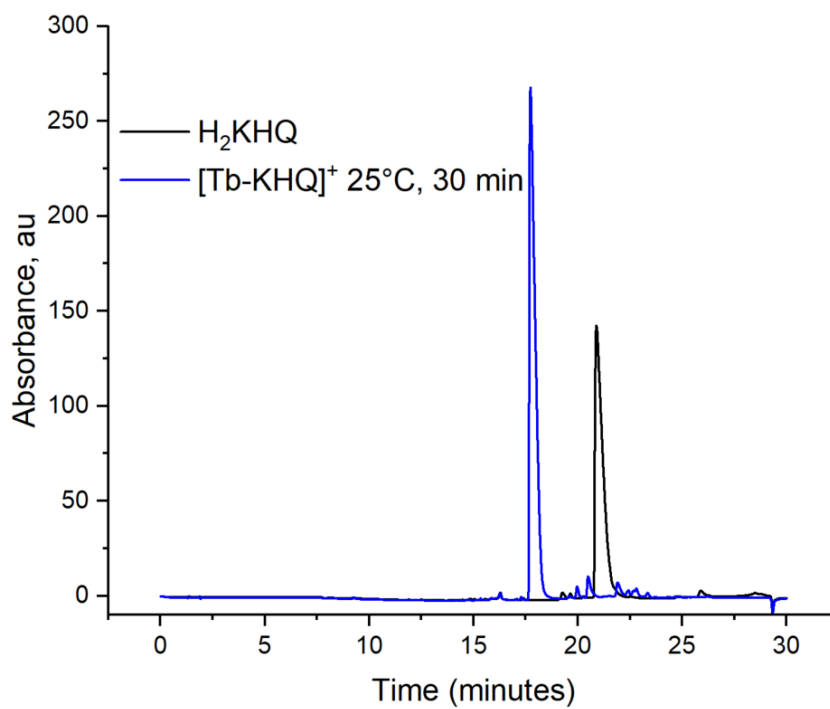


Figure S25. HPLC chromatogram of $[\text{Tb-KHQ}]^+$. $[\text{Tb-KHQ}]^+$ retention time= 17.7 min, H_2KHQ retention time= 20.9 min.

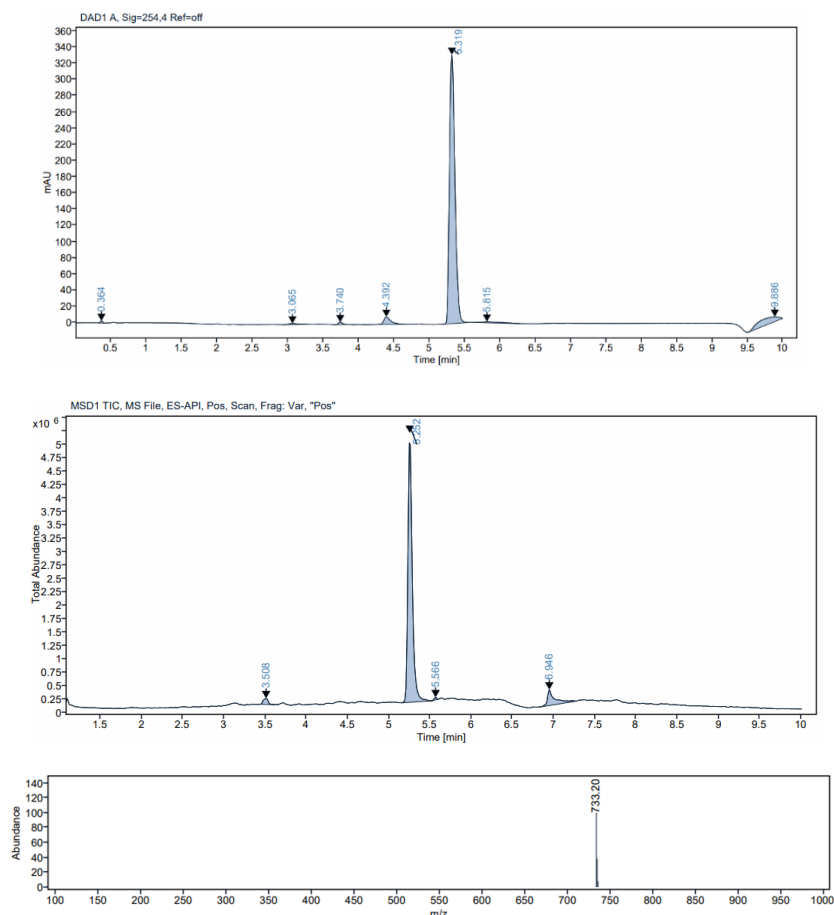


Figure S26. LCMS of **[Tb-KHQ]⁺** Measured in basic methods. retention time= 5.3 min with m/z calcd. for $C_{32}H_{38}N_4TbO_6$ ($[M+H]^+$) at 733.20; found as 733.20.

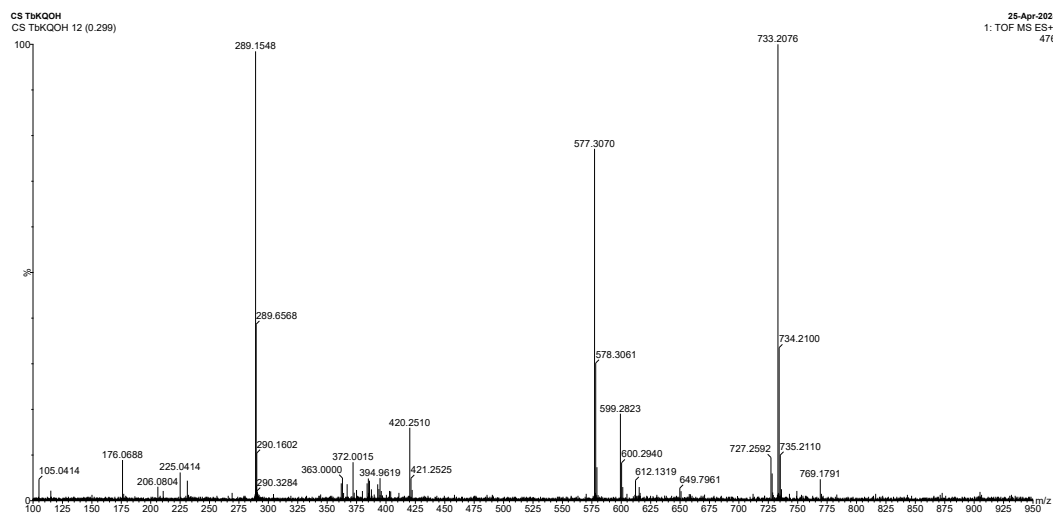


Figure S27. **HRMS(ES-TOF)** of **[Tb-KHQ]⁺** : m/z calcd. for $C_{32}H_{38}N_4TbO_6$ $[M]^+$ at 733.2045; found as 733.2076. m/z calcd. for $C_{32}H_{38}N_4NaO_6$ $[M]^+$ at 599.2689; found as 599.2844. m/z calcd. for $C_{32}H_{38}N_4O_6$ $[M]^+$ at 577.2948; found as 577.3017.

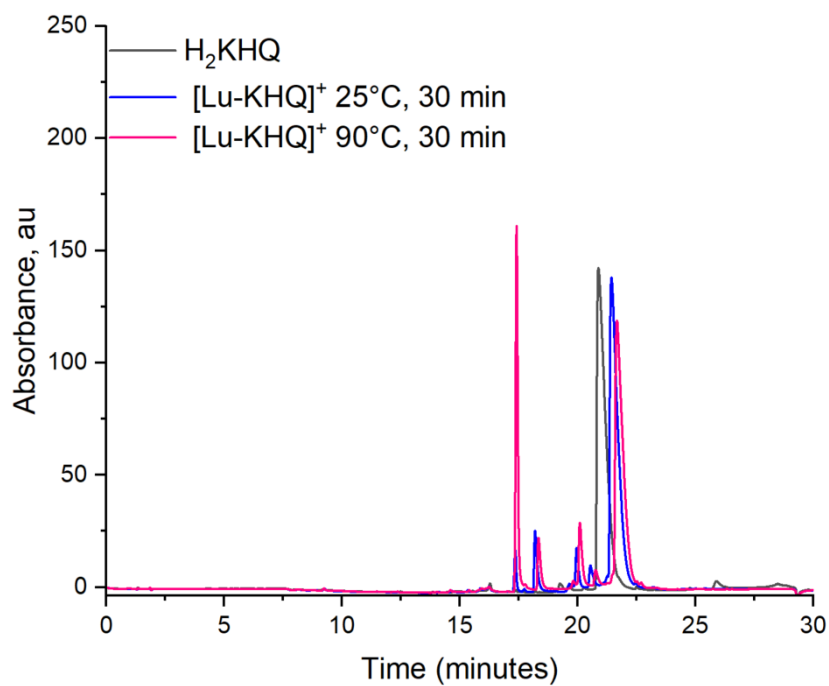


Figure S28. HPLC chromatogram of $[Lu-KHQ]^+$. $[Lu-KHQ]^+$ retention time= 17.4, 18.3, 20.1, 21.6 min, H_2KHQ retention time= 20.9 min.

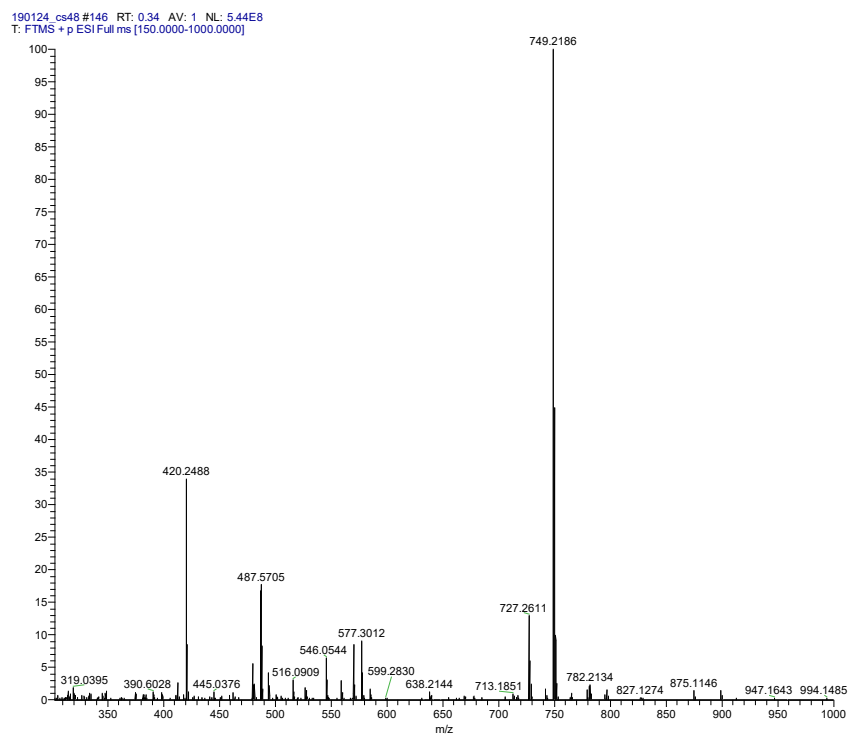


Figure S29. HRMS(ES-TOF) of $[Lu-KHQ]^+$ m/z calcd. for $C_{32}H_{38}N_4LuO_6 [M]^+$ at 749.2199; found as 749.2186.

6. DFT

6.1. Experimental Details

Geometry optimizations using density functional theory (DFT) were performed in Gaussian16 (Revision C.01.).⁸ To investigate the 1:1 complex of Ln^{3+} with the H_2KHQ ligand in different conformational arrangements. Initial geometries for the *syn*-conformer were taken from the crystal structure of $[\text{La-HKHQ}]^{2+}$ with removal of the H8 atom bound to O8 to model the overall +1 charged species. The La^{3+} centre was replaced with other Ln^{3+} ions to investigate the series. The hybrid ωB97XD functional was employed,^{9,10} which includes both dispersion and long-range corrections, and has been shown to give accurate geometries of Ln^{3+} complexes.¹¹ Specifically For C, H, N and O atoms the def2svp (double ζ) basis set was utilised.¹² For Ln^{3+} ions the large-core relativistic effective core potentials (LCRECP) and associated (7s6p5d)/[5s4p3d] basis sets of Dolg *et al.*¹³, were employed. The LCRECP calculation includes 4f electrons in the core (46 + 4fⁿ), leaving the valence 5s, 5p, 5d, and 6s electrons to be considered explicitly, and thus all calculations were carried out in the pseudosinglet state. The use of LCRECP for other Ln^{3+} complexes has been validated by previous studies^{14,15}, and is justified in that 4f orbitals do not have significant contribution to bonding. Geometry optimisations were performed without symmetry constraints (nosymm) and improved numerical integration grid using a pruned grid with 99 radial shells and 590 angular points per shell (int=ultrafine) was used. Additionally, frequency calculations were carried out on optimised structure to confirm, via the absence of imaginary frequencies, that the structures are local minima on the potential energy surface. To simulate the aqueous environment, single point energy corrections using the universal solvation model (SMD)¹⁶ were carried out using water as the solvent, employing the parameterised PCM ionic radii of the Ln^{3+} ions.¹⁷

Thermal corrections and solution phase corrections were applied using Paton's *GoodVibes* software,¹⁸ which incorporates Grimme's quasi-harmonic approximation to the vibrational entropy below a cut-off of 100 cm^{-1} and a frequency scaling factor = 1.0. The entropic terms for the frequencies below the cut-off are obtained from the free-rotor approximation while the standard rigid-rotor harmonic oscillator (RRHO) approximation is retained for those above the cut-off. A dampening function is used to interpolate between these two expressions close to the cut-off frequency. A temperature of 298 K and concentration of 1 M for $[\text{Ln-KHQ}]^+$ and 55.5 M (concentration of pure water) for H_2O was used to correct the gas-phase standard state free energies (G°_{gas} : 298 K, 1 atm) into solution-phase standard state free energies (G°_{gas} : 298 K, 1 mol/L) by the relationship with the ideal gas law (1 atm = 1/24.5 M at 298 K).

Interestingly, for macropa we do not see the conformational change reported by Roca-Sabio *et al.* as ionic radius decreases across the Ln series. Their work reports the La (III) favoured conformation to be $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$, which then destabilizes for the rest of the series, resulting in the $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformation being most stable.¹⁹ Herein, we have also calculated the optimised geometries for the 8 pairs of the three lanthanide ions discussed in this work with macropa. Our work demonstrates the $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ to be the lowest energy form for both $[\text{Ln-KHQ}]^+$ and $[\text{Ln-macropa}]^+$. This may be an artifact of the different theory levels used between both studies, however they both confirm that there exists a number of accessible conformational modes in solution at room temperature.

6.2. Methods

The Gibbs free energies of $[\text{syn-Ln-KHQ}]^+$, $[\text{syn-H}_2\text{O-Ln-KHQ}]^+$ and $[\text{anti-Ln-KHQ}]^+$ were determined from DFT calculations. The values are summarized in Table S1. The Gibbs free energy difference between $[\text{syn-Ln-KHQ}]^+$ and the hydrated form $[\text{syn-H}_2\text{O-Ln-KHQ}]^+$ is calculated by:

$$\Delta G^\circ_{\text{hyd.}} = G^\circ_{\text{aq}}([\text{syn-H}_2\text{O-Ln-KHQ}]^+) - G^\circ_{\text{aq}}([\text{syn-Ln-KHQ}]^+) - G^\circ_{\text{L}}(\text{H}_2\text{O}) \quad \text{Equation S1}$$

The Gibbs energy difference between $[\text{syn-Ln-KHQ}]^+$ and $[\text{anti-Ln-KHQ}]^+$ conformations is calculated by:

$$\Delta G^\circ_{\text{conf.}} = G^\circ_{\text{aq}}([\text{anti-Ln-KHQ}]^+) - G^\circ_{\text{aq}}([\text{syn-Ln-KHQ}]^+) \quad \text{Equation S2}$$

For the Gibbs energy of complexation:

$$\Delta G^\circ_{[\text{Ln-L}]^+} = G^\circ_{\text{gas}}([\text{syn-Ln-L}]^+) - G^\circ_{\text{gas}}(\text{Ln}^{3+}) - G^\circ_{\text{gas}}(\text{L}^{2-}) \quad \text{Equation S3}$$

Where L = KHQ or macropa

The term $G^\circ_g(\text{L}^{2-})$ was determined from a geometry optimisation of an initial guess structure based on the optimised structure of $[\text{syn-La-L}]^+$ and removing the La^{3+} centre. The optimised structure was then verified as a local minimum via a frequency calculation. Whilst the optimised structure of L^{2-} may not represent the global minimum, (and in reality H_2KHQ and $\text{H}_2\text{macropa}$ will exist in different protonation states depending on pH), the value of $G^\circ_g(\text{L}^{2-})$ remains constant for the calculation of $\Delta G^\circ_{[\text{Ln-L}]}$ for all Ln ions, and therefore relative comparisons and observed trends are valid.

Table S2. Free energies in aqueous solution (G°_{aq} , kcal mol⁻¹) of DFT optimised structures and the Gibbs free energy changes (ΔG°_{aq} , kcal mol⁻¹) described by equations S1 and S2. a: $G^\circ(\text{H}_2\text{O}) = -47901.18$ kcal mol⁻¹.

	$G^\circ_{aq}(\text{syn-Ln-KHQ})$	$G^\circ_{aq}(\text{anti-Ln-KHQ})$	$\Delta G^\circ_{conf.}$	$G^\circ_{aq}(\text{syn-H}_2\text{O-Ln-KHQ})$	$\Delta G^\circ_{hyd.}^a$	$G^\circ_{aq}(\text{Ln}^{3+})$
La	-1218165.73	-1218161.53	+ 4.2	-1266054.31	+ 12.6	-19753.40
Ce	-1218564.79	-1218559.91	+ 4.9	-1266452.41	+ 13.6	-20161.55
Pr	-1218965.48	-1218961.53	+ 4.0	-1266854.19	+ 12.5	-20563.87
Nd	-1219352.65	-1219348.62	+ 4.0	-1267241.07	+ 12.8	-20950.34
Sm	-1220119.30	-1220114.51	+ 4.8	-1268005.42	+ 15.1	-21719.57
Eu	-1220493.50	-1220489.08	+ 4.4	-1268379.99	+ 14.7	-22094.39
Gd	-1220865.56	-1220861.21	+ 4.4	-1268752.61	+ 14.1	-22465.58
Tb	-1221233.96	-1221229.29	+ 4.7	-1269120.39	+ 14.8	-22833.59
Dy	-1221601.45	-1221596.79	+ 4.7	-1269488.29	+ 14.3	-23204.94
Ho	-1221965.24	-1221960.06	+ 5.2	-1269851.99	+ 14.4	-23566.13
Er	-1222330.72	-1222326.64	+ 4.1	-1270217.18	+ 14.7	-23933.93
Tm	-1222695.47	-1222690.88	+ 4.6	-1270582.07	+ 14.6	-24300.18
Yb	-1223061.91	-1223056.63	+ 5.3	-1270949.94	+ 13.1	-24668.44
Lu	-1223407.64	-1223402.94	+ 4.7	-1271296.02	+ 12.8	-25014.88

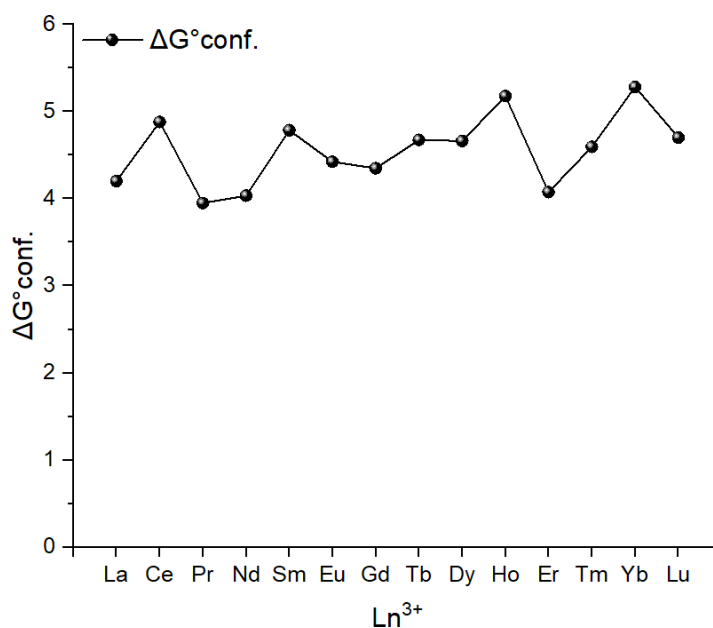


Figure S30. DFT-computed Gibbs free energy difference for the anti/syn conformation equilibrium of $[\text{Ln-KHQ}]^+$ complexes.

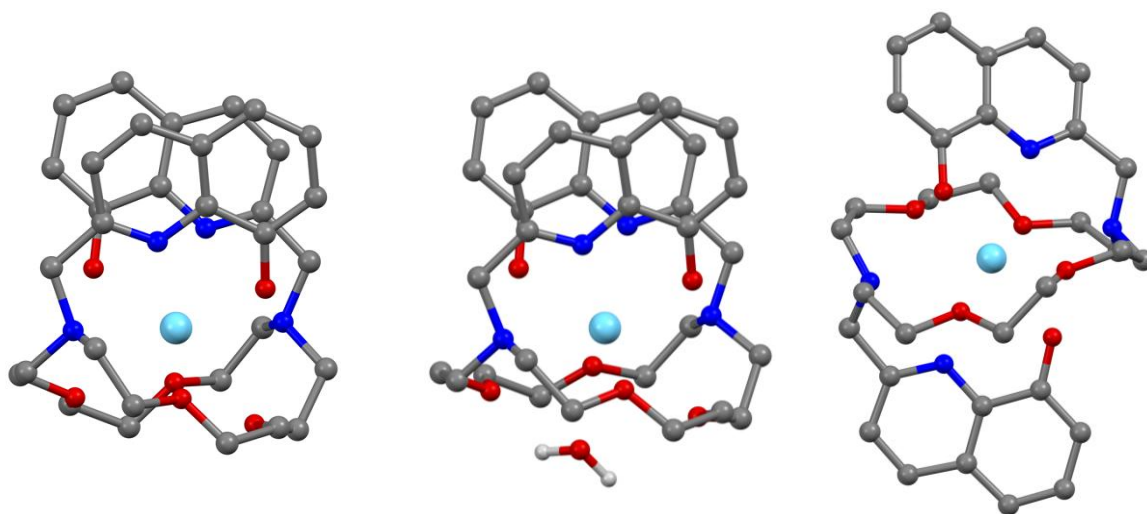


Figure S31. Left to right: $[\text{syn-La-KHQ}]^+$, $[\text{syn-H}_2\text{O-La-KHQ}]^+$, and $[\text{anti-La-KHQ}]^+$ complexes obtained from DFT calculations.

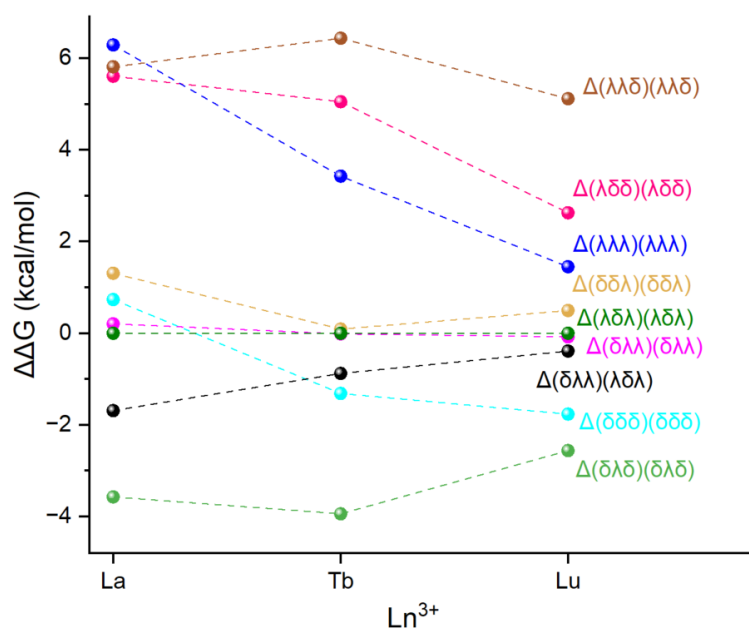


Figure S32. Comparison of relative Gibbs free energies of conformational modes in $[\text{Ln-KHQ}]^+$. $\Delta\Delta\text{G}$ values relative to $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformation.

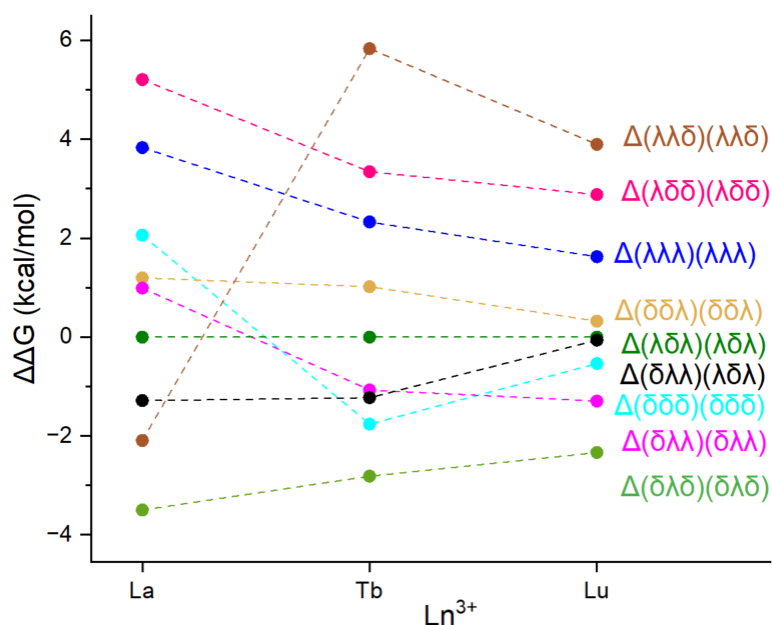


Figure S33. Comparison of relative Gibbs free energies of conformational modes in $[\text{Ln-macropa}]^+$. $\Delta\Delta G$ values relative to $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformation.

6.3. Ligand Strain Analysis

Ligand strain energy ΔG_s° (gas phase standard state) is the standard free energy required to change the free ligand from the relaxed (geometry optimised) conformation, $G^\circ_g(\text{L}^{2-})$, to the conformation found in the Ln^{3+} complex of either KHQ or Macropa in the gas phase, $G^\circ_g(\text{L}_{\text{complex}}^{2-})$. $G^\circ_g(\text{L}_{\text{complex}}^{2-})$ is determined from single point frequency calculations of the frozen ligand structure as found in the metal complex, where the Ln^{3+} ion is removed from the optimised structures of $[\text{Ln-L}]^+$ (where $\text{L} = \text{KHQ}$ or Macropa). It is clear in **Figure S34**, that as the size of the Ln^{3+} ion decreases, ligand strain increases due to a higher degree of folding in the azamacrocyclic ring as the oxygen atoms move closer to accommodate the smaller central metal ion.

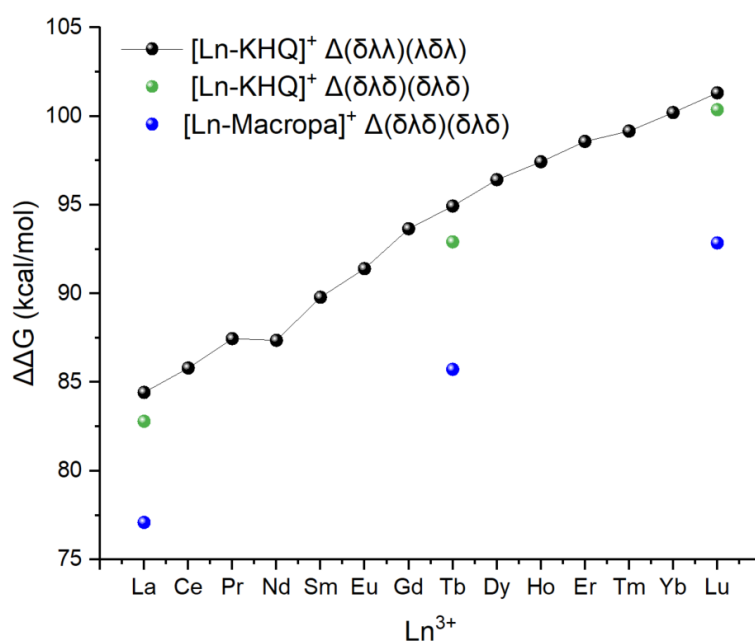


Figure S34. DFT-computed ligand strain energy for $[\text{Ln-KHQ}]^+$ and $[\text{Ln-Macropa}]^+$ complexes.

Table S3. Relative Gibbs free energies for the studied ring conformations of both KHQ and Macropa

Conformation	<i>H₂KHQ</i> , $\Delta\Delta G$ (kcal/mol)			<i>Macropa</i> , $\Delta\Delta G$ (kcal/mol)		
	La	Tb	Lu	La	Tb	Lu
$\Delta(\delta\delta\delta)/(\delta\delta\delta)$	0.735189544	-1.3133199	-1.7640094	2.06274131	-1.7601627	-0.5357797
$\Delta(\delta\delta\lambda)/(\delta\delta\lambda)$	1.309692859	0.09077545	0.4966671	1.197036169	1.01849103	0.32037472
$\Delta(\delta\lambda\delta)/(\delta\lambda\delta)$	-3.57297977	-3.9382088	-2.5607074	-3.497565739	-2.8128844	-2.3351806
$\Delta(\delta\lambda\lambda)/(\delta\lambda\lambda)$	0.203833748	-0.0140939	-0.0771585	0.990742585	-1.0707186	-1.2937479
$\Delta(\lambda\delta\delta)/(\lambda\delta\delta)$	5.608248736	5.05240126	2.62835282	5.205475809	3.34198116	2.88110717
$\Delta(\lambda\delta\lambda)/(\lambda\delta\lambda)$	0	0	0	0	0	0
$\Delta(\lambda\lambda\delta)/(\lambda\lambda\delta)$	5.815107078	6.43620921	5.11767475	-2.091142367	5.83131564	3.89660499
$\Delta(\lambda\lambda\lambda)/(\lambda\lambda\lambda)$	6.29180684	3.42818834	1.45152244	3.831136973	2.32746226	1.62379249
$\Delta(\delta\lambda\lambda)/(\lambda\delta\lambda)$	-1.687735656	-0.8772639	-0.3900533	-1.284743101	-1.2262216	-0.0648782

Table S4. Gas phase comparison of Gibbs free energies of complexation (Equation S3) of [Ln-macropa]⁺ and [Ln-KHQ]⁺. Values given in kcal/mol. $\Delta\Delta G = \Delta G^\circ[\text{Ln-KHQ}] - \Delta G^\circ[\text{Ln-Macropa}]$

<i>Ln</i> ³⁺	$\Delta G^\circ_{[\text{Ln-KHQ}]^+}$	$\Delta G^\circ_{[\text{Ln-Macropa}]^+}$	$\Delta\Delta G$
<i>La</i>	-977.5103024	-978.602168	-1.0918657
<i>Tb</i>	-1029.790587	-1029.894754	-0.1041665
<i>Lu</i>	-1060.424322	-1061.302207	-0.8778851

7. Potentiometric titrations

7.1. Experimental Data

Potentiometric titrations were carried out using a Metrohm Titrando 888 titrator equipped with a combined glass electrode (Metrohm model 6.0260.010) and a Metrohm 801 Stirrer unit. This titration system was controlled by *Tiamo* (ver. 2.34) software. The titration vessel was fitted into a removable glass cell (≈ 70 mL) and thermostated at 25.0 °C ($\text{pKw}(\text{NaCl}, 0.1 \text{ M}) = 13.78$)²⁰ using a circulating water bath. CO₂ was excluded from the vessel prior to and during the titrations by a nitrogen flow, which was passed through an aqueous solution. NaOH (0.1 M) was standardized by potentiometric titration against potassium hydrogen phthalate. Hydrochloric acid (0.1 M) was standardized against Tris (base form). Titration solutions were maintained at a constant ionic strength of 0.1 M with NaCl (prepared by adding 5.8 g NaCl to 1 L de-ionised H₂O). The electrode was calibrated before each titration by titrating a solution of standardized HCl (0.1 M) with standardized NaOH (0.1 M), and the data were analysed using the program *GLEE5* (ver. 3.0.21)²¹ to obtain the standard electrode potential and slope factor.

Ln³⁺ stock solutions were made by dissolving the corresponding chloride salts (98 % purity or higher) in H₂O or standardized HCl (0.1 M, for La³⁺ only). The exact concentrations were determined by complexometric titrations²² with a standardized 0.01 M EDTA solution. The complexometric titrations were performed at pH 5.4 maintained by a HOAc-NaOAc buffer, and the end point was indicated by xylene orange. Ligand aliquots were added directly into the electrolyte solution prior to analysis.

Protonation constant or stability constant determinations were carried out by titrating an acidic solution containing free ligand or both ligand and metal (in 30 mL 0.1 M NaCl) with standardized 0.1 M NaOH. For protonation constant determinations, the ligand concentration was 0.018 mmol. For stability constant determinations, both the ligand and metal ion concentrations were 0.018 mmol. The solutions were inspected throughout the titrations for signs of Ln(OH)₃ precipitation. Titration data were refined with *Hyperquad 2013*²³ software to determine protonation and stability constants. The data points within the pH range of 3 – 10.5 were used for analysis. At least three independent titrations for protonation constant measurements and three titrations for stability constant

measurements were carried out for each L and LnL system. Within the data fitting models for the $[\text{Ln-KHQ}]^+$ complexes, we included the deprotonated complex species (LnLH_{-1} , Figure S31-34), which was necessary to obtain robust fit and values for $\log K_{\text{LnL}}$.

Equilibration between the addition of NaOH aliquots was monitored via the electrode potential. If the system is not at equilibrium, the electrode potential will drift as the system continues to adjust. To ensure that the thermodynamic equilibration is reached after an aliquot of NaOH is added, the next NaOH aliquot was not added until either the electrode drifting is slow (< 0.2 mV/min), or a maximum time limit is reached (2 min for both protonation constant determinations and stability constant determinations).

7.2. Supplementary Data

$$K_{ai} = \frac{[\text{H}_i\text{L}]}{[\text{H}^+][\text{H}_{i-1}\text{L}]}$$

Equation S4. Ligand protonation constants (K_{ai}).
L = fully deprotonated KHQ, i = number of protons

$$K_{\text{LnL}} = \frac{[\text{LnL}]}{[\text{Ln}^{3+}][\text{L}]}$$

Equation S5. Complex stability constants (K_{LnL}).
L = fully deprotonated KHQ, Ln = La, Tb, Lu

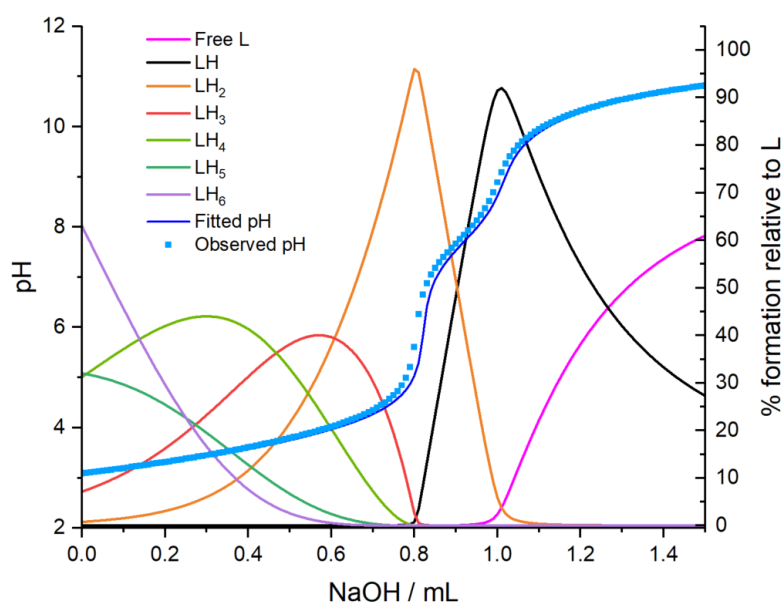


Figure S35. Representative protonation constant determination of H_2KHQ modelled in HySS. H_2KHQ $c = 0.018$ mM. Initial volume $V = 30$ mL. Data fitting and speciation distribution over the pH range shown.

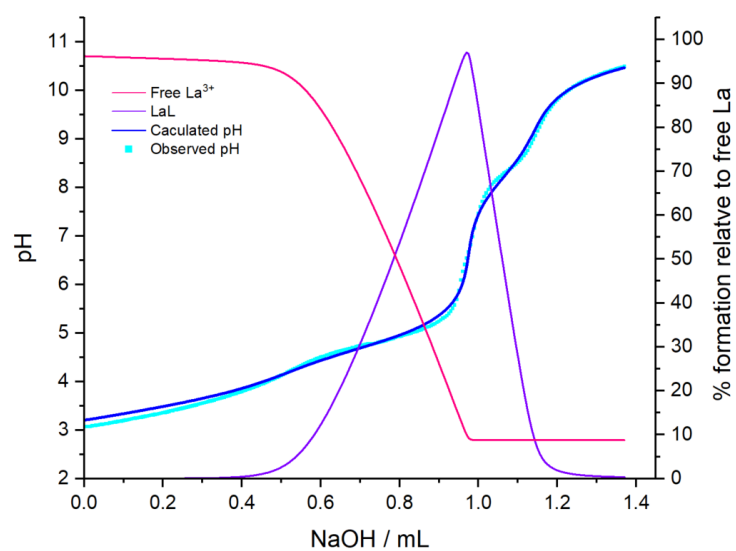


Figure S36. Representative stability constant determination of $[\text{La-KHQ}]^+$ modelled in HySS. H_2KHQ $c = 0.018$ mM, La^{3+} $c = 0.018$ mM. Initial volume $V = 30$ mL. Data fitting and speciation distribution over the pH range shown.

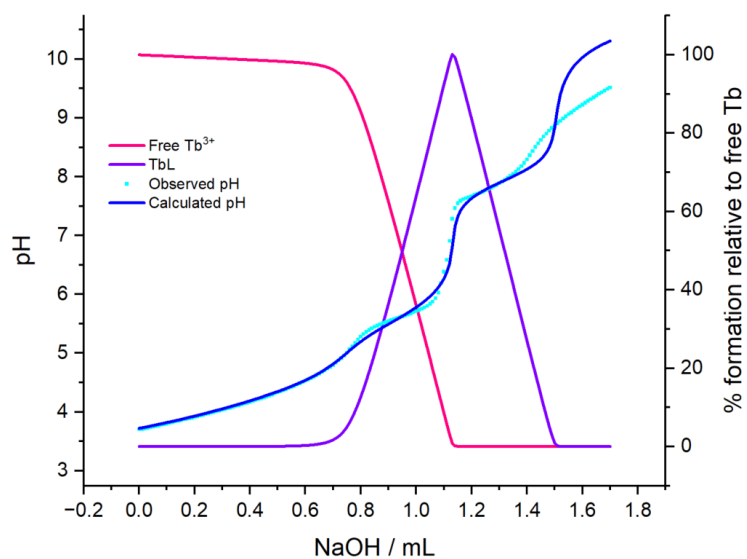


Figure S37. Representative stability constant determination of $[\text{Tb-KHQ}]^+$ modelled in HySS. H_2KHQ $c = 0.018$ mM, Tb^{3+} $c = 0.018$ mM. Initial volume $V = 30$ mL. Data fitting and speciation distribution over the pH range shown.

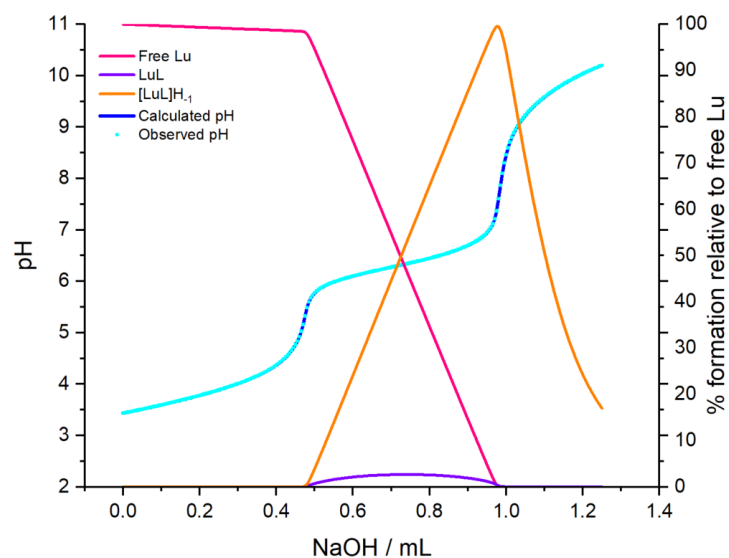


Figure S38. Representative stability constant determination of $[\text{Lu-KHQ}]^+$ modelled in HySS. H_2KHQ $c = 0.018$ mM, Lu^{3+} $c = 0.018$ mM. Initial volume $V = 30$ mL. Data fitting and speciation distribution over the pH range shown.

8. UV-Vis Spectroscopy and Phosphorescence

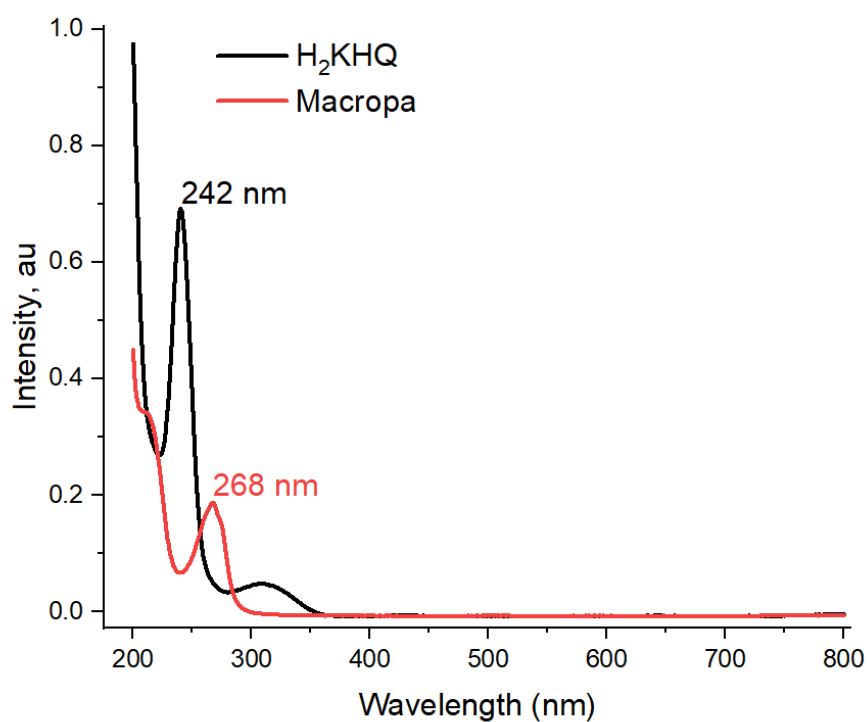


Figure S39. UV-Vis spectrum showing the absorption wavelengths of H_2KHQ and **macropa**. (20 μM , 10 nm slits, H_2O).

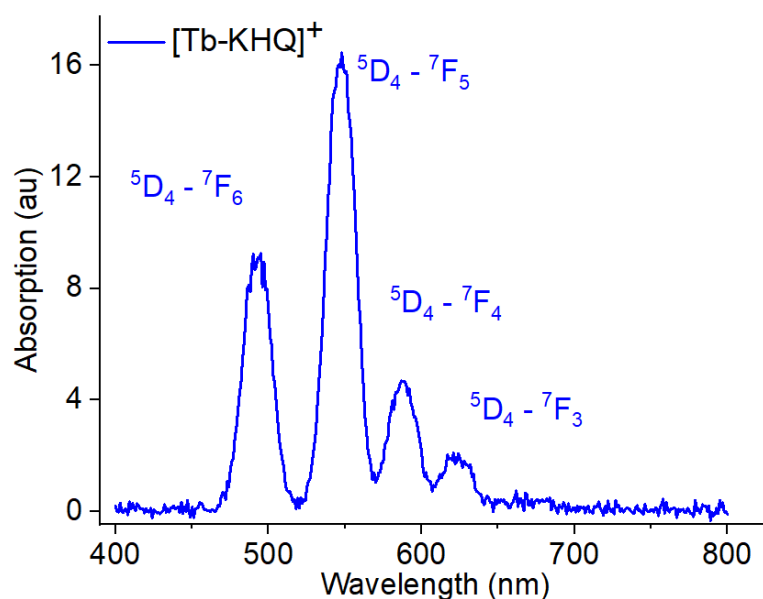


Figure S40. Phosphorescence spectrum for $[\text{Tb-KHQ}]^+$ (H_2O , 20 μM , 20 nm slits, 0.1 ms delay).

9. Radiolabelling

9.1. Experimental Details

Caution: ^{161}Tb emits ionizing radiation and should only be used in a facility in accordance with appropriate safety controls.

Radiolabelling studies of H_2KHQ with $^{161}\text{Tb}^{3+}$ were performed to establish suitable labelling conditions. A 2.5 mM stock solution of H_2KHQ was made by dissolving H_2KHQ in 20 mM NH_4OAc buffer (20 mM, pH 8.5). For labelling experiments, $^{161}\text{Tb}^{3+}$ (1 mM HCl, 2.5 MBq, 10 μL) was added to a solution of H_2KHQ (concentration 1 mM). $V_T = 100 \mu\text{L}$. Reactions were allowed to stand at room temperature or 90 °C for 20 min – 180 min and then monitored by radio-HPLC using mobile phase A: 2mM NH_4OAc in H_2O and mobile phase B: 5 % 2 mM NH_4OAc in H_2O in 95 % MeCN. Gradients are as shown below. Analytical reverse-phase radio-HPLC was performed on an Agilent 1200 Series Liquid Chromatograph (with UV and gamma detectors) using an Agilent Eclipse XDB-C18 column (4.6 $\times$ 150 mm, 5 μm) with a 1 mL/min⁻¹ flow rate and UV spectroscopic detection at 254 nm. Under these conditions $^{161}\text{Tb}^{3+}[\text{Tb-KHQ}]^+$ eluted at 18.33 min while free $^{161}\text{Tb}^{3+}$ eluted during the aqueous phase washes at 1.33 and 29.30 min.

Gradient, min	A, %	B, %
0.00	95	5
5.00	95	5
30.00	5	95
30.10	95	5
33.00	95	5

Radiolabelling studies of **macropa** with $^{161}\text{Tb}^{3+}$ were performed to establish suitable labelling conditions. A 10 mM stock solution of **macropa** was made by dissolving **macropa** in 200 mM NH_4OAc buffer (20 mM, pH 6.5). For labelling experiments, $^{161}\text{Tb}^{3+}$ (2 mM HCl, 5 MBq, 10 μL) was added to a solution of **macropa** (concentration 1 mM). $V_T = 100 \mu\text{L}$. Reactions were allowed to stand at room temperature or 90 °C for 30 min and then monitored by radio-HPLC using mobile phase A: 2mM NH_4OAc in H_2O and mobile phase B: 5 % 2 mM NH_4OAc in H_2O in 95 % MeCN. Gradients are as shown below. Analytical reverse-phase radio-HPLC was performed on an Agilent 1200 Series Liquid Chromatograph (with UV and gamma detectors) using an Agilent Eclipse XDB-C18 column (4.6 $\times$ 150 mm, 5 μm) with a 1 mL/min⁻¹ flow rate and UV spectroscopic detection at 254 nm. Under these conditions $^{161}\text{Tb}^{3+}[\text{Tb-macropa}]^+$ eluted at 11.1 min while free $^{161}\text{Tb}^{3+}$ eluted during the aqueous phase washes at 1.37 and 32.50 min.

Gradient, min	A, %	B, %
0.00	95	5
5.00	95	5
25.00	5	95
30.00	5	95
32.000	95	5
35.00	95	5

9.2. Supplementary Data

Table S5. The RCY values for non-carried added radiolabelling of **H₂KHQ** with ¹⁶¹Tb[Tb³⁺] in NH₄OAc buffer (20 mM, pH 8.5) at room temperature and 90 °C for 20 min – 180 min.

Time, min	Temperature	RCY, %
20	Room temperature	33
180	Room temperature	68
20	90 °C	92

Table S6. The RCY values for non-carried added radiolabelling of **macropa** with ¹⁶¹Tb[Tb³⁺] in NH₄OAc buffer (200 mM, pH 6.5) at room temperature and 90 °C for 20 min – 180 min.

Time, min	Temperature	RCY, %
30	Room temperature	62
30	90 °C	55

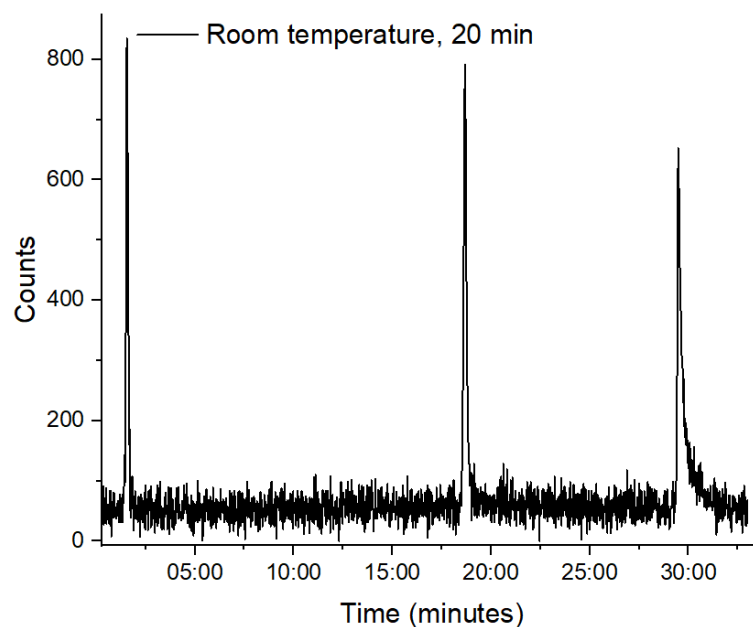


Figure S41. RadioHPLC of H_2KHQ (1 mM, 20 mM NH_4OAc , pH 8.5) with $^{161}\text{Tb}[\text{Tb}^{3+}]$ (3 MBq, 1mM HCl) after 20 minutes at room temperature. RCY = 33 %. $^{161}\text{Tb}[\text{Tb-KHQ}]^+$ retention time = 18.4 min and free $^{161}\text{Tb}[\text{Tb}^{3+}]$ retention time = 1.3 and 29.3 min.

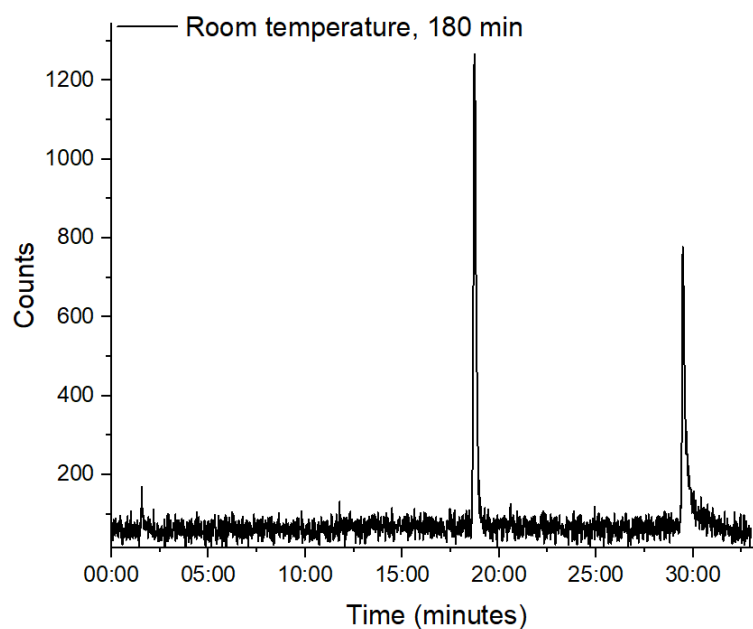


Figure S42. RadioHPLC of H_2KHQ (1 mM, 20 mM NH_4OAc , pH 8.5) with $^{161}\text{Tb}[\text{Tb}^{3+}]$ (3 MBq, 1mM HCl) after 180 minutes at room temperature. RCY = 66 %. $^{161}\text{Tb}[\text{Tb-KHQ}]^+$ retention time = 18.4 min and free $^{161}\text{Tb}[\text{Tb}^{3+}]$ retention time = 1.3 and 29.3 min.

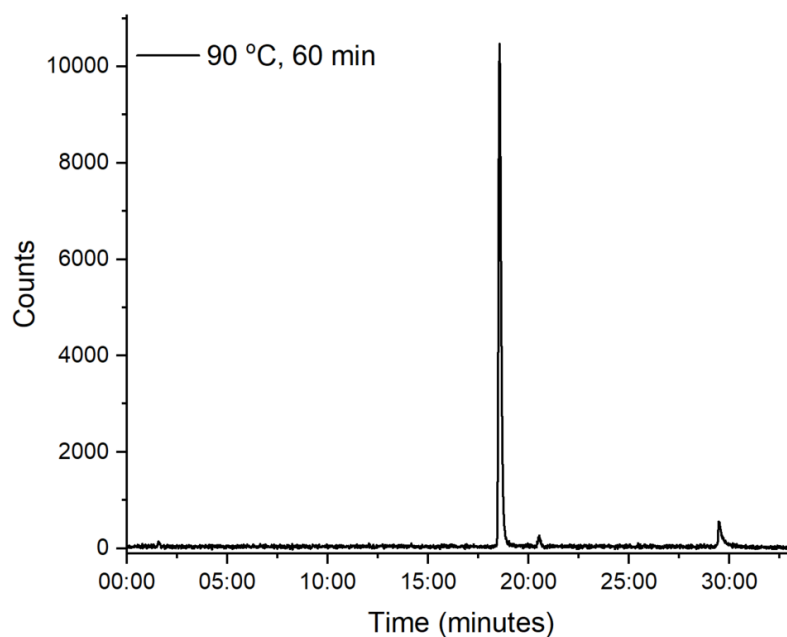


Figure S43. RadioHPLC of **H₂KHQ** (1 mM, 20 mM NH₄OAc, pH 8.5) with ¹⁶¹Tb[Tb³⁺] (3 MBq, 1mM HCl) after 60 minutes at 90 °C. RCY = 92 %. [¹⁶¹Tb][Tb-KHQ]⁺ retention time = 18.3 min and free [¹⁶¹Tb]Tb³⁺ retention time = 29.3 min.

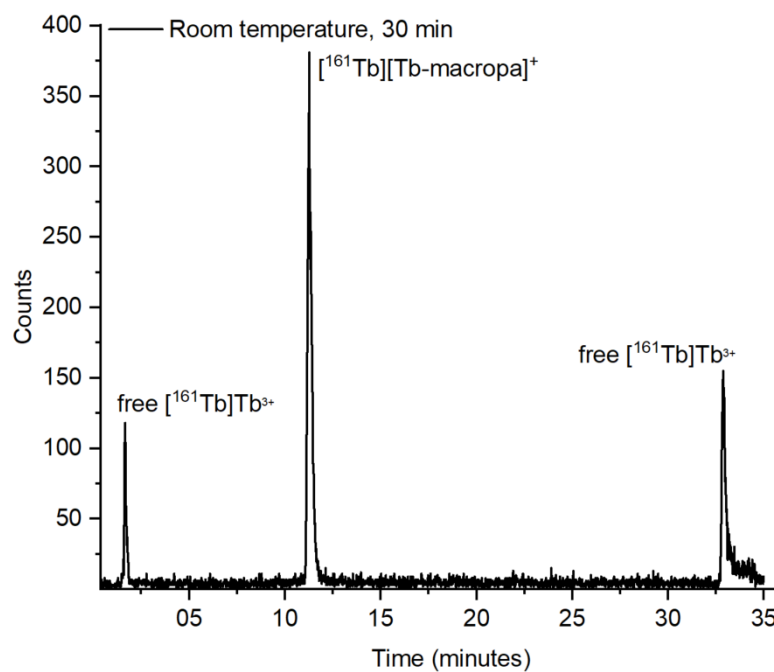


Figure S 44. RadioHPLC of **macropa** (1 mM) with [¹⁶¹Tb]Tb³⁺ (5 MBq, 2 mM HCl) after 30 min at 25 °C. RCY = 62 %. [¹⁶¹Tb][Tb-macropa]⁺ retention time = 11.1 min and free [¹⁶¹Tb]Tb³⁺ retention time = 1.3 and 30.3 min.

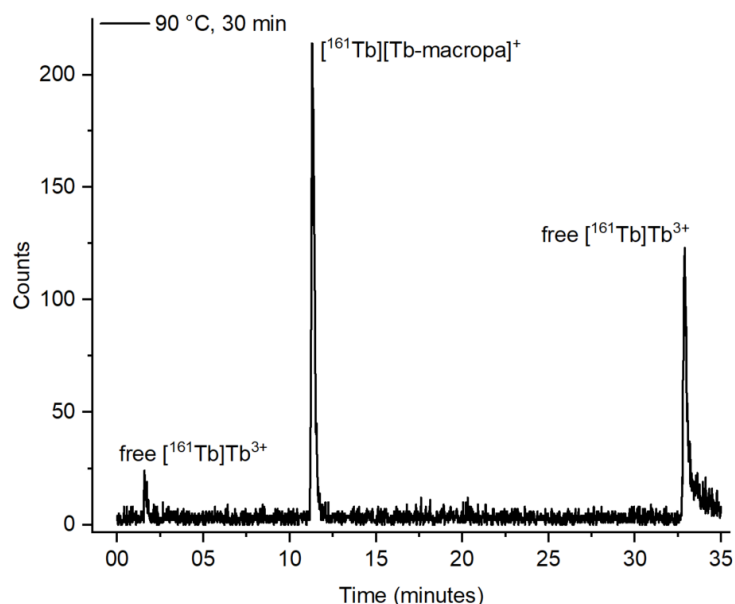


Figure S 45. RadioHPLC of **macropa** (1 mM) with $[^{161}\text{Tb}]\text{Tb}^{3+}$ (5 MBq, 2 mM HCl) after 30 min at 25 °C. RCY = 55 %. $[^{161}\text{Tb}][\text{Tb-macropa}]^+$ retention time = 11.1 min and free $[^{161}\text{Tb}]\text{Tb}^{3+}$ retention time = 1.3 and 30.3 min.

10. References

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11.XYZ Coordinates

Ce-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.50741294

E(SCF)+ZPE(0 K)= -1909.841038

H(298 K)= -1909.807021

G(298 K)= -1909.902171

Lowest Frequency = -50.0982cm⁻¹

C	5.839215	1.391568	17.400938
C	5.673871	1.621101	18.792816
C	5.296247	0.499050	19.575289
H	5.169540	0.617177	20.654405
C	5.057829	-0.713839	18.974486
H	4.723824	-1.574013	19.558321
C	5.236245	-0.837094	17.575066
C	4.815193	-2.094441	16.852618
H	4.955824	-2.976730	17.502110
H	3.722164	-2.017820	16.724715
C	4.466803	-2.479190	14.476246
H	3.711114	-3.244030	14.744697
H	5.013967	-2.821186	13.588921
C	3.748063	-1.194539	14.106094
H	2.983899	-1.428285	13.346112
H	3.236764	-0.733110	14.970192
C	4.208077	0.712336	12.677334
H	3.943999	1.623437	13.240164
H	3.316866	0.347929	12.140248
C	5.304495	1.005426	11.676165
H	5.522228	0.115570	11.060554
H	4.981635	1.827879	11.016529
C	7.369666	2.273664	11.777042
H	6.807751	3.015908	11.185542
H	8.028670	1.721330	11.086877
C	6.457424	-3.342896	15.576012
H	6.871113	-3.426863	14.562872
H	6.026528	-4.324085	15.863246
N	5.660964	0.166408	16.839616
N	5.445029	-2.287279	15.549093
O	6.296926	2.195571	15.226536
O	4.685115	-0.279219	13.565759
O	6.459311	1.385107	12.399845
C	7.763561	-2.226629	12.043133
C	8.874068	-1.371465	11.713481
C	9.691958	-1.634301	10.581509
C	10.722892	-0.698898	10.314903
H	11.377476	-0.851962	9.453360
C	10.877822	0.400268	11.123475
H	11.649735	1.144633	10.919687
C	10.017105	0.566336	12.234239
C	10.179320	1.747691	13.154698
H	10.682152	2.577107	12.619633
H	10.872823	1.440558	13.951969
C	9.180836	2.925607	15.006443
H	9.873651	3.777721	14.853550
H	8.222535	3.330268	15.343041
C	9.759867	2.054325	16.102217

H	9.683578	2.593057	17.062131
H	10.828456	1.834381	15.929888
C	9.741260	-0.126531	16.989721
H	10.582948	-0.550716	16.412475
H	10.147460	0.355079	17.895182
C	8.789363	-1.208020	17.417418
H	8.021343	-0.804054	18.102772
H	9.363987	-1.982142	17.953302
C	7.566903	-3.031767	16.556148
H	8.340816	-3.815381	16.500142
H	7.183381	-3.015959	17.591263
C	8.125055	3.026866	12.857172
H	7.370600	3.530737	13.475626
H	8.752417	3.799931	12.370117
N	9.069065	-0.297722	12.526872
N	8.929805	2.195621	13.762383
O	9.057018	0.821785	16.194253
O	8.157444	-1.764072	16.278824
O	7.029941	-1.916042	13.069044
C	7.547444	-3.333366	11.224052
H	6.710369	-3.995894	11.453980
C	8.378390	-3.597962	10.116077
H	8.170338	-4.478472	9.503570
C	9.432540	-2.775448	9.782385
H	10.061863	-2.983450	8.915535
C	6.155502	2.465732	16.487384
C	6.299225	3.736915	17.049423
H	6.495755	4.581425	16.384990
C	6.164041	3.949484	18.437087
H	6.289325	4.963607	18.824349
C	5.864732	2.926004	19.310907
H	5.748147	3.108739	20.380374

Ce-anti-KHQ(1+)

SCF (RwB97XD) = -1943.05035903
 E(SCF)+ZPE(0 K)= -1942.368398
 H(298 K)= -1942.331048
 G(298 K)= -1942.434339
 Lowest Frequency = 15.5893cm⁻¹

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C	5.673871	1.621101	18.792816
C	5.296247	0.499050	19.575289
H	5.169540	0.617177	20.654405
C	5.057829	-0.713839	18.974486
H	4.723824	-1.574013	19.558321
C	5.236245	-0.837094	17.575066
C	4.815193	-2.094441	16.852618
H	4.955824	-2.976730	17.502110
H	3.722164	-2.017820	16.724715
C	4.466803	-2.479190	14.476246
H	3.711114	-3.244030	14.744697
H	5.013967	-2.821186	13.588921
C	3.748063	-1.194539	14.106094
H	2.983899	-1.428285	13.346112
H	3.236764	-0.733110	14.970192

C	4.208077	0.712336	12.677334
H	3.943999	1.623437	13.240164
H	3.316866	0.347929	12.140248
C	5.304495	1.005426	11.676165
H	5.522228	0.115570	11.060554
H	4.981635	1.827879	11.016529
C	7.369666	2.273664	11.777042
H	6.807751	3.015908	11.185542
H	8.028670	1.721330	11.086877
C	6.457424	-3.342896	15.576012
H	6.871113	-3.426863	14.562872
H	6.026528	-4.324085	15.863246
N	5.660964	0.166408	16.839616
N	5.445029	-2.287279	15.549093
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C	10.722892	-0.698898	10.314903
H	11.377476	-0.851962	9.453360
C	10.877822	0.400268	11.123475
H	11.649735	1.144633	10.919687
C	10.017105	0.566336	12.234239
C	10.179320	1.747691	13.154698
H	10.682152	2.577107	12.619633
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C	9.180836	2.925607	15.006443
H	9.873651	3.777721	14.853550
H	8.222535	3.330268	15.343041
C	9.759867	2.054325	16.102217
H	9.683578	2.593057	17.062131
H	10.828456	1.834381	15.929888
C	9.741260	-0.126531	16.989721
H	10.582948	-0.550716	16.412475
H	10.147460	0.355079	17.895182
C	8.789363	-1.208020	17.417418
H	8.021343	-0.804054	18.102772
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C	7.566903	-3.031767	16.556148
H	8.340816	-3.815381	16.500142
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H	7.370600	3.530737	13.475626
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O	8.157444	-1.764072	16.278824
O	7.029941	-1.916042	13.069044
C	7.547444	-3.333366	11.224052
H	6.710369	-3.995894	11.453980
C	8.378390	-3.597962	10.116077
H	8.170338	-4.478472	9.503570
C	9.432540	-2.775448	9.782385
H	10.061863	-2.983450	8.915535

C	6.155502	2.465732	16.487384
C	6.299225	3.736915	17.049423
H	6.495755	4.581425	16.384990
C	6.164041	3.949484	18.437087
H	6.289325	4.963607	18.824349
C	5.864732	2.926004	19.310907
H	5.748147	3.108739	20.380374
Ce	7.101623	0.004712	14.512866

Ce3+_Ion

SCF (RwB97XD) = -30.8172967268
 E(SCF)+ZPE(0 K)= -30.817297
 H(298 K)= -30.814936
 G(298 K)= -30.834283

Ce	0.887400	3.945900	9.220400
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Ce-syn-KHQ_Ligand(2-)

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 E(SCF)+ZPE(0 K)= -1909.846041
 H(298 K)= -1909.810738
 G(298 K)= -1909.909183
 Lowest Frequency = -37.7082cm⁻¹

N	3.120387	2.590545	9.213233
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C	4.249211	0.621776	9.912644
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C	5.341511	1.364971	10.296833
H	6.209164	0.874121	10.744240
C	5.369729	2.770223	10.092519
C	4.204490	3.340674	9.527197
C	4.093030	4.752139	9.245957
O	2.962678	5.203360	8.775381
C	5.210775	5.530306	9.538387
H	5.181501	6.599185	9.314229
C	6.369440	4.959873	10.111882
H	7.216606	5.614163	10.331460
C	6.466122	3.615627	10.399862
H	7.370829	3.194908	10.841731
N	1.910260	4.436571	11.584699
C	2.522639	5.554144	11.903434
C	3.500551	5.589948	12.924397
H	4.007470	6.527192	13.159534
C	3.807878	4.430185	13.595932
H	4.573559	4.432272	14.375444
C	3.119416	3.223282	13.302581
C	2.152441	3.292076	12.271891
C	1.365876	2.149991	11.879347
O	0.527926	2.290495	10.888757
C	1.592171	0.967376	12.578533
H	0.999659	0.084751	12.326687
C	2.565905	0.898648	13.599900
H	2.713345	-0.053329	14.115610
C	3.328336	1.986983	13.965305

H	4.074213	1.914712	14.758557
C	1.893616	0.546618	8.899406
H	2.181869	-0.430985	8.463916
H	1.272897	0.348186	9.784810
N	1.098272	1.331518	7.946146
C	1.811341	1.464369	6.672099
H	1.810156	0.510480	6.107755
H	2.857342	1.714306	6.890556
C	1.252214	2.551077	5.779561
H	1.914009	2.653640	4.902035
H	0.242004	2.313518	5.398900
O	1.210143	3.769583	6.493442
C	0.982172	4.897687	5.674259
H	-0.022716	4.830960	5.218425
H	1.731676	4.937325	4.864596
C	1.103386	6.141784	6.513517
H	2.121988	6.227067	6.927931
H	0.873748	7.019450	5.886758
O	0.160786	6.042847	7.575569
C	-0.183514	7.264457	8.204961
H	-1.217481	7.148877	8.546108
H	-0.183281	8.078862	7.461101
C	0.768186	7.639035	9.333963
H	1.770473	7.754130	8.898038
H	0.469798	8.632732	9.726438
N	0.874886	6.645692	10.404030
C	2.159622	6.782688	11.104439
H	2.164338	7.671247	11.766290
H	2.942730	6.926471	10.348111
C	-0.214193	6.687671	11.382973
H	-0.347211	7.709097	11.793498
H	0.077788	6.038121	12.218296
C	-1.562125	6.206391	10.880251
H	-2.213171	6.031343	11.754369
H	-2.068827	6.957615	10.250367
O	-1.398565	5.000975	10.158780
C	-2.605431	4.407515	9.711442
H	-2.857249	4.787409	8.704910
H	-3.431329	4.665527	10.394462
C	-2.447878	2.910544	9.707538
H	-2.174178	2.564564	10.719871
H	-3.407961	2.447847	9.416763
O	-1.434304	2.532830	8.796067
C	-1.231588	1.123101	8.810813
H	-2.188387	0.617444	8.591812
H	-0.889667	0.831741	9.816348
C	-0.230314	0.747377	7.745454
H	-0.176368	-0.357079	7.684232
H	-0.625364	1.094108	6.780947

Ce-syn-KHQ(1+)

SCF (RwB97XD) = -1943.06342609

E(SCF)+ZPE(0 K)= -1942.380887

H(298 K)= -1942.343934

G(298 K)= -1942.444617

Lowest Frequency = 35.6606cm⁻¹

Ce	0.907874	3.974727	9.194455
N	3.120387	2.590545	9.213233
C	3.132225	1.284401	9.354883
C	4.249211	0.621776	9.912644
H	4.233545	-0.461754	10.040348
C	5.341511	1.364971	10.296833
H	6.209164	0.874121	10.744240
C	5.369729	2.770223	10.092519
C	4.204490	3.340674	9.527197
C	4.093030	4.752139	9.245957
O	2.962678	5.203360	8.775381
C	5.210775	5.530306	9.538387
H	5.181501	6.599185	9.314229
C	6.369440	4.959873	10.111882
H	7.216606	5.614163	10.331460
C	6.466122	3.615627	10.399862
H	7.370829	3.194908	10.841731
N	1.910260	4.436571	11.584699
C	2.522639	5.554144	11.903434
C	3.500551	5.589948	12.924397
H	4.007470	6.527192	13.159534
C	3.807878	4.430185	13.595932
H	4.573559	4.432272	14.375444
C	3.119416	3.223282	13.302581
C	2.152441	3.292076	12.271891
C	1.365876	2.149991	11.879347
O	0.527926	2.290495	10.888757
C	1.592171	0.967376	12.578533
H	0.999659	0.084751	12.326687
C	2.565905	0.898648	13.599900
H	2.713345	-0.053329	14.115610
C	3.328336	1.986983	13.965305
H	4.074213	1.914712	14.758557
C	1.893616	0.546618	8.899406
H	2.181869	-0.430985	8.463916
H	1.272897	0.348186	9.784810
N	1.098272	1.331518	7.946146
C	1.811341	1.464369	6.672099
H	1.810156	0.510480	6.107755
H	2.857342	1.714306	6.890556
C	1.252214	2.551077	5.779561
H	1.914009	2.653640	4.902035
H	0.242004	2.313518	5.398900
O	1.210143	3.769583	6.493442
C	0.982172	4.897687	5.674259
H	-0.022716	4.830960	5.218425
H	1.731676	4.937325	4.864596
C	1.103386	6.141784	6.513517
H	2.121988	6.227067	6.927931
H	0.873748	7.019450	5.886758
O	0.160786	6.042847	7.575569
C	-0.183514	7.264457	8.204961
H	-1.217481	7.148877	8.546108
H	-0.183281	8.078862	7.461101
C	0.768186	7.639035	9.333963
H	1.770473	7.754130	8.898038

H	0.469798	8.632732	9.726438
N	0.874886	6.645692	10.404030
C	2.159622	6.782688	11.104439
H	2.164338	7.671247	11.766290
H	2.942730	6.926471	10.348111
C	-0.214193	6.687671	11.382973
H	-0.347211	7.709097	11.793498
H	0.077788	6.038121	12.218296
C	-1.562125	6.206391	10.880251
H	-2.213171	6.031343	11.754369
H	-2.068827	6.957615	10.250367
O	-1.398565	5.000975	10.158780
C	-2.605431	4.407515	9.711442
H	-2.857249	4.787409	8.704910
H	-3.431329	4.665527	10.394462
C	-2.447878	2.910544	9.707538
H	-2.174178	2.564564	10.719871
H	-3.407961	2.447847	9.416763
O	-1.434304	2.532830	8.796067
C	-1.231588	1.123101	8.810813
H	-2.188387	0.617444	8.591812
H	-0.889667	0.831741	9.816348
C	-0.230314	0.747377	7.745454
H	-0.176368	-0.357079	7.684232
H	-0.625364	1.094108	6.780947

Ce-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2019.42687097
 E(SCF)+ZPE(0 K)= -2018.718659
 H(298 K)= -2018.679328
 G(298 K)= -2018.783906
 Lowest Frequency = 32.2166cm⁻¹

Ce	0.903315	4.000833	9.071929
N	3.103868	2.580916	9.117116
C	3.108503	1.269641	9.197786
C	4.228522	0.569794	9.702379
H	4.206376	-0.519296	9.767383
C	5.329313	1.281788	10.116571
H	6.199747	0.761945	10.524065
C	5.357427	2.696581	10.003921
C	4.192734	3.305322	9.476086
C	4.090510	4.733184	9.292798
O	2.972699	5.224304	8.834346
C	5.204980	5.487346	9.652576
H	5.176258	6.569896	9.507810
C	6.361054	4.876926	10.187443
H	7.206972	5.512645	10.459888
C	6.455234	3.514958	10.372391
H	7.356958	3.060547	10.786105
N	1.814701	4.481215	11.546299
C	2.348435	5.619451	11.924854
C	3.220400	5.699339	13.036830
H	3.650546	6.661346	13.320606
C	3.525754	4.554666	13.731427
H	4.210930	4.589725	14.581849

C	2.941078	3.316097	13.359702
C	2.066094	3.345346	12.246770
C	1.390184	2.161478	11.782768
O	0.614471	2.265195	10.742211
C	1.637188	0.981106	12.479742
H	1.129488	0.066462	12.164049
C	2.521214	0.954647	13.580586
H	2.688683	0.004555	14.093609
C	3.170924	2.085127	14.025306
H	3.848672	2.049215	14.879828
C	1.855015	0.550361	8.759138
H	2.124984	-0.410207	8.276522
H	1.278914	0.318877	9.664125
N	1.019246	1.362946	7.864319
C	1.691202	1.480662	6.559941
H	1.549857	0.558302	5.963002
H	2.768814	1.587142	6.740426
C	1.254225	2.664794	5.728589
H	1.798430	2.629976	4.768231
H	0.172533	2.643569	5.503604
O	1.564115	3.861891	6.410333
C	1.407163	5.007935	5.602045
H	0.433029	4.963181	5.080456
H	2.204481	5.043316	4.838316
C	1.477443	6.256481	6.444399
H	2.434241	6.297539	6.989828
H	1.377759	7.133348	5.781786
O	0.395340	6.225333	7.369952
C	0.062562	7.452606	7.983686
H	-1.008159	7.400859	8.223238
H	0.186537	8.282369	7.266303
C	0.907026	7.739637	9.211306
H	1.952835	7.797116	8.880583
H	0.634496	8.740866	9.603128
N	0.846372	6.719977	10.263344
C	2.060082	6.834707	11.084815
H	2.019431	7.735301	11.729120
H	2.912681	6.953210	10.403299
C	-0.335348	6.811027	11.127361
H	-0.571449	7.867074	11.369001
H	-0.088501	6.312580	12.074960
C	-1.606786	6.156011	10.618937
H	-2.366934	6.262465	11.412435
H	-2.018127	6.645637	9.719272
O	-1.387501	4.782527	10.356810
C	-2.574759	4.010118	10.366730
H	-3.228027	4.315228	9.525925
H	-3.129931	4.198141	11.302034
C	-2.261799	2.535995	10.297048
H	-1.595589	2.250042	11.126032
H	-3.211074	1.974581	10.367582
O	-1.613361	2.255379	9.073028
C	-1.235100	0.899574	8.905269
H	-2.135841	0.285345	8.726276
H	-0.748089	0.555305	9.829107
C	-0.313701	0.767126	7.706492
H	-0.228441	-0.311094	7.462744

H	-0.803440	1.242984	6.843855
O	-1.139874	4.002695	7.273416
H	-1.804228	3.427682	7.686220
H	-1.540678	4.822377	6.971335

Dy-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.48319972
 E(SCF)+ZPE(0 K)= -1909.817631
 H(298 K)= -1909.783201
 G(298 K)= -1909.881087
 Lowest Frequency = -76.3671cm⁻¹

C	5.784349	1.423899	17.325255
C	5.435402	1.678492	18.676013
C	5.110831	0.545787	19.467534
H	4.831747	0.684551	20.514941
C	5.109804	-0.705562	18.904941
H	4.817865	-1.583415	19.484850
C	5.489321	-0.855929	17.547746
C	5.480964	-2.224163	16.914123
H	6.319359	-2.794835	17.343355
H	4.571286	-2.764975	17.241679
C	4.302554	-2.148552	14.771277
H	3.555761	-2.810504	15.252457
H	4.465399	-2.504588	13.745930
C	3.712776	-0.751610	14.656923
H	2.753616	-0.826620	14.118698
H	3.519140	-0.284452	15.636732
C	4.116126	1.063893	13.063065
H	4.017443	2.002600	13.632357
H	3.134727	0.772637	12.654283
C	5.101990	1.232686	11.922104
H	5.149101	0.316380	11.311194
H	4.786456	2.081222	11.293131
C	7.319141	2.261500	11.770963
H	6.793511	2.960887	11.100278
H	7.948128	1.601789	11.150801
C	6.401094	-3.334691	14.984130
H	6.332125	-3.344590	13.894645
H	6.028316	-4.310502	15.355325
N	5.855368	0.165644	16.808175
N	5.594826	-2.214799	15.461762
O	6.292706	2.198554	15.162688
O	4.612797	0.045209	13.910521
O	6.372595	1.492330	12.488266
C	7.572850	-2.059962	12.118363
C	8.864059	-1.429110	12.038843
C	9.907364	-1.975070	11.248510
C	11.097332	-1.206754	11.157779
H	11.932531	-1.578456	10.559048
C	11.176257	0.010698	11.785695
H	12.065242	0.637261	11.689486
C	10.082275	0.460644	12.566084
C	10.151378	1.800842	13.253444
H	10.617924	2.533403	12.565674
H	10.859310	1.708818	14.092011

C	9.031053	3.004433	15.013630
H	9.775333	3.822750	14.940669
H	8.065915	3.452575	15.257272
C	9.464088	2.079328	16.150323
H	9.120494	2.493506	17.111457
H	10.562201	2.000640	16.193145
C	9.856851	-0.264011	16.314188
H	10.570814	-0.388363	15.479319
H	10.420435	-0.009623	17.226691
C	9.116941	-1.548689	16.564574
H	8.498909	-1.464311	17.477346
H	9.860195	-2.349050	16.713118
C	7.865209	-3.205743	15.400736
H	8.500585	-3.746664	14.681618
H	8.029289	-3.652837	16.394328
C	8.121115	3.078348	12.772244
H	7.398060	3.685422	13.331836
H	8.788827	3.764967	12.215410
N	8.992638	-0.256367	12.719435
N	8.871575	2.286108	13.752411
O	8.933613	0.760667	15.998331
O	8.286363	-1.841038	15.456926
O	6.645648	-1.483612	12.818714
C	7.414206	-3.262989	11.428355
H	6.438535	-3.753485	11.451152
C	8.471511	-3.822479	10.681396
H	8.299635	-4.765154	10.156381
C	9.700520	-3.206189	10.578398
H	10.502318	-3.637784	9.977101
C	6.026151	2.496744	16.396601
C	5.956978	3.796412	16.901553
H	6.112400	4.632123	16.215643
C	5.653892	4.039237	18.257248
H	5.609147	5.073657	18.606243
C	5.392852	3.015458	19.143058
H	5.135547	3.218423	20.183885

Dy-anti-KHQ(1+)

SCF (RwB97XD) = -1947.89729577

E(SCF)+ZPE(0 K)= -1947.214853

H(298 K)= -1947.177531

G(298 K)= -1947.280724

Lowest Frequency = 18.9282cm⁻¹

C	5.784349	1.423899	17.325255
C	5.435402	1.678492	18.676013
C	5.110831	0.545787	19.467534
H	4.831747	0.684551	20.514941
C	5.109804	-0.705562	18.904941
H	4.817865	-1.583415	19.484850
C	5.489321	-0.855929	17.547746
C	5.480964	-2.224163	16.914123
H	6.319359	-2.794835	17.343355
H	4.571286	-2.764975	17.241679
C	4.302554	-2.148552	14.771277
H	3.555761	-2.810504	15.252457

H	4.465399	-2.504588	13.745930
C	3.712776	-0.751610	14.656923
H	2.753616	-0.826620	14.118698
H	3.519140	-0.284452	15.636732
C	4.116126	1.063893	13.063065
H	4.017443	2.002600	13.632357
H	3.134727	0.772637	12.654283
C	5.101990	1.232686	11.922104
H	5.149101	0.316380	11.311194
H	4.786456	2.081222	11.293131
C	7.319141	2.261500	11.770963
H	6.793511	2.960887	11.100278
H	7.948128	1.601789	11.150801
C	6.401094	-3.334691	14.984130
H	6.332125	-3.344590	13.894645
H	6.028316	-4.310502	15.355325
N	5.855368	0.165644	16.808175
N	5.594826	-2.214799	15.461762
O	6.292706	2.198554	15.162688
O	4.612797	0.045209	13.910521
O	6.372595	1.492330	12.488266
C	7.572850	-2.059962	12.118363
C	8.864059	-1.429110	12.038843
C	9.907364	-1.975070	11.248510
C	11.097332	-1.206754	11.157779
H	11.932531	-1.578456	10.559048
C	11.176257	0.010698	11.785695
H	12.065242	0.637261	11.689486
C	10.082275	0.460644	12.566084
C	10.151378	1.800842	13.253444
H	10.617924	2.533403	12.565674
H	10.859310	1.708818	14.092011
C	9.031053	3.004433	15.013630
H	9.775333	3.822750	14.940669
H	8.065915	3.452575	15.257272
C	9.464088	2.079328	16.150323
H	9.120494	2.493506	17.111457
H	10.562201	2.000640	16.193145
C	9.856851	-0.264011	16.314188
H	10.570814	-0.388363	15.479319
H	10.420435	-0.009623	17.226691
C	9.116941	-1.548689	16.564574
H	8.498909	-1.464311	17.477346
H	9.860195	-2.349050	16.713118
C	7.865209	-3.205743	15.400736
H	8.500585	-3.746664	14.681618
H	8.029289	-3.652837	16.394328
C	8.121115	3.078348	12.772244
H	7.398060	3.685422	13.331836
H	8.788827	3.764967	12.215410
N	8.992638	-0.256367	12.719435
N	8.871575	2.286108	13.752411
O	8.933613	0.760667	15.998331
O	8.286363	-1.841038	15.456926
O	6.645648	-1.483612	12.818714
C	7.414206	-3.262989	11.428355
H	6.438535	-3.753485	11.451152

C	8.471511	-3.822479	10.681396
H	8.299635	-4.765154	10.156381
C	9.700520	-3.206189	10.578398
H	10.502318	-3.637784	9.977101
C	6.026151	2.496744	16.396601
C	5.956978	3.796412	16.901553
H	6.112400	4.632123	16.215643
C	5.653892	4.039237	18.257248
H	5.609147	5.073657	18.606243
C	5.392852	3.015458	19.143058
H	5.135547	3.218423	20.183885
Dy	7.009308	0.130182	14.427695

Dy3+_lon

SCF (RwB97XD) = -35.5745387418
 E(SCF)+ZPE(0 K)= -35.574539
 H(298 K)= -35.572178
 G(298 K)= -35.591750

Dy	0.887400	3.945900	9.220400
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Dy-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.49860017
 E(SCF)+ZPE(0 K)= -1909.830380
 H(298 K)= -1909.795428
 G(298 K)= -1909.892250
 Lowest Frequency = -38.3594cm⁻¹

N	3.077487	2.633192	9.275769
C	3.128542	1.331072	9.450146
C	4.278456	0.712580	9.990433
H	4.289576	-0.366297	10.152659
C	5.371683	1.487869	10.303286
H	6.265794	1.029035	10.732200
C	5.366676	2.882092	10.034333
C	4.165002	3.406508	9.506276
C	4.011944	4.795171	9.158863
O	2.841546	5.190906	8.738555
C	5.128683	5.606281	9.336330
H	5.069773	6.659621	9.052626
C	6.327552	5.084258	9.875206
H	7.174979	5.761161	10.007711
C	6.462686	3.760762	10.234432
H	7.398252	3.379319	10.646667
N	1.969027	4.404649	11.529020
C	2.617957	5.497719	11.861265
C	3.599906	5.486981	12.878223
H	4.143014	6.402636	13.117299
C	3.857222	4.314060	13.549646
H	4.622371	4.282613	14.329057
C	3.105399	3.143884	13.263966
C	2.152265	3.258551	12.227263
C	1.295190	2.171176	11.841209
O	0.487477	2.370120	10.835110
C	1.427125	0.986601	12.558072

H	0.773893	0.144277	12.318865
C	2.390493	0.866371	13.586759
H	2.467437	-0.085425	14.117825
C	3.226795	1.902736	13.941212
H	3.960489	1.788592	14.740872
C	1.911915	0.554532	9.006047
H	2.229605	-0.426363	8.598917
H	1.276515	0.360001	9.880771
N	1.131920	1.308567	8.022546
C	1.866227	1.438600	6.764670
H	1.886334	0.484622	6.200735
H	2.905515	1.703514	6.995283
C	1.296570	2.516687	5.872950
H	1.974973	2.658345	5.013715
H	0.305323	2.249482	5.463376
O	1.190464	3.722926	6.600455
C	0.869194	4.821218	5.774283
H	-0.156862	4.701814	5.380110
H	1.566859	4.872725	4.920317
C	0.986765	6.084992	6.577014
H	2.024664	6.233224	6.914949
H	0.662479	6.934178	5.953554
O	0.132451	5.959319	7.707718
C	-0.220769	7.189524	8.317708
H	-1.241206	7.069041	8.693545
H	-0.258081	7.982693	7.553257
C	0.760556	7.605342	9.404170
H	1.740444	7.748821	8.928576
H	0.445149	8.590797	9.804615
N	0.934532	6.615363	10.462191
C	2.243281	6.749362	11.107056
H	2.272311	7.616803	11.795932
H	2.996514	6.921531	10.327822
C	-0.115455	6.616508	11.479111
H	-0.256059	7.623901	11.920659
H	0.211787	5.951361	12.287737
C	-1.462151	6.123536	10.987170
H	-2.078305	5.837858	11.856918
H	-2.014415	6.911592	10.446721
O	-1.280842	5.003224	10.141092
C	-2.475181	4.529321	9.543703
H	-2.567749	4.949017	8.525818
H	-3.351141	4.846180	10.131548
C	-2.438306	3.028539	9.512593
H	-2.330080	2.643314	10.541566
H	-3.382227	2.645665	9.084814
O	-1.342473	2.597175	8.733118
C	-1.216976	1.180071	8.802116
H	-2.187977	0.718871	8.550882
H	-0.941287	0.907243	9.832140
C	-0.187287	0.719191	7.803489
H	-0.144960	-0.387157	7.816842
H	-0.540773	1.004070	6.803799

Dy-syn-KHQ(1+)

SCF (RwB97XD) = -1947.90817749

E(SCF)+ZPE(0 K)= -1947.224145
 H(298 K)= -1947.187584
 G(298 K)= -1947.286971
 Lowest Frequency = 40.3200cm⁻¹

Dy	0.948624	3.966089	9.242925
N	3.077487	2.633192	9.275769
C	3.128542	1.331072	9.450146
C	4.278456	0.712580	9.990433
H	4.289576	-0.366297	10.152659
C	5.371683	1.487869	10.303286
H	6.265794	1.029035	10.732200
C	5.366676	2.882092	10.034333
C	4.165002	3.406508	9.506276
C	4.011944	4.795171	9.158863
O	2.841546	5.190906	8.738555
C	5.128683	5.606281	9.336330
H	5.069773	6.659621	9.052626
C	6.327552	5.084258	9.875206
H	7.174979	5.761161	10.007711
C	6.462686	3.760762	10.234432
H	7.398252	3.379319	10.646667
N	1.969027	4.404649	11.529020
C	2.617957	5.497719	11.861265
C	3.599906	5.486981	12.878223
H	4.143014	6.402636	13.117299
C	3.857222	4.314060	13.549646
H	4.622371	4.282613	14.329057
C	3.105399	3.143884	13.263966
C	2.152265	3.258551	12.227263
C	1.295190	2.171176	11.841209
O	0.487477	2.370120	10.835110
C	1.427125	0.986601	12.558072
H	0.773893	0.144277	12.318865
C	2.390493	0.866371	13.586759
H	2.467437	-0.085425	14.117825
C	3.226795	1.902736	13.941212
H	3.960489	1.788592	14.740872
C	1.911915	0.554532	9.006047
H	2.229605	-0.426363	8.598917
H	1.276515	0.360001	9.880771
N	1.131920	1.308567	8.022546
C	1.866227	1.438600	6.764670
H	1.886334	0.484622	6.200735
H	2.905515	1.703514	6.995283
C	1.296570	2.516687	5.872950
H	1.974973	2.658345	5.013715
H	0.305323	2.249482	5.463376
O	1.190464	3.722926	6.600455
C	0.869194	4.821218	5.774283
H	-0.156862	4.701814	5.380110
H	1.566859	4.872725	4.920317
C	0.986765	6.084992	6.577014
H	2.024664	6.233224	6.914949
H	0.662479	6.934178	5.953554
O	0.132451	5.959319	7.707718
C	-0.220769	7.189524	8.317708

H	-1.241206	7.069041	8.693545
H	-0.258081	7.982693	7.553257
C	0.760556	7.605342	9.404170
H	1.740444	7.748821	8.928576
H	0.445149	8.590797	9.804615
N	0.934532	6.615363	10.462191
C	2.243281	6.749362	11.107056
H	2.272311	7.616803	11.795932
H	2.996514	6.921531	10.327822
C	-0.115455	6.616508	11.479111
H	-0.256059	7.623901	11.920659
H	0.211787	5.951361	12.287737
C	-1.462151	6.123536	10.987170
H	-2.078305	5.837858	11.856918
H	-2.014415	6.911592	10.446721
O	-1.280842	5.003224	10.141092
C	-2.475181	4.529321	9.543703
H	-2.567749	4.949017	8.525818
H	-3.351141	4.846180	10.131548
C	-2.438306	3.028539	9.512593
H	-2.330080	2.643314	10.541566
H	-3.382227	2.645665	9.084814
O	-1.342473	2.597175	8.733118
C	-1.216976	1.180071	8.802116
H	-2.187977	0.718871	8.550882
H	-0.941287	0.907243	9.832140
C	-0.187287	0.719191	7.803489
H	-0.144960	-0.387157	7.816842
H	-0.540773	1.004070	6.803799

Dy-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2024.26905011
 E(SCF)+ZPE(0 K)= -2023.559437
 H(298 K)= -2023.520632
 G(298 K)= -2023.624716
 Lowest Frequency = 22.3421cm⁻¹

Dy	1.017858	4.021475	9.092705
N	3.093586	2.621892	9.132507
C	3.109777	1.309831	9.217551
C	4.253038	0.620331	9.682368
H	4.237554	-0.468476	9.752930
C	5.369914	1.337164	10.042495
H	6.258860	0.822176	10.414673
C	5.389587	2.749944	9.910312
C	4.199280	3.347334	9.432991
C	4.084295	4.767119	9.225292
O	2.938528	5.233647	8.808743
C	5.208544	5.534933	9.511143
H	5.169004	6.613830	9.344113
C	6.393016	4.937358	9.999144
H	7.249655	5.580308	10.214840
C	6.501454	3.579764	10.206084
H	7.425523	3.136696	10.580923
N	1.843455	4.489404	11.479470
C	2.371044	5.617767	11.895241

C	3.172405	5.677588	13.059618
H	3.603953	6.630326	13.370994
C	3.399110	4.528567	13.779078
H	4.025025	4.551177	14.674424
C	2.796825	3.307423	13.379418
C	2.009338	3.357370	12.206053
C	1.305614	2.208083	11.708656
O	0.613930	2.354491	10.615196
C	1.431197	1.027817	12.434875
H	0.894705	0.136065	12.101654
C	2.234583	0.974613	13.597210
H	2.311845	0.026294	14.134307
C	2.913075	2.074928	14.073131
H	3.523617	2.015476	14.975612
C	1.857378	0.579117	8.800827
H	2.134521	-0.381698	8.322254
H	1.289209	0.343626	9.708408
N	1.016200	1.380957	7.905457
C	1.690664	1.489377	6.602809
H	1.535970	0.571238	6.002789
H	2.770458	1.579970	6.778180
C	1.268326	2.681809	5.782168
H	1.794231	2.638933	4.812022
H	0.182435	2.681858	5.578051
O	1.614078	3.872254	6.458214
C	1.448555	5.004633	5.632935
H	0.477469	4.938626	5.107288
H	2.247542	5.037852	4.870868
C	1.489134	6.268348	6.448939
H	2.444770	6.347951	6.989577
H	1.362520	7.128168	5.768618
O	0.410715	6.224233	7.376262
C	0.079830	7.455414	7.981561
H	-0.987308	7.405574	8.235386
H	0.194269	8.279439	7.256244
C	0.940422	7.744035	9.194980
H	1.981533	7.807822	8.851462
H	0.669023	8.740621	9.598929
N	0.893871	6.714331	10.235291
C	2.106369	6.836611	11.055993
H	2.061475	7.734966	11.702753
H	2.960892	6.958898	10.378070
C	-0.290121	6.787895	11.097105
H	-0.557458	7.841119	11.316415
H	-0.034915	6.317107	12.056332
C	-1.537681	6.085802	10.597494
H	-2.310525	6.211097	11.376052
H	-1.946644	6.534103	9.675340
O	-1.296100	4.707684	10.390094
C	-2.498025	3.954001	10.427184
H	-3.163079	4.274536	9.601199
H	-3.026409	4.162708	11.373685
C	-2.254636	2.467557	10.352165
H	-1.541364	2.163874	11.132827
H	-3.221931	1.956248	10.510930
O	-1.728835	2.145956	9.085416
C	-1.243908	0.828597	8.928504

H	-2.089614	0.141669	8.744734
H	-0.738139	0.522358	9.855443
C	-0.303980	0.757346	7.737217
H	-0.184848	-0.312056	7.468605
H	-0.804205	1.235818	6.882198
O	-0.929688	3.950575	7.512439
H	-1.607953	3.361202	7.895554
H	-1.298382	4.780322	7.195715

Er-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.47998499
 E(SCF)+ZPE(0 K)= -1909.814116
 H(298 K)= -1909.779809
 G(298 K)= -1909.877020
 Lowest Frequency = -69.1480cm⁻¹

C	5.802381	1.416955	17.312594
C	5.460667	1.674548	18.664392
C	5.151858	0.542463	19.462982
H	4.879760	0.682776	20.512006
C	5.155535	-0.710673	18.904307
H	4.873983	-1.588707	19.489011
C	5.524368	-0.862983	17.544491
C	5.516948	-2.231146	16.911867
H	6.374556	-2.791132	17.316894
H	4.623344	-2.784407	17.262472
C	4.287209	-2.136186	14.798170
H	3.540869	-2.781438	15.302242
H	4.418822	-2.505533	13.773117
C	3.716372	-0.731207	14.683374
H	2.751763	-0.794847	14.153681
H	3.536901	-0.257371	15.662320
C	4.125478	1.061505	13.067368
H	4.026104	2.005932	13.626831
H	3.144697	0.766124	12.660258
C	5.112815	1.217737	11.926161
H	5.158444	0.296143	11.323350
H	4.800538	2.061967	11.290010
C	7.329729	2.244180	11.769737
H	6.803108	2.934912	11.091055
H	7.961814	1.580742	11.157116
C	6.385770	-3.334242	14.957568
H	6.281742	-3.348735	13.871207
H	6.027933	-4.309808	15.343668
N	5.879093	0.158116	16.798691
N	5.593593	-2.215893	15.458125
O	6.293686	2.182581	15.144878
O	4.620233	0.051251	13.926230
O	6.383688	1.478398	12.491556
C	7.563968	-2.044648	12.134620
C	8.860803	-1.424814	12.069329
C	9.908453	-1.979378	11.291234
C	11.105534	-1.220653	11.214229
H	11.945286	-1.599542	10.626488
C	11.185046	-0.002346	11.840356
H	12.079165	0.618214	11.753327

C	10.084544	0.457723	12.605556
C	10.151090	1.801155	13.286152
H	10.632593	2.527084	12.601458
H	10.844568	1.711469	14.137348
C	9.008616	3.016053	15.020009
H	9.770065	3.819377	14.959821
H	8.047926	3.485425	15.238623
C	9.394660	2.086485	16.173477
H	8.990300	2.485382	17.117024
H	10.489546	2.026151	16.276257
C	9.838808	-0.256631	16.273963
H	10.544451	-0.358432	15.429307
H	10.409085	-0.009493	17.184010
C	9.117617	-1.554486	16.510668
H	8.515777	-1.496130	17.436065
H	9.871121	-2.350353	16.627821
C	7.863778	-3.197444	15.326030
H	8.480415	-3.704744	14.567260
H	8.068951	-3.673349	16.298162
C	8.127072	3.073668	12.764377
H	7.402164	3.691955	13.308987
H	8.800503	3.749862	12.201554
N	8.988900	-0.252074	12.749518
N	8.866021	2.293241	13.761029
O	8.896659	0.759011	15.986082
O	8.270200	-1.829542	15.411850
O	6.636640	-1.461868	12.829119
C	7.400695	-3.243611	11.438853
H	6.419951	-3.724287	11.448192
C	8.461728	-3.812044	10.703803
H	8.286976	-4.751779	10.174502
C	9.698138	-3.208067	10.617644
H	10.503000	-3.646740	10.025639
C	6.028006	2.486857	16.377314
C	5.945866	3.788645	16.874280
H	6.086469	4.622270	16.182687
C	5.649865	4.035365	18.231032
H	5.595536	5.071107	18.574663
C	5.407654	3.013647	19.124510
H	5.156043	3.219634	20.166130

Er-anti-KHQ(1+)

SCF (RwB97XD) = -1949.06281829

E(SCF)+ZPE(0 K)= -1948.380232

H(298 K)= -1948.342976

G(298 K)= -1948.446060

Lowest Frequency = 14.5571cm⁻¹

C	5.802381	1.416955	17.312594
C	5.460667	1.674548	18.664392
C	5.151858	0.542463	19.462982
H	4.879760	0.682776	20.512006
C	5.155535	-0.710673	18.904307
H	4.873983	-1.588707	19.489011
C	5.524368	-0.862983	17.544491
C	5.516948	-2.231146	16.911867

H	6.374556	-2.791132	17.316894
H	4.623344	-2.784407	17.262472
C	4.287209	-2.136186	14.798170
H	3.540869	-2.781438	15.302242
H	4.418822	-2.505533	13.773117
C	3.716372	-0.731207	14.683374
H	2.751763	-0.794847	14.153681
H	3.536901	-0.257371	15.662320
C	4.125478	1.061505	13.067368
H	4.026104	2.005932	13.626831
H	3.144697	0.766124	12.660258
C	5.112815	1.217737	11.926161
H	5.158444	0.296143	11.323350
H	4.800538	2.061967	11.290010
C	7.329729	2.244180	11.769737
H	6.803108	2.934912	11.091055
H	7.961814	1.580742	11.157116
C	6.385770	-3.334242	14.957568
H	6.281742	-3.348735	13.871207
H	6.027933	-4.309808	15.343668
N	5.879093	0.158116	16.798691
N	5.593593	-2.215893	15.458125
O	6.293686	2.182581	15.144878
O	4.620233	0.051251	13.926230
O	6.383688	1.478398	12.491556
C	7.563968	-2.044648	12.134620
C	8.860803	-1.424814	12.069329
C	9.908453	-1.979378	11.291234
C	11.105534	-1.220653	11.214229
H	11.945286	-1.599542	10.626488
C	11.185046	-0.002346	11.840356
H	12.079165	0.618214	11.753327
C	10.084544	0.457723	12.605556
C	10.151090	1.801155	13.286152
H	10.632593	2.527084	12.601458
H	10.844568	1.711469	14.137348
C	9.008616	3.016053	15.020009
H	9.770065	3.819377	14.959821
H	8.047926	3.485425	15.238623
C	9.394660	2.086485	16.173477
H	8.990300	2.485382	17.117024
H	10.489546	2.026151	16.276257
C	9.838808	-0.256631	16.273963
H	10.544451	-0.358432	15.429307
H	10.409085	-0.009493	17.184010
C	9.117617	-1.554486	16.510668
H	8.515777	-1.496130	17.436065
H	9.871121	-2.350353	16.627821
C	7.863778	-3.197444	15.326030
H	8.480415	-3.704744	14.567260
H	8.068951	-3.673349	16.298162
C	8.127072	3.073668	12.764377
H	7.402164	3.691955	13.308987
H	8.800503	3.749862	12.201554
N	8.988900	-0.252074	12.749518
N	8.866021	2.293241	13.761029
O	8.896659	0.759011	15.986082

O	8.270200	-1.829542	15.411850
O	6.636640	-1.461868	12.829119
C	7.400695	-3.243611	11.438853
H	6.419951	-3.724287	11.448192
C	8.461728	-3.812044	10.703803
H	8.286976	-4.751779	10.174502
C	9.698138	-3.208067	10.617644
H	10.503000	-3.646740	10.025639
C	6.028006	2.486857	16.377314
C	5.945866	3.788645	16.874280
H	6.086469	4.622270	16.182687
C	5.649865	4.035365	18.231032
H	5.595536	5.071107	18.574663
C	5.407654	3.013647	19.124510
H	5.156043	3.219634	20.166130
Er	6.998241	0.133823	14.421425

Er3+_lon

SCF (Rwb97XD) = -36.7207183585
 E(SCF)+ZPE(0 K)= -36.720718
 H(298 K)= -36.718358
 G(298 K)= -36.737946

Er	0.887400	3.945900	9.220400
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Er-syn-KHQ_Ligand(2-)

SCF (Rwb97XD) = -1910.49525541
 E(SCF)+ZPE(0 K)= -1909.826993
 H(298 K)= -1909.792062
 G(298 K)= -1909.888826
 Lowest Frequency = -39.2690cm-1

N	3.067758	2.630927	9.307560
C	3.124047	1.331578	9.502337
C	4.278317	0.725480	10.047090
H	4.292587	-0.350549	10.226952
C	5.372187	1.507782	10.339795
H	6.269773	1.058088	10.771121
C	5.363152	2.896365	10.044018
C	4.156711	3.408487	9.515512
C	3.999036	4.788563	9.140217
O	2.823385	5.171542	8.722613
C	5.115678	5.604935	9.289282
H	5.053205	6.651657	8.982816
C	6.319815	5.095827	9.829337
H	7.167596	5.776230	9.939667
C	6.459544	3.780672	10.216150
H	7.399162	3.409300	10.628344
N	1.974548	4.425747	11.511860
C	2.628184	5.518558	11.836395
C	3.602776	5.513266	12.860308
H	4.150495	6.428175	13.091573
C	3.845636	4.347805	13.550075
H	4.604437	4.321112	14.335841
C	3.084298	3.181088	13.276231

C	2.141666	3.289728	12.229797
C	1.274168	2.207958	11.854493
O	0.479156	2.403706	10.837538
C	1.382820	1.034190	12.592050
H	0.719801	0.196905	12.362357
C	2.336588	0.918698	13.630575
H	2.396250	-0.024805	14.178362
C	3.183990	1.949530	13.974486
H	3.909308	1.838994	14.782248
C	1.911013	0.544054	9.068835
H	2.232936	-0.444500	8.683987
H	1.269669	0.366140	9.942692
N	1.139069	1.278694	8.066301
C	1.881089	1.390111	6.812363
H	1.904143	0.429213	6.260295
H	2.919320	1.657641	7.044528
C	1.315206	2.457087	5.905792
H	1.999016	2.593035	5.049891
H	0.327948	2.181968	5.491825
O	1.198840	3.670472	6.619649
C	0.861451	4.751109	5.777354
H	-0.168158	4.617857	5.396961
H	1.548914	4.791214	4.914538
C	0.979646	6.030046	6.554152
H	2.020047	6.192346	6.876758
H	0.641932	6.864557	5.918211
O	0.139748	5.920670	7.696855
C	-0.211798	7.162922	8.283640
H	-1.232037	7.052776	8.663025
H	-0.248952	7.940707	7.503744
C	0.771854	7.598511	9.359773
H	1.750206	7.734526	8.878947
H	0.456262	8.590291	9.744354
N	0.949052	6.625879	10.431852
C	2.259107	6.764439	11.070499
H	2.292915	7.637895	11.751568
H	3.010997	6.927471	10.288128
C	-0.098859	6.637248	11.449703
H	-0.243755	7.649674	11.878268
H	0.230990	5.984317	12.267061
C	-1.442815	6.132308	10.962260
H	-2.056266	5.843080	11.832666
H	-2.000701	6.915965	10.421287
O	-1.255676	5.012812	10.115927
C	-2.444697	4.552713	9.497544
H	-2.507998	4.964707	8.474292
H	-3.327856	4.888313	10.063555
C	-2.429887	3.052106	9.479245
H	-2.352001	2.674443	10.513727
H	-3.368836	2.678792	9.032433
O	-1.322171	2.599352	8.729999
C	-1.214189	1.182499	8.827021
H	-2.187988	0.728142	8.574273
H	-0.952984	0.926430	9.865008
C	-0.179675	0.690014	7.849292
H	-0.143979	-0.415880	7.891040
H	-0.522721	0.950982	6.839541

Er-syn-KHQ(1+)

SCF (RwB97XD) = -1949.07221369

E(SCF)+ZPE(0 K)= -1948.388008

H(298 K)= -1948.351482

G(298 K)= -1948.450720

Lowest Frequency = 38.3129cm⁻¹

Er	0.961654	3.959611	9.250540
N	3.067758	2.630927	9.307560
C	3.124047	1.331578	9.502337
C	4.278317	0.725480	10.047090
H	4.292587	-0.350549	10.226952
C	5.372187	1.507782	10.339795
H	6.269773	1.058088	10.771121
C	5.363152	2.896365	10.044018
C	4.156711	3.408487	9.515512
C	3.999036	4.788563	9.140217
O	2.823385	5.171542	8.722613
C	5.115678	5.604935	9.289282
H	5.053205	6.651657	8.982816
C	6.319815	5.095827	9.829337
H	7.167596	5.776230	9.939667
C	6.459544	3.780672	10.216150
H	7.399162	3.409300	10.628344
N	1.974548	4.425747	11.511860
C	2.628184	5.518558	11.836395
C	3.602776	5.513266	12.860308
H	4.150495	6.428175	13.091573
C	3.845636	4.347805	13.550075
H	4.604437	4.321112	14.335841
C	3.084298	3.181088	13.276231
C	2.141666	3.289728	12.229797
C	1.274168	2.207958	11.854493
O	0.479156	2.403706	10.837538
C	1.382820	1.034190	12.592050
H	0.719801	0.196905	12.362357
C	2.336588	0.918698	13.630575
H	2.396250	-0.024805	14.178362
C	3.183990	1.949530	13.974486
H	3.909308	1.838994	14.782248
C	1.911013	0.544054	9.068835
H	2.232936	-0.444500	8.683987
H	1.269669	0.366140	9.942692
N	1.139069	1.278694	8.066301
C	1.881089	1.390111	6.812363
H	1.904143	0.429213	6.260295
H	2.919320	1.657641	7.044528
C	1.315206	2.457087	5.905792
H	1.999016	2.593035	5.049891
H	0.327948	2.181968	5.491825
O	1.198840	3.670472	6.619649
C	0.861451	4.751109	5.777354
H	-0.168158	4.617857	5.396961
H	1.548914	4.791214	4.914538
C	0.979646	6.030046	6.554152

H	2.020047	6.192346	6.876758
H	0.641932	6.864557	5.918211
O	0.139748	5.920670	7.696855
C	-0.211798	7.162922	8.283640
H	-1.232037	7.052776	8.663025
H	-0.248952	7.940707	7.503744
C	0.771854	7.598511	9.359773
H	1.750206	7.734526	8.878947
H	0.456262	8.590291	9.744354
N	0.949052	6.625879	10.431852
C	2.259107	6.764439	11.070499
H	2.292915	7.637895	11.751568
H	3.010997	6.927471	10.288128
C	-0.098859	6.637248	11.449703
H	-0.243755	7.649674	11.878268
H	0.230990	5.984317	12.267061
C	-1.442815	6.132308	10.962260
H	-2.056266	5.843080	11.832666
H	-2.000701	6.915965	10.421287
O	-1.255676	5.012812	10.115927
C	-2.444697	4.552713	9.497544
H	-2.507998	4.964707	8.474292
H	-3.327856	4.888313	10.063555
C	-2.429887	3.052106	9.479245
H	-2.352001	2.674443	10.513727
H	-3.368836	2.678792	9.032433
O	-1.322171	2.599352	8.729999
C	-1.214189	1.182499	8.827021
H	-2.187988	0.728142	8.574273
H	-0.952984	0.926430	9.865008
C	-0.179675	0.690014	7.849292
H	-0.143979	-0.415880	7.891040
H	-0.522721	0.950982	6.839541

Er-syn-H2O-KHQ(1+)

SCF (RwB97XD) = -2025.43321683
 E(SCF)+ZPE(0 K)= -2024.723033
 H(298 K)= -2024.684419
 G(298 K)= -2024.788122
 Lowest Frequency = 22.2619cm⁻¹

Er	1.052664	4.020938	9.101749
N	3.098357	2.626794	9.128092
C	3.116523	1.314064	9.207885
C	4.266126	0.624480	9.656476
H	4.252403	-0.464620	9.722689
C	5.387425	1.340522	10.004733
H	6.281289	0.824559	10.363548
C	5.404893	2.753537	9.875959
C	4.208183	3.351114	9.416025
C	4.089789	4.770345	9.210560
O	2.937503	5.233720	8.807314
C	5.216100	5.539394	9.482409
H	5.173551	6.618359	9.316805
C	6.407523	4.941930	9.954045
H	7.266454	5.585265	10.159084

C	6.519930	3.584175	10.157627
H	7.449499	3.141563	10.519145
N	1.849827	4.488796	11.468950
C	2.369136	5.617138	11.895657
C	3.145005	5.676052	13.077053
H	3.570789	6.628422	13.397323
C	3.352558	4.527499	13.803519
H	3.957945	4.550245	14.712868
C	2.754093	3.307988	13.393557
C	1.994661	3.358758	12.202338
C	1.291839	2.214674	11.693668
O	0.623627	2.367373	10.586363
C	1.390414	1.035863	12.425679
H	0.853288	0.147404	12.084789
C	2.167808	0.980414	13.605933
H	2.224925	0.033499	14.147955
C	2.844553	2.076636	14.093495
H	3.433543	2.015093	15.010035
C	1.862245	0.582998	8.797630
H	2.138657	-0.377041	8.316922
H	1.298532	0.345047	9.707156
N	1.017716	1.385588	7.907151
C	1.687474	1.496421	6.602709
H	1.527102	0.581478	5.999230
H	2.768489	1.582095	6.773223
C	1.266213	2.693670	5.789344
H	1.784452	2.650770	4.815073
H	0.178774	2.699569	5.593569
O	1.622832	3.881079	6.465247
C	1.455370	5.012538	5.638789
H	0.485563	4.942686	5.111191
H	2.255453	5.047403	4.877941
C	1.487893	6.278176	6.451139
H	2.440876	6.362272	6.995558
H	1.362719	7.135488	5.767191
O	0.405067	6.233973	7.372421
C	0.082170	7.464122	7.983266
H	-0.983794	7.418378	8.242605
H	0.196544	8.290346	7.260306
C	0.950333	7.744350	9.192911
H	1.990432	7.803318	8.845489
H	0.686425	8.741187	9.601247
N	0.902276	6.712223	10.230472
C	2.113193	6.835308	11.053359
H	2.068098	7.734762	11.698461
H	2.969595	6.954826	10.377344
C	-0.284091	6.785640	11.089656
H	-0.559036	7.839194	11.297192
H	-0.028296	6.327374	12.054809
C	-1.525529	6.069050	10.595590
H	-2.303878	6.206779	11.366794
H	-1.929947	6.499107	9.662575
O	-1.277934	4.689192	10.415114
C	-2.480531	3.936874	10.453481
H	-3.147873	4.260318	9.630332
H	-3.005915	4.145365	11.401907
C	-2.246970	2.448817	10.373370

H	-1.518765	2.141915	11.138579
H	-3.213657	1.944389	10.555648
O	-1.755181	2.120549	9.094454
C	-1.241751	0.814528	8.934040
H	-2.073448	0.110856	8.750328
H	-0.728670	0.515739	9.859206
C	-0.302231	0.760258	7.740590
H	-0.179749	-0.306357	7.462147
H	-0.807258	1.243372	6.891025
O	-0.880810	3.937545	7.576990
H	-1.558977	3.341803	7.955464
H	-1.247119	4.765862	7.253169

Eu-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.49304572
 E(SCF)+ZPE(0 K)= -1909.826943
 H(298 K)= -1909.792771
 G(298 K)= -1909.889425
 Lowest Frequency = -58.3213cm⁻¹

C	5.893881	1.358735	17.382362
C	5.770320	1.550629	18.782360
C	5.498722	0.391240	19.555298
H	5.409693	0.479421	20.640986
C	5.308871	-0.819687	18.936486
H	5.048555	-1.710442	19.512002
C	5.434924	-0.904254	17.527371
C	5.049989	-2.176335	16.810013
H	5.428090	-3.049829	17.367191
H	3.950868	-2.255958	16.892703
C	4.301869	-2.262079	14.493000
H	3.547419	-3.010168	14.807977
H	4.677581	-2.539321	13.500374
C	3.626916	-0.907915	14.362553
H	2.736927	-1.015946	13.721889
H	3.298222	-0.507982	15.337989
C	4.057259	0.954990	12.836974
H	3.857427	1.905891	13.357596
H	3.129176	0.596223	12.363222
C	5.117221	1.146385	11.771088
H	5.276174	0.213241	11.205552
H	4.799853	1.947183	11.082706
C	7.275671	2.275054	11.716019
H	6.760354	2.968338	11.030567
H	7.914562	1.609183	11.112344
C	6.402889	-3.303606	15.140766
H	6.601756	-3.315821	14.064654
H	6.010116	-4.301423	15.424967
N	5.773337	0.134971	16.798301
N	5.445636	-2.233742	15.406549
O	6.204518	2.225424	15.210532
O	4.535496	-0.000416	13.764530
O	6.315061	1.517211	12.427977
C	7.605503	-2.085584	12.101559
C	8.871886	-1.411398	11.996871
C	9.913448	-1.920921	11.179613

C	11.074113	-1.113428	11.060982
H	11.905227	-1.454969	10.439069
C	11.129355	0.103060	11.693391
H	11.994962	0.758433	11.578251
C	10.043085	0.512348	12.506014
C	10.097383	1.844712	13.209036
H	10.565149	2.589635	12.535529
H	10.798409	1.741703	14.051464
C	8.971906	3.065509	14.954297
H	9.685361	3.908002	14.852048
H	7.995368	3.483008	15.207622
C	9.458029	2.180328	16.094879
H	9.169875	2.632418	17.057891
H	10.556675	2.090086	16.081237
C	9.788216	-0.143484	16.454022
H	10.518765	-0.371601	15.655998
H	10.337798	0.188916	17.349900
C	9.002571	-1.369840	16.820967
H	8.357015	-1.165696	17.695394
H	9.712475	-2.171434	17.085829
C	7.696156	-3.095466	15.900107
H	8.452652	-3.818791	15.553732
H	7.542180	-3.264203	16.979924
C	8.057364	3.100700	12.722874
H	7.320258	3.696347	13.277686
H	8.718640	3.799066	12.172938
N	8.979121	-0.238324	12.681726
N	8.812775	2.319849	13.707884
O	8.904855	0.867335	16.009329
O	8.194937	-1.770087	15.729144
O	6.669486	-1.534444	12.813178
C	7.473694	-3.296330	11.421592
H	6.518653	-3.823601	11.474808
C	8.531034	-3.819585	10.648924
H	8.380835	-4.769828	10.131034
C	9.732888	-3.158272	10.513240
H	10.534443	-3.561168	9.892023
C	6.094321	2.466937	16.481359
C	6.167973	3.736538	17.058776
H	6.275369	4.603201	16.402737
C	6.077708	3.914875	18.454967
H	6.146246	4.928350	18.857626
C	5.890404	2.856558	19.318665
H	5.806267	3.011509	20.395545

Eu-anti-KHQ(1+)

SCF (RwB97XD) = -1946.12802516

E(SCF)+ZPE(0 K)= -1945.445655

H(298 K)= -1945.408424

G(298 K)= -1945.511570

Lowest Frequency = 13.7953cm⁻¹

C	5.893881	1.358735	17.382362
C	5.770320	1.550629	18.782360
C	5.498722	0.391240	19.555298
H	5.409693	0.479421	20.640986

C	5.308871	-0.819687	18.936486
H	5.048555	-1.710442	19.512002
C	5.434924	-0.904254	17.527371
C	5.049989	-2.176335	16.810013
H	5.428090	-3.049829	17.367191
H	3.950868	-2.255958	16.892703
C	4.301869	-2.262079	14.493000
H	3.547419	-3.010168	14.807977
H	4.677581	-2.539321	13.500374
C	3.626916	-0.907915	14.362553
H	2.736927	-1.015946	13.721889
H	3.298222	-0.507982	15.337989
C	4.057259	0.954990	12.836974
H	3.857427	1.905891	13.357596
H	3.129176	0.596223	12.363222
C	5.117221	1.146385	11.771088
H	5.276174	0.213241	11.205552
H	4.799853	1.947183	11.082706
C	7.275671	2.275054	11.716019
H	6.760354	2.968338	11.030567
H	7.914562	1.609183	11.112344
C	6.402889	-3.303606	15.140766
H	6.601756	-3.315821	14.064654
H	6.010116	-4.301423	15.424967
N	5.773337	0.134971	16.798301
N	5.445636	-2.233742	15.406549
O	6.204518	2.225424	15.210532
O	4.535496	-0.000416	13.764530
O	6.315061	1.517211	12.427977
C	7.605503	-2.085584	12.101559
C	8.871886	-1.411398	11.996871
C	9.913448	-1.920921	11.179613
C	11.074113	-1.113428	11.060982
H	11.905227	-1.454969	10.439069
C	11.129355	0.103060	11.693391
H	11.994962	0.758433	11.578251
C	10.043085	0.512348	12.506014
C	10.097383	1.844712	13.209036
H	10.565149	2.589635	12.535529
H	10.798409	1.741703	14.051464
C	8.971906	3.065509	14.954297
H	9.685361	3.908002	14.852048
H	7.995368	3.483008	15.207622
C	9.458029	2.180328	16.094879
H	9.169875	2.632418	17.057891
H	10.556675	2.090086	16.081237
C	9.788216	-0.143484	16.454022
H	10.518765	-0.371601	15.655998
H	10.337798	0.188916	17.349900
C	9.002571	-1.369840	16.820967
H	8.357015	-1.165696	17.695394
H	9.712475	-2.171434	17.085829
C	7.696156	-3.095466	15.900107
H	8.452652	-3.818791	15.553732
H	7.542180	-3.264203	16.979924
C	8.057364	3.100700	12.722874
H	7.320258	3.696347	13.277686

H	8.718640	3.799066	12.172938
N	8.979121	-0.238324	12.681726
N	8.812775	2.319849	13.707884
O	8.904855	0.867335	16.009329
O	8.194937	-1.770087	15.729144
O	6.669486	-1.534444	12.813178
C	7.473694	-3.296330	11.421592
H	6.518653	-3.823601	11.474808
C	8.531034	-3.819585	10.648924
H	8.380835	-4.769828	10.131034
C	9.732888	-3.158272	10.513240
H	10.534443	-3.561168	9.892023
C	6.094321	2.466937	16.481359
C	6.167973	3.736538	17.058776
H	6.275369	4.603201	16.402737
C	6.077708	3.914875	18.454967
H	6.146246	4.928350	18.857626
C	5.890404	2.856558	19.318665
H	5.806267	3.011509	20.395545
Eu	6.952111	0.143012	14.422929

Eu3+_Ion

SCF (RwB97XD) = -33.8359439519
 E(SCF)+ZPE(0 K)= -33.835944
 H(298 K)= -33.833583
 G(298 K)= -33.853056

Eu 0.887400 3.945900 9.220400

Eu-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.50396308
 E(SCF)+ZPE(0 K)= -1909.835880
 H(298 K)= -1909.800017
 G(298 K)= -1909.900246
 Lowest Frequency = -33.1976cm-1

N	3.092205	2.619667	9.262318
C	3.128091	1.316262	9.427915
C	4.264132	0.682751	9.980348
H	4.264415	-0.397584	10.133136
C	5.356762	1.447100	10.320590
H	6.239786	0.977379	10.760538
C	5.365777	2.844999	10.070577
C	4.178647	3.384901	9.524195
C	4.041940	4.781312	9.196298
O	2.885839	5.195259	8.754525
C	5.159704	5.581628	9.415149
H	5.113015	6.640308	9.149546
C	6.343015	5.043233	9.971097
H	7.190954	5.712630	10.134908
C	6.462489	3.712702	10.309481
H	7.386121	3.318180	10.736092
N	1.942321	4.415436	11.548067
C	2.579999	5.516329	11.875772
C	3.560251	5.520446	12.894604

H	4.092491	6.442862	13.132194
C	3.832703	4.351507	13.566510
H	4.597896	4.330655	14.346227
C	3.100733	3.169311	13.278314
C	2.143606	3.269418	12.242902
C	1.309741	2.163669	11.853397
O	0.493369	2.343871	10.850925
C	1.471547	0.978836	12.564699
H	0.838185	0.122826	12.320600
C	2.437434	0.875224	13.592084
H	2.536715	-0.077269	14.118206
C	3.249877	1.928957	13.950902
H	3.987115	1.828121	14.749093
C	1.905263	0.553877	8.974736
H	2.213634	-0.426371	8.559225
H	1.270493	0.359133	9.850269
N	1.125499	1.319480	7.997408
C	1.859248	1.447804	6.737375
H	1.873679	0.492854	6.175003
H	2.899975	1.706757	6.968745
C	1.298581	2.528131	5.841274
H	1.976286	2.655357	4.979244
H	0.302672	2.271190	5.436398
O	1.211237	3.739108	6.563239
C	0.928632	4.848570	5.737204
H	-0.087464	4.747506	5.313358
H	1.651149	4.896984	4.903907
C	1.041433	6.104597	6.554980
H	2.071189	6.231689	6.926223
H	0.751559	6.964929	5.929658
O	0.149830	5.983610	7.657552
C	-0.207733	7.209404	8.272669
H	-1.233080	7.085015	8.634346
H	-0.234186	8.009707	7.514826
C	0.759633	7.614817	9.376209
H	1.748119	7.752734	8.916709
H	0.445482	8.601712	9.773770
N	0.911054	6.623026	10.438323
C	2.210265	6.759935	11.105260
H	2.227633	7.634652	11.785191
H	2.975495	6.923560	10.335637
C	-0.153858	6.638322	11.441337
H	-0.289916	7.649941	11.874462
H	0.158235	5.975284	12.258023
C	-1.500776	6.154319	10.941535
H	-2.131979	5.904976	11.811831
H	-2.034646	6.933703	10.370777
O	-1.324417	5.005331	10.134622
C	-2.524133	4.489776	9.584203
H	-2.668500	4.896589	8.567107
H	-3.387110	4.786211	10.201716
C	-2.445765	2.989225	9.566037
H	-2.284190	2.616868	10.592860
H	-3.396147	2.577948	9.181149
O	-1.372247	2.577271	8.744925
C	-1.220705	1.162045	8.795294
H	-2.186368	0.686156	8.550572

H	-0.926986	0.881243	9.818426
C	-0.195689	0.731663	7.777355
H	-0.148269	-0.374555	7.763688
H	-0.559049	1.039619	6.787953

Eu-syn-KHQ(1+)

SCF (RwB97XD) = -1946.14081393
 E(SCF)+ZPE(0 K)= -1945.457290
 H(298 K)= -1945.420629
 G(298 K)= -1945.520270
 Lowest Frequency = 39.4672cm⁻¹

Eu	0.935166	3.969669	9.224383
N	3.092205	2.619667	9.262318
C	3.128091	1.316262	9.427915
C	4.264132	0.682751	9.980348
H	4.264415	-0.397584	10.133136
C	5.356762	1.447100	10.320590
H	6.239786	0.977379	10.760538
C	5.365777	2.844999	10.070577
C	4.178647	3.384901	9.524195
C	4.041940	4.781312	9.196298
O	2.885839	5.195259	8.754525
C	5.159704	5.581628	9.415149
H	5.113015	6.640308	9.149546
C	6.343015	5.043233	9.971097
H	7.190954	5.712630	10.134908
C	6.462489	3.712702	10.309481
H	7.386121	3.318180	10.736092
N	1.942321	4.415436	11.548067
C	2.579999	5.516329	11.875772
C	3.560251	5.520446	12.894604
H	4.092491	6.442862	13.132194
C	3.832703	4.351507	13.566510
H	4.597896	4.330655	14.346227
C	3.100733	3.169311	13.278314
C	2.143606	3.269418	12.242902
C	1.309741	2.163669	11.853397
O	0.493369	2.343871	10.850925
C	1.471547	0.978836	12.564699
H	0.838185	0.122826	12.320600
C	2.437434	0.875224	13.592084
H	2.536715	-0.077269	14.118206
C	3.249877	1.928957	13.950902
H	3.987115	1.828121	14.749093
C	1.905263	0.553877	8.974736
H	2.213634	-0.426371	8.559225
H	1.270493	0.359133	9.850269
N	1.125499	1.319480	7.997408
C	1.859248	1.447804	6.737375
H	1.873679	0.492854	6.175003
H	2.899975	1.706757	6.968745
C	1.298581	2.528131	5.841274
H	1.976286	2.655357	4.979244
H	0.302672	2.271190	5.436398
O	1.211237	3.739108	6.563239

C	0.928632	4.848570	5.737204
H	-0.087464	4.747506	5.313358
H	1.651149	4.896984	4.903907
C	1.041433	6.104597	6.554980
H	2.071189	6.231689	6.926223
H	0.751559	6.964929	5.929658
O	0.149830	5.983610	7.657552
C	-0.207733	7.209404	8.272669
H	-1.233080	7.085015	8.634346
H	-0.234186	8.009707	7.514826
C	0.759633	7.614817	9.376209
H	1.748119	7.752734	8.916709
H	0.445482	8.601712	9.773770
N	0.911054	6.623026	10.438323
C	2.210265	6.759935	11.105260
H	2.227633	7.634652	11.785191
H	2.975495	6.923560	10.335637
C	-0.153858	6.638322	11.441337
H	-0.289916	7.649941	11.874462
H	0.158235	5.975284	12.258023
C	-1.500776	6.154319	10.941535
H	-2.131979	5.904976	11.811831
H	-2.034646	6.933703	10.370777
O	-1.324417	5.005331	10.134622
C	-2.524133	4.489776	9.584203
H	-2.668500	4.896589	8.567107
H	-3.387110	4.786211	10.201716
C	-2.445765	2.989225	9.566037
H	-2.284190	2.616868	10.592860
H	-3.396147	2.577948	9.181149
O	-1.372247	2.577271	8.744925
C	-1.220705	1.162045	8.795294
H	-2.186368	0.686156	8.550572
H	-0.926986	0.881243	9.818426
C	-0.195689	0.731663	7.777355
H	-0.148269	-0.374555	7.763688
H	-0.559049	1.039619	6.787953

Eu-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2022.50218869

E(SCF)+ZPE(0 K)= -2021.792981

H(298 K)= -2021.754049

G(298 K)= -2021.857993

Lowest Frequency = 23.7271cm⁻¹

Eu	0.971322	4.015376	9.083076
N	3.091833	2.609572	9.126933
C	3.104753	1.297835	9.209622
C	4.239454	0.604991	9.690318
H	4.221928	-0.483950	9.758521
C	5.349848	1.320515	10.072072
H	6.231957	0.804137	10.458312
C	5.372104	2.734097	9.947188
C	4.191028	3.334865	9.450302
C	4.079771	4.757360	9.251790
O	2.943258	5.231278	8.819891

C	5.200119	5.521351	9.564951
H	5.164192	6.601629	9.405938
C	6.374589	4.919900	10.071080
H	7.227093	5.560905	10.308062
C	6.478405	3.560774	10.270513
H	7.394569	3.114388	10.660540
N	1.833036	4.483575	11.501642
C	2.365505	5.613844	11.905259
C	3.197606	5.677077	13.047986
H	3.630760	6.632086	13.350116
C	3.455242	4.527342	13.754930
H	4.106593	4.551444	14.631898
C	2.856672	3.301291	13.364584
C	2.032591	3.347971	12.215677
C	1.336609	2.187829	11.729671
O	0.611006	2.323339	10.657106
C	1.507828	1.004547	12.442439
H	0.979774	0.105563	12.115261
C	2.345035	0.956890	13.580102
H	2.456421	0.005832	14.106312
C	3.016057	2.066541	14.044961
H	3.654729	2.012204	14.928106
C	1.853036	0.571384	8.782348
H	2.128552	-0.387898	8.300026
H	1.281211	0.334578	9.687684
N	1.014278	1.378792	7.888051
C	1.689082	1.491557	6.585412
H	1.539027	0.572642	5.985447
H	2.768050	1.587270	6.763327
C	1.261956	2.682393	5.763133
H	1.794050	2.644198	4.796193
H	0.177261	2.676125	5.552448
O	1.596063	3.873441	6.443972
C	1.436935	5.011883	5.625744
H	0.465493	4.955503	5.099794
H	2.236640	5.045376	4.864465
C	1.488660	6.268779	6.453258
H	2.445034	6.333984	6.995214
H	1.369944	7.136129	5.781245
O	0.409913	6.225738	7.380926
C	0.073883	7.454675	7.988557
H	-0.994738	7.401209	8.235905
H	0.190445	8.280986	7.266171
C	0.926294	7.744051	9.208176
H	1.969134	7.809807	8.870204
H	0.650697	8.740625	9.609370
N	0.876685	6.715472	10.250159
C	2.089970	6.833919	11.070355
H	2.045771	7.730694	11.719548
H	2.943175	6.958895	10.391172
C	-0.305805	6.791851	11.113575
H	-0.562988	7.845272	11.344318
H	-0.052789	6.308223	12.067037
C	-1.561119	6.107060	10.608305
H	-2.329076	6.221298	11.393185
H	-1.972403	6.573434	9.696316
O	-1.326454	4.731121	10.375367

C	-2.523445	3.970807	10.408129
H	-3.188086	4.286938	9.580248
H	-3.056663	4.171690	11.353474
C	-2.254801	2.489041	10.331941
H	-1.558009	2.190939	11.130091
H	-3.216686	1.958548	10.456350
O	-1.681989	2.187564	9.079754
C	-1.243087	0.854342	8.914417
H	-2.112102	0.197467	8.729014
H	-0.745990	0.527686	9.839146
C	-0.309246	0.763192	7.720830
H	-0.200346	-0.308926	7.459453
H	-0.805448	1.241659	6.863457
O	-1.004817	3.977460	7.425322
H	-1.681769	3.395607	7.815100
H	-1.379759	4.806316	7.114447

Gd-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.49129446
 E(SCF)+ZPE(0 K)= -1909.825221
 H(298 K)= -1909.791015
 G(298 K)= -1909.887464
 Lowest Frequency = -64.7640cm⁻¹

C	5.888399	1.358144	17.374758
C	5.754251	1.551641	18.773181
C	5.489794	0.391081	19.547084
H	5.392926	0.480457	20.631986
C	5.315686	-0.822240	18.929243
H	5.060029	-1.714579	19.504410
C	5.451452	-0.908439	17.520832
C	5.085365	-2.188384	16.807787
H	5.507485	-3.050017	17.350937
H	3.991830	-2.304936	16.920773
C	4.282364	-2.235488	14.506612
H	3.525756	-2.977124	14.831493
H	4.632779	-2.509251	13.503658
C	3.621169	-0.872645	14.399205
H	2.716897	-0.965347	13.776439
H	3.318632	-0.474142	15.383543
C	4.048375	0.992504	12.873032
H	3.867495	1.941552	13.403774
H	3.109889	0.646864	12.410202
C	5.096236	1.178728	11.794148
H	5.236453	0.247480	11.220682
H	4.779565	1.988228	11.115777
C	7.269004	2.281668	11.720451
H	6.755049	2.968997	11.028180
H	7.908224	1.609703	11.123846
C	6.385434	-3.305489	15.091712
H	6.546337	-3.316056	14.009904
H	5.996015	-4.301773	15.385445
N	5.784673	0.131891	16.791439
N	5.446235	-2.230030	15.394679
O	6.198443	2.222679	15.203282
O	4.529713	0.024958	13.786571

O	6.307104	1.530200	12.437620
C	7.597944	-2.071327	12.122009
C	8.875569	-1.414294	12.046502
C	9.937311	-1.950954	11.274153
C	11.111029	-1.158900	11.179431
H	11.958904	-1.522490	10.593678
C	11.158302	0.070269	11.787151
H	12.034227	0.714390	11.687025
C	10.049288	0.508992	12.552861
C	10.091647	1.862025	13.217139
H	10.545368	2.589982	12.516027
H	10.802291	1.796477	14.055645
C	8.954057	3.074673	14.960988
H	9.674879	3.912558	14.873482
H	7.977872	3.498390	15.204422
C	9.418341	2.176482	16.103756
H	9.090273	2.606323	17.063670
H	10.517688	2.106443	16.124883
C	9.817223	-0.163072	16.320309
H	10.490466	-0.351326	15.463541
H	10.425893	0.138977	17.187891
C	9.070053	-1.412206	16.690780
H	8.479813	-1.247302	17.611347
H	9.802803	-2.214875	16.879640
C	7.707036	-3.109543	15.804513
H	8.449674	-3.825644	15.415524
H	7.595730	-3.297385	16.886579
C	8.051092	3.114331	12.721417
H	7.314546	3.714017	13.272497
H	8.712225	3.808971	12.166570
N	8.973690	-0.228537	12.710784
N	8.805365	2.337533	13.709400
O	8.892954	0.853406	15.982849
O	8.198216	-1.781128	15.638701
O	6.647192	-1.499313	12.796308
C	7.473301	-3.291393	11.456804
H	6.509654	-3.804850	11.484358
C	8.549139	-3.841192	10.729571
H	8.403727	-4.797934	10.222385
C	9.763885	-3.197994	10.624363
H	10.580633	-3.621781	10.037802
C	6.079789	2.466491	16.473061
C	6.135343	3.738399	17.047058
H	6.236189	4.604517	16.389278
C	6.035644	3.918845	18.442313
H	6.090207	4.933865	18.843159
C	5.855891	2.860081	19.307103
H	5.763822	3.016285	20.383151

Gd-anti-KHQ(1+)

SCF (RwB97XD) = -1946.72250111

E(SCF)+ZPE(0 K)= -1946.039988

H(298 K)= -1946.002763

G(298 K)= -1946.105950

Lowest Frequency = 15.9917cm⁻¹

C	5.888399	1.358144	17.374758
C	5.754251	1.551641	18.773181
C	5.489794	0.391081	19.547084
H	5.392926	0.480457	20.631986
C	5.315686	-0.822240	18.929243
H	5.060029	-1.714579	19.504410
C	5.451452	-0.908439	17.520832
C	5.085365	-2.188384	16.807787
H	5.507485	-3.050017	17.350937
H	3.991830	-2.304936	16.920773
C	4.282364	-2.235488	14.506612
H	3.525756	-2.977124	14.831493
H	4.632779	-2.509251	13.503658
C	3.621169	-0.872645	14.399205
H	2.716897	-0.965347	13.776439
H	3.318632	-0.474142	15.383543
C	4.048375	0.992504	12.873032
H	3.867495	1.941552	13.403774
H	3.109889	0.646864	12.410202
C	5.096236	1.178728	11.794148
H	5.236453	0.247480	11.220682
H	4.779565	1.988228	11.115777
C	7.269004	2.281668	11.720451
H	6.755049	2.968997	11.028180
H	7.908224	1.609703	11.123846
C	6.385434	-3.305489	15.091712
H	6.546337	-3.316056	14.009904
H	5.996015	-4.301773	15.385445
N	5.784673	0.131891	16.791439
N	5.446235	-2.230030	15.394679
O	6.198443	2.222679	15.203282
O	4.529713	0.024958	13.786571
O	6.307104	1.530200	12.437620
C	7.597944	-2.071327	12.122009
C	8.875569	-1.414294	12.046502
C	9.937311	-1.950954	11.274153
C	11.111029	-1.158900	11.179431
H	11.958904	-1.522490	10.593678
C	11.158302	0.070269	11.787151
H	12.034227	0.714390	11.687025
C	10.049288	0.508992	12.552861
C	10.091647	1.862025	13.217139
H	10.545368	2.589982	12.516027
H	10.802291	1.796477	14.055645
C	8.954057	3.074673	14.960988
H	9.674879	3.912558	14.873482
H	7.977872	3.498390	15.204422
C	9.418341	2.176482	16.103756
H	9.090273	2.606323	17.063670
H	10.517688	2.106443	16.124883
C	9.817223	-0.163072	16.320309
H	10.490466	-0.351326	15.463541
H	10.425893	0.138977	17.187891
C	9.070053	-1.412206	16.690780
H	8.479813	-1.247302	17.611347
H	9.802803	-2.214875	16.879640
C	7.707036	-3.109543	15.804513

H	8.449674	-3.825644	15.415524
H	7.595730	-3.297385	16.886579
C	8.051092	3.114331	12.721417
H	7.314546	3.714017	13.272497
H	8.712225	3.808971	12.166570
N	8.973690	-0.228537	12.710784
N	8.805365	2.337533	13.709400
O	8.892954	0.853406	15.982849
O	8.198216	-1.781128	15.638701
O	6.647192	-1.499313	12.796308
C	7.473301	-3.291393	11.456804
H	6.509654	-3.804850	11.484358
C	8.549139	-3.841192	10.729571
H	8.403727	-4.797934	10.222385
C	9.763885	-3.197994	10.624363
H	10.580633	-3.621781	10.037802
C	6.079789	2.466491	16.473061
C	6.135343	3.738399	17.047058
H	6.236189	4.604517	16.389278
C	6.035644	3.918845	18.442313
H	6.090207	4.933865	18.843159
C	5.855891	2.860081	19.307103
H	5.763822	3.016285	20.383151
Gd	6.937053	0.153056	14.414948

Gd3+_lon

SCF (RwB97XD) = -34.4205805528
 E(SCF)+ZPE(0 K)= -34.420581
 H(298 K)= -34.418220
 G(298 K)= -34.437739

Gd 0.887400 3.945900 9.220400

Gd-syn-KHQ_Ligand(2--)

SCF (RwB97XD) = -1910.50238230
 E(SCF)+ZPE(0 K)= -1909.834576
 H(298 K)= -1909.799504
 G(298 K)= -1909.896666
 Lowest Frequency = -34.3686cm-1

N	3.084613	2.623514	9.259552
C	3.124866	1.320136	9.425535
C	4.266497	0.689535	9.969567
H	4.269801	-0.390629	10.123476
C	5.360917	1.455959	10.299308
H	6.248406	0.988258	10.732368
C	5.365839	2.853177	10.045736
C	4.172877	3.390071	9.509583
C	4.031184	4.784857	9.178344
O	2.869619	5.194755	8.747408
C	5.150096	5.587310	9.382264
H	5.099751	6.644873	9.112904
C	6.339540	5.052153	9.928398
H	7.188423	5.722996	10.080974
C	6.463826	3.723082	10.270695

H	7.392203	3.331171	10.689330
N	1.957159	4.408023	11.541699
C	2.600587	5.505318	11.870509
C	3.585481	5.501993	12.884791
H	4.122849	6.421413	13.122432
C	3.855083	4.330251	13.553063
H	4.623480	4.303906	14.329455
C	3.114824	3.152924	13.266287
C	2.154759	3.260378	12.234613
C	1.311466	2.161514	11.847277
O	0.493952	2.350062	10.847230
C	1.465979	0.975207	12.557429
H	0.824865	0.124299	12.315749
C	2.435131	0.863711	13.581113
H	2.528903	-0.089716	14.106538
C	3.257192	1.910841	13.937312
H	3.996503	1.803788	14.732768
C	1.902023	0.554863	8.977828
H	2.211278	-0.425100	8.562226
H	1.269788	0.359232	9.854890
N	1.119531	1.319091	8.002464
C	1.849172	1.449660	6.740818
H	1.862292	0.496142	6.175953
H	2.890589	1.708797	6.968734
C	1.283511	2.531724	5.850404
H	1.958345	2.664514	4.986967
H	0.287242	2.273407	5.447330
O	1.194279	3.739976	6.576838
C	0.897642	4.847783	5.753628
H	-0.123144	4.742489	5.342177
H	1.609693	4.898077	4.911506
C	1.015903	6.104735	6.568393
H	2.049550	6.236522	6.926535
H	0.714357	6.963020	5.945836
O	0.139102	5.981411	7.682383
C	-0.213433	7.208176	8.298841
H	-1.236461	7.086231	8.667524
H	-0.244127	8.007515	7.540255
C	0.762058	7.613684	9.394927
H	1.746545	7.753930	8.927688
H	0.449374	8.599458	9.796521
N	0.923104	6.620034	10.453122
C	2.227650	6.753383	11.109060
H	2.251702	7.624308	11.793684
H	2.986793	6.920653	10.334312
C	-0.133737	6.629679	11.464090
H	-0.268808	7.639128	11.902604
H	0.185272	5.963742	12.275656
C	-1.482693	6.145380	10.970070
H	-2.106894	5.883934	11.841802
H	-2.023062	6.929180	10.411664
O	-1.308582	5.006316	10.148388
C	-2.508939	4.506250	9.585335
H	-2.639552	4.919488	8.568949
H	-3.374239	4.808608	10.196553
C	-2.445150	3.005508	9.560356
H	-2.297641	2.626932	10.587021

H	-3.395234	2.604656	9.163903
O	-1.367040	2.587953	8.748359
C	-1.225083	1.171728	8.801841
H	-2.193807	0.702061	8.557327
H	-0.934190	0.891415	9.825820
C	-0.202202	0.732165	7.786082
H	-0.157300	-0.374197	7.779473
H	-0.565295	1.034341	6.794844

Gd-syn-KHQ(1+)

SCF (RwB97XD) = -1946.73483415

E(SCF)+ZPE(0 K)= -1946.051088

H(298 K)= -1946.014471

G(298 K)= -1946.113965

Lowest Frequency = 40.2146cm⁻¹

Gd	0.938251	3.969188	9.233516
N	3.084613	2.623514	9.259552
C	3.124866	1.320136	9.425535
C	4.266497	0.689535	9.969567
H	4.269801	-0.390629	10.123476
C	5.360917	1.455959	10.299308
H	6.248406	0.988258	10.732368
C	5.365839	2.853177	10.045736
C	4.172877	3.390071	9.509583
C	4.031184	4.784857	9.178344
O	2.869619	5.194755	8.747408
C	5.150096	5.587310	9.382264
H	5.099751	6.644873	9.112904
C	6.339540	5.052153	9.928398
H	7.188423	5.722996	10.080974
C	6.463826	3.723082	10.270695
H	7.392203	3.331171	10.689330
N	1.957159	4.408023	11.541699
C	2.600587	5.505318	11.870509
C	3.585481	5.501993	12.884791
H	4.122849	6.421413	13.122432
C	3.855083	4.330251	13.553063
H	4.623480	4.303906	14.329455
C	3.114824	3.152924	13.266287
C	2.154759	3.260378	12.234613
C	1.311466	2.161514	11.847277
O	0.493952	2.350062	10.847230
C	1.465979	0.975207	12.557429
H	0.824865	0.124299	12.315749
C	2.435131	0.863711	13.581113
H	2.528903	-0.089716	14.106538
C	3.257192	1.910841	13.937312
H	3.996503	1.803788	14.732768
C	1.902023	0.554863	8.977828
H	2.211278	-0.425100	8.562226
H	1.269788	0.359232	9.854890
N	1.119531	1.319091	8.002464
C	1.849172	1.449660	6.740818
H	1.862292	0.496142	6.175953
H	2.890589	1.708797	6.968734

C	1.283511	2.531724	5.850404
H	1.958345	2.664514	4.986967
H	0.287242	2.273407	5.447330
O	1.194279	3.739976	6.576838
C	0.897642	4.847783	5.753628
H	-0.123144	4.742489	5.342177
H	1.609693	4.898077	4.911506
C	1.015903	6.104735	6.568393
H	2.049550	6.236522	6.926535
H	0.714357	6.963020	5.945836
O	0.139102	5.981411	7.682383
C	-0.213433	7.208176	8.298841
H	-1.236461	7.086231	8.667524
H	-0.244127	8.007515	7.540255
C	0.762058	7.613684	9.394927
H	1.746545	7.753930	8.927688
H	0.449374	8.599458	9.796521
N	0.923104	6.620034	10.453122
C	2.227650	6.753383	11.109060
H	2.251702	7.624308	11.793684
H	2.986793	6.920653	10.334312
C	-0.133737	6.629679	11.464090
H	-0.268808	7.639128	11.902604
H	0.185272	5.963742	12.275656
C	-1.482693	6.145380	10.970070
H	-2.106894	5.883934	11.841802
H	-2.023062	6.929180	10.411664
O	-1.308582	5.006316	10.148388
C	-2.508939	4.506250	9.585335
H	-2.639552	4.919488	8.568949
H	-3.374239	4.808608	10.196553
C	-2.445150	3.005508	9.560356
H	-2.297641	2.626932	10.587021
H	-3.395234	2.604656	9.163903
O	-1.367040	2.587953	8.748359
C	-1.225083	1.171728	8.801841
H	-2.193807	0.702061	8.557327
H	-0.934190	0.891415	9.825820
C	-0.202202	0.732165	7.786082
H	-0.157300	-0.374197	7.779473
H	-0.565295	1.034341	6.794844

Gd-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2023.09605905

E(SCF)+ZPE(0 K)= -2022.386826

H(298 K)= -2022.347888

G(298 K)= -2022.452139

Lowest Frequency = 21.7548cm⁻¹

Gd	0.985970	4.017722	9.086093
N	3.091677	2.614122	9.126416
C	3.105247	1.302218	9.209346
C	4.242147	0.609848	9.685420
H	4.224848	-0.479076	9.753915
C	5.354483	1.325282	10.061679
H	6.238310	0.808938	10.444018

C	5.376375	2.738679	9.935367
C	4.192984	3.339008	9.443804
C	4.081095	4.760961	9.243582
O	2.942302	5.233303	8.815738
C	5.202681	5.525560	9.550080
H	5.166099	6.605583	9.389537
C	6.379683	4.924626	10.051137
H	7.233458	5.565845	10.282854
C	6.484407	3.565768	10.251801
H	7.402579	3.119845	10.637599
N	1.836839	4.484281	11.493750
C	2.367596	5.613802	11.901907
C	3.190601	5.675342	13.051212
H	3.623067	6.629562	13.356778
C	3.439467	4.525344	13.761092
H	4.083358	4.548479	14.643578
C	2.840099	3.300877	13.367091
C	2.026687	3.349245	12.210921
C	1.328722	2.192429	11.720747
O	0.613043	2.331850	10.642038
C	1.486642	1.009521	12.436934
H	0.956230	0.112762	12.107451
C	2.313959	0.959549	13.581936
H	2.415448	0.008913	14.110881
C	2.987021	2.066284	14.050732
H	3.617454	2.009916	14.939645
C	1.853231	0.574638	8.785190
H	2.129191	-0.384427	8.302612
H	1.283287	0.337004	9.691356
N	1.012796	1.381089	7.892079
C	1.686536	1.493155	6.588913
H	1.534284	0.574906	5.988469
H	2.765968	1.586778	6.765198
C	1.260447	2.685112	5.768324
H	1.790116	2.646218	4.800080
H	0.175252	2.680795	5.560082
O	1.598615	3.875457	6.448435
C	1.438743	5.012486	5.628227
H	0.467682	4.953970	5.101685
H	2.238655	5.045323	4.867161
C	1.487903	6.271271	6.452432
H	2.443690	6.339256	6.994933
H	1.368529	7.136676	5.777979
O	0.408459	6.228911	7.379052
C	0.076458	7.458525	7.987486
H	-0.991704	7.407894	8.237319
H	0.193463	8.284689	7.265002
C	0.932527	7.744947	9.204962
H	1.974794	7.809016	8.864924
H	0.659889	8.741531	9.608137
N	0.882756	6.715221	10.245628
C	2.095449	6.834142	11.066599
H	2.050683	7.730864	11.715771
H	2.949365	6.958969	10.388336
C	-0.300730	6.791027	11.107881
H	-0.562318	7.844557	11.332884
H	-0.047033	6.313601	12.064304

C	-1.552588	6.098450	10.604961
H	-2.322918	6.217752	11.386819
H	-1.962684	6.556306	9.688029
O	-1.314561	4.721311	10.384011
C	-2.512993	3.962912	10.420504
H	-3.180324	4.281755	9.595775
H	-3.041847	4.164993	11.368089
C	-2.253113	2.479629	10.341815
H	-1.548646	2.178442	11.131815
H	-3.216694	1.955463	10.479313
O	-1.698886	2.173155	9.082762
C	-1.245011	0.845263	8.917834
H	-2.106519	0.178726	8.732031
H	-0.744938	0.523413	9.842566
C	-0.309475	0.762352	7.724634
H	-0.196709	-0.308630	7.460061
H	-0.807489	1.241008	6.868399
O	-0.982231	3.973728	7.460512
H	-1.659223	3.386938	7.845047
H	-1.355402	4.800239	7.141238

H2O

SCF (RwB97XD) = -76.3370013200
 E(SCF)+ZPE(0 K)= -76.315287
 H(298 K)= -76.311507
 G(298 K)= -76.333588
 Lowest Frequency = 1645.6741cm⁻¹

O	-2.815524	-1.087365	0.000000
H	-1.855311	-1.036742	0.000000
H	-3.088329	-0.165332	0.000000

Ho-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.48146758
 E(SCF)+ZPE(0 K)= -1909.815236
 H(298 K)= -1909.781069
 G(298 K)= -1909.877846
 Lowest Frequency = -71.6505cm⁻¹

C	5.790852	1.423152	17.318744
C	5.441411	1.680062	18.668820
C	5.125269	0.547857	19.464343
H	4.846222	0.687958	20.511573
C	5.131481	-0.705168	18.905289
H	4.845390	-1.583119	19.487908
C	5.510017	-0.857141	17.548155
C	5.510390	-2.225621	16.915992
H	6.367902	-2.781749	17.326293
H	4.616998	-2.782132	17.261792
C	4.290725	-2.137230	14.796271
H	3.545369	-2.785415	15.297910
H	4.428336	-2.506624	13.772014
C	3.714048	-0.734948	14.677596
H	2.750429	-0.804231	14.146650
H	3.531259	-0.259587	15.655270

C	4.120523	1.062864	13.065968
H	4.021275	2.004727	13.629883
H	3.139586	0.769238	12.657810
C	5.107614	1.224749	11.925161
H	5.154591	0.305102	11.319390
H	4.793711	2.070417	11.291652
C	7.323725	2.255577	11.773564
H	6.797106	2.951473	11.100091
H	7.955128	1.595892	11.155977
C	6.388185	-3.333330	14.967430
H	6.293810	-3.345316	13.880037
H	6.022766	-4.307839	15.349082
N	5.869347	0.164321	16.805040
N	5.595149	-2.212045	15.462101
O	6.293402	2.191095	15.153719
O	4.616000	0.048640	13.919613
O	6.378025	1.485714	12.491278
C	7.568275	-2.052001	12.128281
C	8.862730	-1.427171	12.057562
C	9.909777	-1.979009	11.276522
C	11.103836	-1.216052	11.194148
H	11.942534	-1.592617	10.603407
C	11.182135	0.002762	11.819446
H	12.074174	0.625822	11.728906
C	10.083265	0.459375	12.589087
C	10.150265	1.802163	13.271280
H	10.621996	2.531128	12.583135
H	10.852841	1.713578	14.114965
C	9.019973	3.007821	15.021359
H	9.774066	3.817704	14.956137
H	8.057713	3.467766	15.253287
C	9.428139	2.077488	16.165283
H	9.050351	2.480399	17.118140
H	10.524950	2.010154	16.241121
C	9.855190	-0.266907	16.274841
H	10.555555	-0.373145	15.426238
H	10.431940	-0.021165	17.181271
C	9.129899	-1.561341	16.518058
H	8.530655	-1.497624	17.444890
H	9.881258	-2.359137	16.636532
C	7.862855	-3.204277	15.349162
H	8.482522	-3.725704	14.602457
H	8.054896	-3.670575	16.328724
C	8.122338	3.077583	12.773382
H	7.397553	3.687911	13.327054
H	8.792059	3.761054	12.215015
N	8.990086	-0.253447	12.736440
N	8.868027	2.289776	13.759951
O	8.916892	0.753518	15.990553
O	8.278493	-1.838643	15.422841
O	6.639808	-1.471317	12.823033
C	7.408396	-3.253919	11.436590
H	6.429898	-3.739050	11.451013
C	8.469032	-3.819355	10.698809
H	8.296500	-4.761232	10.172581
C	9.702279	-3.209867	10.606116
H	10.506794	-3.646204	10.011916

C	6.024196	2.493780	16.385848
C	5.944849	3.795001	16.884884
H	6.093006	4.629135	16.195471
C	5.641284	4.040791	18.240095
H	5.588760	5.076219	18.584970
C	5.389382	3.018671	19.130427
H	5.131756	3.224000	20.170708

Ho-anti-KHQ(1+)

SCF (RwB97XD) = -1948.47895604
 E(SCF)+ZPE(0 K)= -1947.796181
 H(298 K)= -1947.758987
 G(298 K)= -1947.861504
 Lowest Frequency = 19.3098cm⁻¹

C	5.790852	1.423152	17.318744
C	5.441411	1.680062	18.668820
C	5.125269	0.547857	19.464343
H	4.846222	0.687958	20.511573
C	5.131481	-0.705168	18.905289
H	4.845390	-1.583119	19.487908
C	5.510017	-0.857141	17.548155
C	5.510390	-2.225621	16.915992
H	6.367902	-2.781749	17.326293
H	4.616998	-2.782132	17.261792
C	4.290725	-2.137230	14.796271
H	3.545369	-2.785415	15.297910
H	4.428336	-2.506624	13.772014
C	3.714048	-0.734948	14.677596
H	2.750429	-0.804231	14.146650
H	3.531259	-0.259587	15.655270
C	4.120523	1.062864	13.065968
H	4.021275	2.004727	13.629883
H	3.139586	0.769238	12.657810
C	5.107614	1.224749	11.925161
H	5.154591	0.305102	11.319390
H	4.793711	2.070417	11.291652
C	7.323725	2.255577	11.773564
H	6.797106	2.951473	11.100091
H	7.955128	1.595892	11.155977
C	6.388185	-3.333330	14.967430
H	6.293810	-3.345316	13.880037
H	6.022766	-4.307839	15.349082
N	5.869347	0.164321	16.805040
N	5.595149	-2.212045	15.462101
O	6.293402	2.191095	15.153719
O	4.616000	0.048640	13.919613
O	6.378025	1.485714	12.491278
C	7.568275	-2.052001	12.128281
C	8.862730	-1.427171	12.057562
C	9.909777	-1.979009	11.276522
C	11.103836	-1.216052	11.194148
H	11.942534	-1.592617	10.603407
C	11.182135	0.002762	11.819446
H	12.074174	0.625822	11.728906
C	10.083265	0.459375	12.589087

C	10.150265	1.802163	13.271280
H	10.621996	2.531128	12.583135
H	10.852841	1.713578	14.114965
C	9.019973	3.007821	15.021359
H	9.774066	3.817704	14.956137
H	8.057713	3.467766	15.253287
C	9.428139	2.077488	16.165283
H	9.050351	2.480399	17.118140
H	10.524950	2.010154	16.241121
C	9.855190	-0.266907	16.274841
H	10.555555	-0.373145	15.426238
H	10.431940	-0.021165	17.181271
C	9.129899	-1.561341	16.518058
H	8.530655	-1.497624	17.444890
H	9.881258	-2.359137	16.636532
C	7.862855	-3.204277	15.349162
H	8.482522	-3.725704	14.602457
H	8.054896	-3.670575	16.328724
C	8.122338	3.077583	12.773382
H	7.397553	3.687911	13.327054
H	8.792059	3.761054	12.215015
N	8.990086	-0.253447	12.736440
N	8.868027	2.289776	13.759951
O	8.916892	0.753518	15.990553
O	8.278493	-1.838643	15.422841
O	6.639808	-1.471317	12.823033
C	7.408396	-3.253919	11.436590
H	6.429898	-3.739050	11.451013
C	8.469032	-3.819355	10.698809
H	8.296500	-4.761232	10.172581
C	9.702279	-3.209867	10.606116
H	10.506794	-3.646204	10.011916
C	6.024196	2.493780	16.385848
C	5.944849	3.795001	16.884884
H	6.093006	4.629135	16.195471
C	5.641284	4.040791	18.240095
H	5.588760	5.076219	18.584970
C	5.389382	3.018671	19.130427
H	5.131756	3.224000	20.170708
Ho	7.003080	0.131991	14.425158

Ho3+_lon

SCF (RwB97XD) = -36.1463484872
 E(SCF)+ZPE(0 K)= -36.146348
 H(298 K)= -36.143988
 G(298 K)= -36.163568

Ho 0.887400 3.945900 9.220400

Ho-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.49687183
 E(SCF)+ZPE(0 K)= -1909.828594
 H(298 K)= -1909.793653
 G(298 K)= -1909.890642
 Lowest Frequency = -39.4109cm⁻¹

N	3.072879	2.635546	9.281730
C	3.127685	1.333602	9.457449
C	4.281289	0.718359	9.993454
H	4.294980	-0.360251	10.157231
C	5.375065	1.495799	10.299081
H	6.272124	1.039180	10.724189
C	5.366629	2.889137	10.026090
C	4.161088	3.410222	9.503958
C	4.004098	4.796968	9.152321
O	2.829903	5.188351	8.738461
C	5.120626	5.610410	9.318702
H	5.058616	6.662457	9.030917
C	6.323662	5.091941	9.851999
H	7.171132	5.770358	9.976162
C	6.462729	3.770118	10.215738
H	7.401473	3.391528	10.623341
N	1.974415	4.402832	11.524216
C	2.625507	5.493840	11.859311
C	3.604911	5.479313	12.878618
H	4.150156	6.393234	13.119453
C	3.856245	4.305570	13.551011
H	4.619055	4.271510	14.332601
C	3.099855	3.138689	13.264165
C	2.150847	3.257047	12.224341
C	1.288372	2.174853	11.837348
O	0.485729	2.379018	10.828147
C	1.409825	0.990729	12.556441
H	0.751656	0.152295	12.317141
C	2.369615	0.866147	13.588177
H	2.438808	-0.085181	14.121129
C	3.211533	1.897650	13.943437
H	3.941945	1.780046	14.745593
C	1.912574	0.553767	9.015491
H	2.232397	-0.428006	8.612069
H	1.275903	0.360875	9.889578
N	1.134300	1.304386	8.028922
C	1.870172	1.433987	6.772507
H	1.891175	0.480365	6.207948
H	2.909238	1.699102	7.003816
C	1.300239	2.512367	5.881759
H	1.979515	2.657105	5.023715
H	0.310173	2.243753	5.470254
O	1.190225	3.717356	6.610775
C	0.859741	4.812417	5.784199
H	-0.168419	4.688266	5.396955
H	1.551526	4.864318	4.925488
C	0.977854	6.078449	6.582538
H	2.017287	6.231925	6.912971
H	0.645853	6.924469	5.958879
O	0.131898	5.952624	7.719293
C	-0.220029	7.184655	8.326627
H	-1.239810	7.066411	8.704865
H	-0.258632	7.975413	7.559846
C	0.763917	7.603370	9.409400
H	1.742214	7.746964	8.930650
H	0.448536	8.589131	9.809224

N	0.941618	6.614805	10.467415
C	2.251787	6.747591	11.108378
H	2.283434	7.613286	11.799364
H	3.003241	6.921292	10.327857
C	-0.106015	6.613529	11.486183
H	-0.248840	7.620434	11.928185
H	0.223950	5.949331	12.294381
C	-1.451681	6.117068	10.994798
H	-2.065025	5.822733	11.863604
H	-2.008123	6.906483	10.460718
O	-1.267892	5.003612	10.140020
C	-2.459973	4.541276	9.529214
H	-2.537705	4.964065	8.511361
H	-3.339423	4.864102	10.108398
C	-2.434756	3.040711	9.494522
H	-2.341913	2.652304	10.523788
H	-3.376411	2.665929	9.054714
O	-1.333006	2.603432	8.727198
C	-1.215598	1.185948	8.801740
H	-2.188161	0.729236	8.548435
H	-0.945422	0.915520	9.833805
C	-0.184579	0.715696	7.809199
H	-0.144685	-0.390624	7.830168
H	-0.534440	0.994319	6.806502

Ho-syn-KHQ(1+)

SCF (RwB97XD) = -1948.48910366
 E(SCF)+ZPE(0 K)= -1947.804956
 H(298 K)= -1947.768422
 G(298 K)= -1947.867795
 Lowest Frequency = 38.7977cm⁻¹

Ho	0.954420	3.965434	9.248529
N	3.072879	2.635546	9.281730
C	3.127685	1.333602	9.457449
C	4.281289	0.718359	9.993454
H	4.294980	-0.360251	10.157231
C	5.375065	1.495799	10.299081
H	6.272124	1.039180	10.724189
C	5.366629	2.889137	10.026090
C	4.161088	3.410222	9.503958
C	4.004098	4.796968	9.152321
O	2.829903	5.188351	8.738461
C	5.120626	5.610410	9.318702
H	5.058616	6.662457	9.030917
C	6.323662	5.091941	9.851999
H	7.171132	5.770358	9.976162
C	6.462729	3.770118	10.215738
H	7.401473	3.391528	10.623341
N	1.974415	4.402832	11.524216
C	2.625507	5.493840	11.859311
C	3.604911	5.479313	12.878618
H	4.150156	6.393234	13.119453
C	3.856245	4.305570	13.551011
H	4.619055	4.271510	14.332601
C	3.099855	3.138689	13.264165

C	2.150847	3.257047	12.224341
C	1.288372	2.174853	11.837348
O	0.485729	2.379018	10.828147
C	1.409825	0.990729	12.556441
H	0.751656	0.152295	12.317141
C	2.369615	0.866147	13.588177
H	2.438808	-0.085181	14.121129
C	3.211533	1.897650	13.943437
H	3.941945	1.780046	14.745593
C	1.912574	0.553767	9.015491
H	2.232397	-0.428006	8.612069
H	1.275903	0.360875	9.889578
N	1.134300	1.304386	8.028922
C	1.870172	1.433987	6.772507
H	1.891175	0.480365	6.207948
H	2.909238	1.699102	7.003816
C	1.300239	2.512367	5.881759
H	1.979515	2.657105	5.023715
H	0.310173	2.243753	5.470254
O	1.190225	3.717356	6.610775
C	0.859741	4.812417	5.784199
H	-0.168419	4.688266	5.396955
H	1.551526	4.864318	4.925488
C	0.977854	6.078449	6.582538
H	2.017287	6.231925	6.912971
H	0.645853	6.924469	5.958879
O	0.131898	5.952624	7.719293
C	-0.220029	7.184655	8.326627
H	-1.239810	7.066411	8.704865
H	-0.258632	7.975413	7.559846
C	0.763917	7.603370	9.409400
H	1.742214	7.746964	8.930650
H	0.448536	8.589131	9.809224
N	0.941618	6.614805	10.467415
C	2.251787	6.747591	11.108378
H	2.283434	7.613286	11.799364
H	3.003241	6.921292	10.327857
C	-0.106015	6.613529	11.486183
H	-0.248840	7.620434	11.928185
H	0.223950	5.949331	12.294381
C	-1.451681	6.117068	10.994798
H	-2.065025	5.822733	11.863604
H	-2.008123	6.906483	10.460718
O	-1.267892	5.003612	10.140020
C	-2.459973	4.541276	9.529214
H	-2.537705	4.964065	8.511361
H	-3.339423	4.864102	10.108398
C	-2.434756	3.040711	9.494522
H	-2.341913	2.652304	10.523788
H	-3.376411	2.665929	9.054714
O	-1.333006	2.603432	8.727198
C	-1.215598	1.185948	8.801740
H	-2.188161	0.729236	8.548435
H	-0.945422	0.915520	9.833805
C	-0.184579	0.715696	7.809199
H	-0.144685	-0.390624	7.830168
H	-0.534440	0.994319	6.806502

Ho-syn-H2O-KHQ(1+)

SCF (RwB97XD) = -2024.85000471

E(SCF)+ZPE(0 K)= -2024.140106

H(298 K)= -2024.101389

G(298 K)= -2024.205472

Lowest Frequency = 21.0601cm⁻¹

Ho	1.035358	4.022451	9.097534
N	3.096167	2.625603	9.130364
C	3.113701	1.313173	9.212429
C	4.260483	0.623765	9.668559
H	4.246128	-0.465213	9.736681
C	5.379617	1.340314	10.022422
H	6.271307	0.824920	10.387410
C	5.397865	2.753229	9.892151
C	4.203982	3.350588	9.424223
C	4.087072	4.770079	9.217762
O	2.937801	5.234921	8.808352
C	5.212393	5.538655	9.496109
H	5.171110	6.617584	9.329828
C	6.400698	4.941255	9.975285
H	7.258535	5.584483	10.185248
C	6.511390	3.583578	10.180368
H	7.438482	3.140809	10.548015
N	1.846669	4.488996	11.474510
C	2.370089	5.617188	11.896257
C	3.158295	5.676142	13.069528
H	3.587015	6.628542	13.385792
C	3.374889	4.527126	13.792390
H	3.990161	4.549494	14.695089
C	2.774392	3.307003	13.387080
C	2.001529	3.357765	12.204310
C	1.298093	2.211431	11.700688
O	0.618701	2.361543	10.599936
C	1.409413	1.031709	12.429743
H	0.872479	0.141808	12.092324
C	2.199226	0.976944	13.601537
H	2.265825	0.029204	14.141052
C	2.876992	2.074897	14.083831
H	3.476290	2.014013	14.993715
C	1.860563	0.581961	8.798879
H	2.137689	-0.378367	8.319230
H	1.294673	0.344964	9.707376
N	1.017632	1.383998	7.905926
C	1.690029	1.493860	6.602556
H	1.532874	0.577268	6.000765
H	2.770377	1.582264	6.775733
C	1.268132	2.688554	5.785444
H	1.790370	2.645749	4.813301
H	0.181487	2.691331	5.585406
O	1.618983	3.877534	6.461470
C	1.450787	5.009456	5.636081
H	0.479912	4.940921	5.110317
H	2.249575	5.044440	4.873864
C	1.487128	6.273860	6.450620

H	2.441771	6.356132	6.992512
H	1.360220	7.132564	5.768863
O	0.407186	6.228990	7.375809
C	0.080389	7.459756	7.983812
H	-0.986117	7.412154	8.240558
H	0.194737	8.284788	7.259577
C	0.945112	7.744106	9.195106
H	1.985623	7.805626	8.849372
H	0.677448	8.740663	9.601626
N	0.898174	6.712843	10.233705
C	2.109713	6.835854	11.055733
H	2.064234	7.734598	11.701847
H	2.965240	6.957230	10.378926
C	-0.287207	6.785417	11.093957
H	-0.558860	7.838587	11.307919
H	-0.031767	6.320422	12.055953
C	-1.531281	6.075897	10.596282
H	-2.306838	6.206131	11.371428
H	-1.938382	6.515952	9.669266
O	-1.286156	4.697065	10.400642
C	-2.488471	3.943923	10.439664
H	-3.155372	4.265879	9.615664
H	-3.014362	4.152919	11.387576
C	-2.250766	2.456542	10.362416
H	-1.529292	2.151293	11.134716
H	-3.217949	1.949370	10.534389
O	-1.743726	2.130840	9.089048
C	-1.241788	0.820074	8.930707
H	-2.079100	0.122929	8.747395
H	-0.731322	0.518993	9.856675
C	-0.302264	0.759303	7.738010
H	-0.181131	-0.308229	7.462724
H	-0.805343	1.241620	6.886785
O	-0.904515	3.941546	7.543960
H	-1.581674	3.348467	7.926078
H	-1.273218	4.771156	7.226547

KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.64998644
 E(SCF)+ZPE(0 K)= -1909.977650
 H(298 K)= -1909.940357
 G(298 K)= -1910.045908
 Lowest Frequency = 15.3711cm⁻¹

N	3.968043	4.472791	8.323716
C	3.696370	3.190266	8.433335
C	4.631210	2.204829	8.023147
H	4.360679	1.151660	8.125221
C	5.836427	2.608185	7.505214
H	6.580029	1.869277	7.185557
C	6.143236	3.990758	7.366170
C	5.137202	4.905508	7.801905
C	5.316315	6.375879	7.669172
O	4.432144	7.187689	8.014756
C	6.577763	6.760570	7.106534
H	6.754290	7.835171	6.996420

C	7.545502	5.835822	6.705212
H	8.485667	6.213418	6.282002
C	7.363905	4.464706	6.816253
H	8.128398	3.753198	6.490658
N	1.686954	2.875098	12.420157
C	1.561549	4.158214	12.688270
C	0.980204	4.598723	13.906673
H	0.926428	5.669473	14.124254
C	0.490369	3.674561	14.794518
H	0.026127	3.993118	15.734278
C	0.596167	2.287151	14.514997
C	1.248963	1.938181	13.286983
C	1.489982	0.509906	12.936334
O	2.111935	0.171553	11.913356
C	0.947443	-0.429242	13.878632
H	1.086877	-1.487749	13.639433
C	0.295865	-0.043200	15.048238
H	-0.080724	-0.824592	15.721157
C	0.112361	1.288937	15.397224
H	-0.388203	1.578695	16.325610
C	2.359766	2.796885	9.025379
H	2.512146	2.448715	10.062933
H	1.737277	3.706912	9.101523
N	1.719483	1.707402	8.304955
C	1.352026	1.938389	6.933386
H	1.225839	0.957694	6.430787
H	2.207916	2.426334	6.431999
C	0.075178	2.734736	6.639820
H	-0.123529	2.706208	5.544781
H	-0.765079	2.249522	7.154616
O	0.108267	4.061895	7.099861
C	0.751208	4.983552	6.262372
H	0.004222	5.454014	5.586570
H	1.507226	4.487386	5.624370
C	1.477269	6.034611	7.062835
H	2.253460	5.554532	7.678937
H	2.011085	6.716703	6.370380
O	0.558772	6.753489	7.847946
C	1.146209	7.507464	8.874392
H	0.320909	8.100618	9.305644
H	1.890083	8.212571	8.455048
C	1.898559	6.748751	9.965527
H	2.808808	6.312893	9.523511
H	2.257451	7.553993	10.657673
N	1.191024	5.724019	10.718199
C	2.112949	5.174803	11.710604
H	2.557616	6.003770	12.314461
H	2.943846	4.711621	11.158482
C	-0.121941	6.106395	11.185526
H	-0.188335	7.197469	11.403545
H	-0.350129	5.589309	12.127032
C	-1.230004	5.714191	10.219102
H	-2.141669	6.320402	10.430125
H	-0.914686	5.904040	9.179963
O	-1.519665	4.352418	10.399186
C	-2.345231	3.821331	9.409208
H	-1.931164	4.029717	8.404045

H	-3.358259	4.286723	9.463076
C	-2.497622	2.317775	9.588917
H	-2.652215	2.107044	10.667071
H	-3.409629	2.003125	9.051229
O	-1.453030	1.555322	9.069749
C	-0.281021	1.494708	9.878408
H	-0.500245	0.882594	10.774263
H	0.003009	2.497432	10.234444
C	0.883354	0.853517	9.127896
H	1.517146	0.416365	9.916422
H	0.489572	0.028488	8.506217

La-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.51144960
 E(SCF)+ZPE(0 K)= -1909.844632
 H(298 K)= -1909.809848
 G(298 K)= -1909.907958
 Lowest Frequency = -46.2280cm⁻¹

C	5.836825	1.398865	17.423985
C	5.666446	1.621093	18.816763
C	5.259119	0.501505	19.587498
H	5.126469	0.614285	20.666474
C	5.001730	-0.702571	18.976205
H	4.647465	-1.560279	19.551628
C	5.188634	-0.819147	17.577666
C	4.754492	-2.062646	16.839308
H	4.831322	-2.948285	17.495730
H	3.673469	-1.943457	16.657861
C	4.503028	-2.520915	14.464255
H	3.750538	-3.291211	14.726014
H	5.089895	-2.877983	13.608629
C	3.777487	-1.260849	14.030172
H	3.048600	-1.530961	13.247898
H	3.222800	-0.785145	14.858906
C	4.247290	0.610572	12.566520
H	3.907415	1.518599	13.092808
H	3.406385	0.194471	11.987331
C	5.383449	0.937845	11.623155
H	5.679194	0.048284	11.039735
H	5.059723	1.730090	10.927918
C	7.371619	2.303717	11.801065
H	6.797148	3.055262	11.233392
H	8.032959	1.778570	11.091794
C	6.453888	-3.331470	15.663423
H	6.911980	-3.436679	14.671098
H	6.013164	-4.307063	15.954477
N	5.636089	0.182289	16.852710
N	5.437303	-2.282888	15.566832
O	6.331621	2.209218	15.259909
O	4.717101	-0.341099	13.500844
O	6.474602	1.387585	12.402776
C	7.791653	-2.249362	12.052660
C	8.859403	-1.357598	11.678600
C	9.623125	-1.580837	10.500898
C	10.624477	-0.622553	10.204652

H	11.238014	-0.746344	9.308863
C	10.804539	0.459780	11.030596
H	11.556777	1.218716	10.807927
C	9.994389	0.589665	12.183404
C	10.183337	1.752258	13.122898
H	10.675183	2.591371	12.592807
H	10.894275	1.426503	13.897061
C	9.231872	2.906345	15.015783
H	9.924749	3.757059	14.855604
H	8.282526	3.311244	15.377864
C	9.828813	2.025115	16.092361
H	9.805305	2.573723	17.049504
H	10.883386	1.771709	15.882552
C	9.743215	-0.120058	17.058715
H	10.582098	-0.583645	16.508487
H	10.148728	0.383281	17.952620
C	8.759411	-1.163814	17.508201
H	7.988344	-0.718448	18.163784
H	9.306142	-1.930560	18.082516
C	7.519510	-2.993507	16.681734
H	8.284978	-3.787430	16.691669
H	7.090716	-2.931136	17.697319
C	8.124078	3.035923	12.896471
H	7.367949	3.508193	13.537489
H	8.735547	3.831712	12.426021
N	9.072436	-0.293853	12.500260
N	8.950114	2.191097	13.769443
O	9.092389	0.816653	16.222358
O	8.137584	-1.746179	16.377686
O	7.112888	-1.981765	13.127033
C	7.555294	-3.342545	11.220929
H	6.750981	-4.032606	11.484339
C	8.328347	-3.563057	10.062597
H	8.106666	-4.435191	9.442916
C	9.344975	-2.710075	9.691253
H	9.931870	-2.886313	8.788334
C	6.186276	2.472695	16.521228
C	6.356577	3.735182	17.095380
H	6.579192	4.580137	16.439798
C	6.214852	3.939743	18.483573
H	6.361428	4.947420	18.880106
C	5.883779	2.917042	19.346804
H	5.763166	3.094084	20.416774

La-anti-KHQ(1+)

SCF (RwB97XD) = -1942.41643622

E(SCF)+ZPE(0 K)= -1941.734227

H(298 K)= -1941.696907

G(298 K)= -1941.800071

Lowest Frequency = 16.5511cm⁻¹

C	5.836825	1.398865	17.423985
C	5.666446	1.621093	18.816763
C	5.259119	0.501505	19.587498
H	5.126469	0.614285	20.666474
C	5.001730	-0.702571	18.976205

H	4.647465	-1.560279	19.551628
C	5.188634	-0.819147	17.577666
C	4.754492	-2.062646	16.839308
H	4.831322	-2.948285	17.495730
H	3.673469	-1.943457	16.657861
C	4.503028	-2.520915	14.464255
H	3.750538	-3.291211	14.726014
H	5.089895	-2.877983	13.608629
C	3.777487	-1.260849	14.030172
H	3.048600	-1.530961	13.247898
H	3.222800	-0.785145	14.858906
C	4.247290	0.610572	12.566520
H	3.907415	1.518599	13.092808
H	3.406385	0.194471	11.987331
C	5.383449	0.937845	11.623155
H	5.679194	0.048284	11.039735
H	5.059723	1.730090	10.927918
C	7.371619	2.303717	11.801065
H	6.797148	3.055262	11.233392
H	8.032959	1.778570	11.091794
C	6.453888	-3.331470	15.663423
H	6.911980	-3.436679	14.671098
H	6.013164	-4.307063	15.954477
N	5.636089	0.182289	16.852710
N	5.437303	-2.282888	15.566832
O	6.331621	2.209218	15.259909
O	4.717101	-0.341099	13.500844
O	6.474602	1.387585	12.402776
C	7.791653	-2.249362	12.052660
C	8.859403	-1.357598	11.678600
C	9.623125	-1.580837	10.500898
C	10.624477	-0.622553	10.204652
H	11.238014	-0.746344	9.308863
C	10.804539	0.459780	11.030596
H	11.556777	1.218716	10.807927
C	9.994389	0.589665	12.183404
C	10.183337	1.752258	13.122898
H	10.675183	2.591371	12.592807
H	10.894275	1.426503	13.897061
C	9.231872	2.906345	15.015783
H	9.924749	3.757059	14.855604
H	8.282526	3.311244	15.377864
C	9.828813	2.025115	16.092361
H	9.805305	2.573723	17.049504
H	10.883386	1.771709	15.882552
C	9.743215	-0.120058	17.058715
H	10.582098	-0.583645	16.508487
H	10.148728	0.383281	17.952620
C	8.759411	-1.163814	17.508201
H	7.988344	-0.718448	18.163784
H	9.306142	-1.930560	18.082516
C	7.519510	-2.993507	16.681734
H	8.284978	-3.787430	16.691669
H	7.090716	-2.931136	17.697319
C	8.124078	3.035923	12.896471
H	7.367949	3.508193	13.537489
H	8.735547	3.831712	12.426021

N	9.072436	-0.293853	12.500260
N	8.950114	2.191097	13.769443
O	9.092389	0.816653	16.222358
O	8.137584	-1.746179	16.377686
O	7.112888	-1.981765	13.127033
C	7.555294	-3.342545	11.220929
H	6.750981	-4.032606	11.484339
C	8.328347	-3.563057	10.062597
H	8.106666	-4.435191	9.442916
C	9.344975	-2.710075	9.691253
H	9.931870	-2.886313	8.788334
C	6.186276	2.472695	16.521228
C	6.356577	3.735182	17.095380
H	6.579192	4.580137	16.439798
C	6.214852	3.939743	18.483573
H	6.361428	4.947420	18.880106
C	5.883779	2.917042	19.346804
H	5.763166	3.094084	20.416774
La	7.121697	-0.006201	14.534860

La3+_Ion

SCF (RwB97XD) = -30.1902022435
 E(SCF)+ZPE(0 K)= -30.190202
 H(298 K)= -30.187842
 G(298 K)= -30.207179

La 0.887400 3.945900 9.220400

La-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.51561708
 E(SCF)+ZPE(0 K)= -1909.848424
 H(298 K)= -1909.813132
 G(298 K)= -1909.911373
 Lowest Frequency = -35.9135cm-1

N	3.127379	2.586003	9.199107
C	3.132573	1.279614	9.337873
C	4.243853	0.610559	9.899333
H	4.223548	-0.473323	10.023410
C	5.336015	1.348651	10.293270
H	6.199164	0.853185	10.744285
C	5.369697	2.754957	10.097086
C	4.210825	3.332328	9.525109
C	4.105915	4.746926	9.253660
O	2.982540	5.207520	8.775838
C	5.223234	5.519228	9.563711
H	5.198280	6.590055	9.348512
C	6.375091	4.941420	10.142939
H	7.221749	5.591775	10.375818
C	6.465708	3.594573	10.420605
H	7.365049	3.167743	10.867530
N	1.900300	4.441154	11.593638
C	2.508551	5.561903	11.908789
C	3.486645	5.604591	12.929329
H	3.989123	6.544650	13.162770

C	3.800960	4.447128	13.601317
H	4.567311	4.454061	14.380140
C	3.121086	3.235329	13.308027
C	2.151151	3.297259	12.279305
C	1.374821	2.147382	11.886541
O	0.532108	2.278338	10.898917
C	1.615926	0.965802	12.582942
H	1.032564	0.077569	12.329479
C	2.591818	0.904852	13.602372
H	2.750190	-0.046671	14.115694
C	3.343397	2.000428	13.968651
H	4.091623	1.934528	14.760243
C	1.890502	0.547294	8.882001
H	2.174013	-0.430490	8.443914
H	1.272379	0.350209	9.769645
N	1.092539	1.335352	7.932823
C	1.802064	1.470371	6.656652
H	1.799624	0.516840	6.091744
H	2.848381	1.720274	6.873650
C	1.242807	2.557773	5.764345
H	1.901738	2.655763	4.884186
H	0.230202	2.323551	5.388095
O	1.208673	3.777728	6.476205
C	0.992819	4.909755	5.658957
H	-0.009493	4.850967	5.196568
H	1.748038	4.947264	4.854556
C	1.116458	6.150626	6.503479
H	2.131736	6.224562	6.928746
H	0.902096	7.032510	5.877235
O	0.161691	6.057588	7.555467
C	-0.177891	7.278432	8.188768
H	-1.213917	7.166513	8.525008
H	-0.170226	8.096126	7.448476
C	0.770641	7.644145	9.323460
H	1.775961	7.752250	8.892687
H	0.477558	8.639646	9.715201
N	0.866324	6.650183	10.394784
C	2.148123	6.786415	11.102161
H	2.151572	7.678966	11.758540
H	2.934703	6.923223	10.347959
C	-0.227897	6.697452	11.368327
H	-0.360537	7.720779	11.774103
H	0.060243	6.050482	12.207072
C	-1.575932	6.215756	10.865561
H	-2.230959	6.058361	11.740085
H	-2.076880	6.958789	10.221667
O	-1.415142	4.997679	10.165555
C	-2.622426	4.383182	9.748631
H	-2.904330	4.754632	8.746992
H	-3.435619	4.631028	10.450530
C	-2.441724	2.888365	9.746861
H	-2.132436	2.551311	10.751983
H	-3.402700	2.410250	9.485761
O	-1.449018	2.520800	8.807936
C	-1.232663	1.113035	8.812361
H	-2.186587	0.599441	8.599426
H	-0.878534	0.819267	9.812981

C	-0.237398	0.752252	7.735643
H	-0.182171	-0.351375	7.661354
H	-0.639809	1.109650	6.778033

La-syn-KHQ(1+)

SCF (RwB97XD) = -1942.42891623
 E(SCF)+ZPE(0 K)= -1941.746307
 H(298 K)= -1941.709416
 G(298 K)= -1941.809708
 Lowest Frequency = 35.0894cm⁻¹

La	0.900306	3.977809	9.185785
N	3.127379	2.586003	9.199107
C	3.132573	1.279614	9.337873
C	4.243853	0.610559	9.899333
H	4.223548	-0.473323	10.023410
C	5.336015	1.348651	10.293270
H	6.199164	0.853185	10.744285
C	5.369697	2.754957	10.097086
C	4.210825	3.332328	9.525109
C	4.105915	4.746926	9.253660
O	2.982540	5.207520	8.775838
C	5.223234	5.519228	9.563711
H	5.198280	6.590055	9.348512
C	6.375091	4.941420	10.142939
H	7.221749	5.591775	10.375818
C	6.465708	3.594573	10.420605
H	7.365049	3.167743	10.867530
N	1.900300	4.441154	11.593638
C	2.508551	5.561903	11.908789
C	3.486645	5.604591	12.929329
H	3.989123	6.544650	13.162770
C	3.800960	4.447128	13.601317
H	4.567311	4.454061	14.380140
C	3.121086	3.235329	13.308027
C	2.151151	3.297259	12.279305
C	1.374821	2.147382	11.886541
O	0.532108	2.278338	10.898917
C	1.615926	0.965802	12.582942
H	1.032564	0.077569	12.329479
C	2.591818	0.904852	13.602372
H	2.750190	-0.046671	14.115694
C	3.343397	2.000428	13.968651
H	4.091623	1.934528	14.760243
C	1.890502	0.547294	8.882001
H	2.174013	-0.430490	8.443914
H	1.272379	0.350209	9.769645
N	1.092539	1.335352	7.932823
C	1.802064	1.470371	6.656652
H	1.799624	0.516840	6.091744
H	2.848381	1.720274	6.873650
C	1.242807	2.557773	5.764345
H	1.901738	2.655763	4.884186
H	0.230202	2.323551	5.388095
O	1.208673	3.777728	6.476205
C	0.992819	4.909755	5.658957

H	-0.009493	4.850967	5.196568
H	1.748038	4.947264	4.854556
C	1.116458	6.150626	6.503479
H	2.131736	6.224562	6.928746
H	0.902096	7.032510	5.877235
O	0.161691	6.057588	7.555467
C	-0.177891	7.278432	8.188768
H	-1.213917	7.166513	8.525008
H	-0.170226	8.096126	7.448476
C	0.770641	7.644145	9.323460
H	1.775961	7.752250	8.892687
H	0.477558	8.639646	9.715201
N	0.866324	6.650183	10.394784
C	2.148123	6.786415	11.102161
H	2.151572	7.678966	11.758540
H	2.934703	6.923223	10.347959
C	-0.227897	6.697452	11.368327
H	-0.360537	7.720779	11.774103
H	0.060243	6.050482	12.207072
C	-1.575932	6.215756	10.865561
H	-2.230959	6.058361	11.740085
H	-2.076880	6.958789	10.221667
O	-1.415142	4.997679	10.165555
C	-2.622426	4.383182	9.748631
H	-2.904330	4.754632	8.746992
H	-3.435619	4.631028	10.450530
C	-2.441724	2.888365	9.746861
H	-2.132436	2.551311	10.751983
H	-3.402700	2.410250	9.485761
O	-1.449018	2.520800	8.807936
C	-1.232663	1.113035	8.812361
H	-2.186587	0.599441	8.599426
H	-0.878534	0.819267	9.812981
C	-0.237398	0.752252	7.735643
H	-0.182171	-0.351375	7.661354
H	-0.639809	1.109650	6.778033

La-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2018.79330160

E(SCF)+ZPE(0 K)= -2018.084969

H(298 K)= -2018.045696

G(298 K)= -2018.150270

Lowest Frequency = 23.0026cm⁻¹

La	0.892641	4.001072	9.067559
N	3.110817	2.576732	9.111799
C	3.111367	1.265582	9.192787
C	4.226698	0.562715	9.703497
H	4.201905	-0.526346	9.768090
C	5.325858	1.272441	10.125537
H	6.192581	0.750680	10.538455
C	5.357184	2.687459	10.015931
C	4.197806	3.299741	9.479910
C	4.099924	4.729230	9.301018
O	2.988259	5.226878	8.835361
C	5.213183	5.479230	9.673989

H	5.187205	6.562427	9.533613
C	6.363470	4.864910	10.216171
H	7.208126	5.498056	10.498407
C	6.453537	3.502022	10.396494
H	7.350695	3.044122	10.816241
N	1.809800	4.481514	11.556840
C	2.343189	5.621584	11.930004
C	3.222422	5.705252	13.035990
H	3.651685	6.668685	13.316246
C	3.537116	4.561688	13.727991
H	4.228611	4.599197	14.573180
C	2.955910	3.320382	13.359778
C	2.071202	3.345589	12.254130
C	1.399839	2.156717	11.794164
O	0.614481	2.252904	10.760172
C	1.662453	0.977482	12.487719
H	1.159393	0.059585	12.174083
C	2.555467	0.955802	13.581046
H	2.734436	0.006180	14.091073
C	3.200190	2.090587	14.022083
H	3.885429	2.058782	14.870776
C	1.856465	0.548587	8.753128
H	2.124190	-0.413201	8.271776
H	1.280280	0.320482	9.659129
N	1.020304	1.360924	7.858151
C	1.690769	1.481120	6.553219
H	1.552504	0.558018	5.956708
H	2.767907	1.591798	6.733947
C	1.249722	2.663441	5.720395
H	1.793416	2.628561	4.759794
H	0.167939	2.639820	5.496343
O	1.557372	3.862115	6.400529
C	1.399258	5.009988	5.595010
H	0.423715	4.967724	5.076084
H	2.195002	5.046386	4.829743
C	1.474164	6.256098	6.441300
H	2.430118	6.289524	6.989281
H	1.381188	7.135721	5.781490
O	0.389677	6.228664	7.364759
C	0.059708	7.455118	7.981897
H	-1.011301	7.404521	8.220313
H	0.185845	8.286357	7.266610
C	0.903587	7.739240	9.211037
H	1.950008	7.792705	8.881479
H	0.633905	8.741838	9.601319
N	0.839448	6.721507	10.265022
C	2.052812	6.835262	11.087698
H	2.013114	7.737326	11.729957
H	2.905414	6.950712	10.405511
C	-0.343409	6.813667	11.127515
H	-0.576503	7.869804	11.371638
H	-0.098410	6.311778	12.073777
C	-1.617198	6.163777	10.617058
H	-2.377238	6.270395	11.410594
H	-2.026493	6.656388	9.718159
O	-1.401023	4.790410	10.351930
C	-2.585700	4.014581	10.358799

H	-3.237521	4.316525	9.515799
H	-3.144262	4.200439	11.292497
C	-2.264105	2.541967	10.291238
H	-1.597452	2.260881	11.121693
H	-3.209850	1.974626	10.359813
O	-1.610363	2.262469	9.068739
C	-1.233438	0.904997	8.902997
H	-2.135612	0.292181	8.727029
H	-0.745263	0.563233	9.827112
C	-0.314119	0.767909	7.702979
H	-0.232049	-0.311028	7.461486
H	-0.803754	1.243247	6.840047
O	-1.167890	4.003847	7.244361
H	-1.826577	3.429222	7.666012
H	-1.575872	4.822641	6.949699

Lu-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.47572041
 E(SCF)+ZPE(0 K)= -1909.809129
 H(298 K)= -1909.774289
 G(298 K)= -1909.872107
 Lowest Frequency = -59.0545cm⁻¹

C	5.828291	1.401974	17.294391
C	5.494764	1.663667	18.647186
C	5.201511	0.533143	19.453717
H	4.938531	0.675702	20.504744
C	5.205908	-0.721433	18.898641
H	4.932982	-1.599004	19.488098
C	5.561005	-0.876935	17.535483
C	5.540382	-2.245510	16.904654
H	6.402542	-2.809550	17.294729
H	4.650484	-2.795299	17.270385
C	4.281704	-2.132421	14.808675
H	3.532689	-2.769606	15.319397
H	4.396383	-2.500643	13.781206
C	3.727723	-0.719750	14.705489
H	2.760254	-0.767273	14.179706
H	3.557870	-0.251037	15.688488
C	4.145889	1.062205	13.081531
H	4.054180	2.013249	13.630736
H	3.162204	0.768074	12.680907
C	5.130192	1.199298	11.935614
H	5.166593	0.271780	11.341568
H	4.822788	2.040126	11.292841
C	7.347744	2.219941	11.766395
H	6.817460	2.898098	11.078234
H	7.986157	1.554377	11.162944
C	6.381324	-3.338724	14.935443
H	6.249485	-3.361338	13.852488
H	6.044020	-4.316139	15.335080
N	5.908438	0.142210	16.783230
N	5.593555	-2.227110	15.451700
O	6.303291	2.157801	15.121782
O	4.636994	0.059210	13.950962
O	6.405521	1.454373	12.493712

C	7.549674	-2.024487	12.152240
C	8.852256	-1.417848	12.096394
C	9.897096	-1.977671	11.318855
C	11.101752	-1.230240	11.251344
H	11.941165	-1.614113	10.666394
C	11.187276	-0.014422	11.881188
H	12.086002	0.600145	11.799434
C	10.086447	0.453584	12.641137
C	10.155160	1.800692	13.313331
H	10.651078	2.517730	12.629301
H	10.836053	1.713385	14.174970
C	8.992950	3.030011	15.021001
H	9.765859	3.823118	14.972486
H	8.035184	3.513938	15.218929
C	9.343119	2.098239	16.185254
H	8.903559	2.489896	17.115943
H	10.433965	2.043698	16.325595
C	9.802024	-0.241709	16.285607
H	10.527475	-0.339570	15.457545
H	10.349325	0.008204	17.208779
C	9.080177	-1.542027	16.503797
H	8.463605	-1.490096	17.419591
H	9.832431	-2.337729	16.627394
C	7.868686	-3.181452	15.264480
H	8.473450	-3.646244	14.470094
H	8.112933	-3.686872	16.211910
C	8.137356	3.066794	12.752520
H	7.408781	3.694137	13.281640
H	8.814102	3.734133	12.182834
N	8.985561	-0.248961	12.782210
N	8.867071	2.301719	13.765402
O	8.860870	0.767939	15.975952
O	8.251920	-1.808923	15.388483
O	6.629305	-1.438626	12.853193
C	7.373302	-3.212968	11.442411
H	6.386610	-3.681341	11.441997
C	8.431244	-3.787456	10.707393
H	8.247702	-4.719634	10.167847
C	9.675637	-3.198395	10.634265
H	10.478260	-3.641616	10.042615
C	6.037437	2.468396	16.352522
C	5.940652	3.772377	16.840304
H	6.065214	4.603187	16.142314
C	5.652715	4.023999	18.197959
H	5.588030	5.061096	18.535587
C	5.431373	3.004914	19.099802
H	5.186234	3.214361	20.142270

Lu-anti-KHQ(1+)

SCF (RwB97XD) = -1950.78065488

E(SCF)+ZPE(0 K)= -1950.097712

H(298 K)= -1950.060544

G(298 K)= -1950.163137

Lowest Frequency = 22.7375cm⁻¹

C	5.828291	1.401974	17.294391
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C	5.494764	1.663667	18.647186
C	5.201511	0.533143	19.453717
H	4.938531	0.675702	20.504744
C	5.205908	-0.721433	18.898641
H	4.932982	-1.599004	19.488098
C	5.561005	-0.876935	17.535483
C	5.540382	-2.245510	16.904654
H	6.402542	-2.809550	17.294729
H	4.650484	-2.795299	17.270385
C	4.281704	-2.132421	14.808675
H	3.532689	-2.769606	15.319397
H	4.396383	-2.500643	13.781206
C	3.727723	-0.719750	14.705489
H	2.760254	-0.767273	14.179706
H	3.557870	-0.251037	15.688488
C	4.145889	1.062205	13.081531
H	4.054180	2.013249	13.630736
H	3.162204	0.768074	12.680907
C	5.130192	1.199298	11.935614
H	5.166593	0.271780	11.341568
H	4.822788	2.040126	11.292841
C	7.347744	2.219941	11.766395
H	6.817460	2.898098	11.078234
H	7.986157	1.554377	11.162944
C	6.381324	-3.338724	14.935443
H	6.249485	-3.361338	13.852488
H	6.044020	-4.316139	15.335080
N	5.908438	0.142210	16.783230
N	5.593555	-2.227110	15.451700
O	6.303291	2.157801	15.121782
O	4.636994	0.059210	13.950962
O	6.405521	1.454373	12.493712
C	7.549674	-2.024487	12.152240
C	8.852256	-1.417848	12.096394
C	9.897096	-1.977671	11.318855
C	11.101752	-1.230240	11.251344
H	11.941165	-1.614113	10.666394
C	11.187276	-0.014422	11.881188
H	12.086002	0.600145	11.799434
C	10.086447	0.453584	12.641137
C	10.155160	1.800692	13.313331
H	10.651078	2.517730	12.629301
H	10.836053	1.713385	14.174970
C	8.992950	3.030011	15.021001
H	9.765859	3.823118	14.972486
H	8.035184	3.513938	15.218929
C	9.343119	2.098239	16.185254
H	8.903559	2.489896	17.115943
H	10.433965	2.043698	16.325595
C	9.802024	-0.241709	16.285607
H	10.527475	-0.339570	15.457545
H	10.349325	0.008204	17.208779
C	9.080177	-1.542027	16.503797
H	8.463605	-1.490096	17.419591
H	9.832431	-2.337729	16.627394
C	7.868686	-3.181452	15.264480
H	8.473450	-3.646244	14.470094

H	8.112933	-3.686872	16.211910
C	8.137356	3.066794	12.752520
H	7.408781	3.694137	13.281640
H	8.814102	3.734133	12.182834
N	8.985561	-0.248961	12.782210
N	8.867071	2.301719	13.765402
O	8.860870	0.767939	15.975952
O	8.251920	-1.808923	15.388483
O	6.629305	-1.438626	12.853193
C	7.373302	-3.212968	11.442411
H	6.386610	-3.681341	11.441997
C	8.431244	-3.787456	10.707393
H	8.247702	-4.719634	10.167847
C	9.675637	-3.198395	10.634265
H	10.478260	-3.641616	10.042615
C	6.037437	2.468396	16.352522
C	5.940652	3.772377	16.840304
H	6.065214	4.603187	16.142314
C	5.652715	4.023999	18.197959
H	5.588030	5.061096	18.535587
C	5.431373	3.004914	19.099802
H	5.186234	3.214361	20.142270
Lu	6.995365	0.136430	14.416843

Lu3+_lon

SCF (RwB97XD) = -38.4130689912
 E(SCF)+ZPE(0 K)= -38.413069
 H(298 K)= -38.410709
 G(298 K)= -38.430372

Lu 0.887400 3.945900 9.220400

Lu-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.49104648
 E(SCF)+ZPE(0 K)= -1909.822476
 H(298 K)= -1909.787618
 G(298 K)= -1909.884447
 Lowest Frequency = -38.5807cm-1

N	3.070425	2.662721	9.310581
C	3.151155	1.361520	9.486371
C	4.318930	0.768313	10.016252
H	4.351668	-0.309728	10.181001
C	5.402836	1.563656	10.310517
H	6.310839	1.123001	10.729188
C	5.369667	2.954624	10.029095
C	4.150441	3.453041	9.517867
C	3.969139	4.832873	9.156018
O	2.782381	5.199685	8.754838
C	5.074333	5.665094	9.298128
H	4.993053	6.712881	8.999853
C	6.291741	5.169769	9.821546
H	7.130700	5.861623	9.927765
C	6.454573	3.854042	10.196820
H	7.403975	3.493379	10.595878

N	1.968979	4.396556	11.516282
C	2.613136	5.485683	11.871266
C	3.575995	5.463537	12.905855
H	4.116895	6.376031	13.161405
C	3.814559	4.286157	13.577048
H	4.563823	4.247298	14.371416
C	3.057862	3.123745	13.274145
C	2.129429	3.249901	12.217614
C	1.263884	2.178024	11.814388
O	0.483892	2.396682	10.790331
C	1.357472	0.992997	12.534983
H	0.693761	0.161926	12.285640
C	2.298555	0.858472	13.583254
H	2.348017	-0.093412	14.117358
C	3.145256	1.880649	13.953665
H	3.859671	1.754806	14.768860
C	1.955377	0.556542	9.038297
H	2.298846	-0.423450	8.649686
H	1.309261	0.359666	9.904311
N	1.183106	1.286948	8.035957
C	1.932588	1.430291	6.791656
H	1.971953	0.481656	6.219353
H	2.966120	1.706214	7.034634
C	1.356784	2.508231	5.905527
H	2.042348	2.673302	5.056128
H	0.375928	2.226859	5.480694
O	1.217363	3.705297	6.642878
C	0.847878	4.786850	5.816087
H	-0.183928	4.636779	5.447818
H	1.522445	4.848622	4.944409
C	0.951033	6.060407	6.601769
H	1.991534	6.241394	6.912977
H	0.588706	6.892796	5.976780
O	0.128019	5.925565	7.753499
C	-0.234547	7.159760	8.351561
H	-1.255617	7.042420	8.726474
H	-0.274184	7.944211	7.578796
C	0.743288	7.591953	9.433597
H	1.720183	7.744935	8.955146
H	0.416057	8.574728	9.831533
N	0.930122	6.605924	10.490126
C	2.236950	6.745457	11.132669
H	2.261457	7.603090	11.833970
H	2.988735	6.934372	10.356204
C	-0.120847	6.582411	11.503315
H	-0.288562	7.585102	11.946276
H	0.217724	5.924883	12.313117
C	-1.451543	6.058125	10.998957
H	-2.059844	5.726749	11.857741
H	-2.026201	6.845145	10.481267
O	-1.238824	4.971125	10.115987
C	-2.413080	4.534490	9.452777
H	-2.440513	4.969134	8.437437
H	-3.309771	4.865760	9.999281
C	-2.409135	3.035474	9.401003
H	-2.364954	2.634883	10.428854
H	-3.337209	2.678810	8.919018

O	-1.282916	2.593002	8.674992
C	-1.175833	1.175874	8.765345
H	-2.145733	0.722854	8.495670
H	-0.930439	0.914108	9.805658
C	-0.126442	0.687761	7.801869
H	-0.084263	-0.417845	7.846657
H	-0.458018	0.943162	6.786893

Lu-syn-KHQ(1+)

SCF (RwB97XD) = -1950.78795512
 E(SCF)+ZPE(0 K)= -1950.103118
 H(298 K)= -1950.066708
 G(298 K)= -1950.165834
 Lowest Frequency = 40.4148cm⁻¹

Lu	0.976655	3.964926	9.268324
N	3.070425	2.662721	9.310581
C	3.151155	1.361520	9.486371
C	4.318930	0.768313	10.016252
H	4.351668	-0.309728	10.181001
C	5.402836	1.563656	10.310517
H	6.310839	1.123001	10.729188
C	5.369667	2.954624	10.029095
C	4.150441	3.453041	9.517867
C	3.969139	4.832873	9.156018
O	2.782381	5.199685	8.754838
C	5.074333	5.665094	9.298128
H	4.993053	6.712881	8.999853
C	6.291741	5.169769	9.821546
H	7.130700	5.861623	9.927765
C	6.454573	3.854042	10.196820
H	7.403975	3.493379	10.595878
N	1.968979	4.396556	11.516282
C	2.613136	5.485683	11.871266
C	3.575995	5.463537	12.905855
H	4.116895	6.376031	13.161405
C	3.814559	4.286157	13.577048
H	4.563823	4.247298	14.371416
C	3.057862	3.123745	13.274145
C	2.129429	3.249901	12.217614
C	1.263884	2.178024	11.814388
O	0.483892	2.396682	10.790331
C	1.357472	0.992997	12.534983
H	0.693761	0.161926	12.285640
C	2.298555	0.858472	13.583254
H	2.348017	-0.093412	14.117358
C	3.145256	1.880649	13.953665
H	3.859671	1.754806	14.768860
C	1.955377	0.556542	9.038297
H	2.298846	-0.423450	8.649686
H	1.309261	0.359666	9.904311
N	1.183106	1.286948	8.035957
C	1.932588	1.430291	6.791656
H	1.971953	0.481656	6.219353
H	2.966120	1.706214	7.034634
C	1.356784	2.508231	5.905527

H	2.042348	2.673302	5.056128
H	0.375928	2.226859	5.480694
O	1.217363	3.705297	6.642878
C	0.847878	4.786850	5.816087
H	-0.183928	4.636779	5.447818
H	1.522445	4.848622	4.944409
C	0.951033	6.060407	6.601769
H	1.991534	6.241394	6.912977
H	0.588706	6.892796	5.976780
O	0.128019	5.925565	7.753499
C	-0.234547	7.159760	8.351561
H	-1.255617	7.042420	8.726474
H	-0.274184	7.944211	7.578796
C	0.743288	7.591953	9.433597
H	1.720183	7.744935	8.955146
H	0.416057	8.574728	9.831533
N	0.930122	6.605924	10.490126
C	2.236950	6.745457	11.132669
H	2.261457	7.603090	11.833970
H	2.988735	6.934372	10.356204
C	-0.120847	6.582411	11.503315
H	-0.288562	7.585102	11.946276
H	0.217724	5.924883	12.313117
C	-1.451543	6.058125	10.998957
H	-2.059844	5.726749	11.857741
H	-2.026201	6.845145	10.481267
O	-1.238824	4.971125	10.115987
C	-2.413080	4.534490	9.452777
H	-2.440513	4.969134	8.437437
H	-3.309771	4.865760	9.999281
C	-2.409135	3.035474	9.401003
H	-2.364954	2.634883	10.428854
H	-3.337209	2.678810	8.919018
O	-1.282916	2.593002	8.674992
C	-1.175833	1.175874	8.765345
H	-2.145733	0.722854	8.495670
H	-0.930439	0.914108	9.805658
C	-0.126442	0.687761	7.801869
H	-0.084263	-0.417845	7.846657
H	-0.458018	0.943162	6.786893

Lu-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2027.14968320

E(SCF)+ZPE(0 K)= -2026.439895

H(298 K)= -2026.401148

G(298 K)= -2026.505439

Lowest Frequency = 21.4374cm⁻¹

Lu	1.095201	4.009959	9.123682
N	3.102931	2.626951	9.126609
C	3.124484	1.313274	9.197202
C	4.283155	0.624037	9.621985
H	4.272811	-0.465511	9.680906
C	5.409824	1.339754	9.954289
H	6.310696	0.822847	10.293702
C	5.423400	2.753233	9.831537

C	4.217607	3.350462	9.396804
C	4.093085	4.768945	9.194827
O	2.931490	5.226984	8.810728
C	5.221689	5.540386	9.446677
H	5.174419	6.619442	9.283224
C	6.422990	4.943756	9.894782
H	7.284517	5.588233	10.084622
C	6.542013	3.585818	10.093295
H	7.479475	3.144571	10.435546
N	1.854673	4.485916	11.460456
C	2.361375	5.616493	11.897244
C	3.105563	5.678859	13.098484
H	3.521825	6.632587	13.427062
C	3.292913	4.533073	13.835279
H	3.873283	4.559581	14.760690
C	2.702861	3.312972	13.415430
C	1.976802	3.360168	12.203967
C	1.279055	2.219066	11.684071
O	0.637800	2.375261	10.560980
C	1.350101	1.043458	12.423365
H	0.815758	0.156582	12.074163
C	2.096588	0.989927	13.624008
H	2.133395	0.045736	14.172430
C	2.766892	2.084549	14.123764
H	3.330332	2.024154	15.056282
C	1.867067	0.582978	8.794765
H	2.141003	-0.376542	8.311486
H	1.307817	0.343632	9.706577
N	1.020880	1.389219	7.910343
C	1.685429	1.502266	6.603915
H	1.518263	0.590646	5.997073
H	2.767826	1.581778	6.768997
C	1.266617	2.704518	5.797099
H	1.776289	2.659112	4.818319
H	0.177670	2.716319	5.609039
O	1.635972	3.888847	6.470640
C	1.466998	5.019233	5.642889
H	0.500178	4.944546	5.110203
H	2.270070	5.057184	4.885281
C	1.487154	6.287437	6.450830
H	2.432962	6.372765	7.007349
H	1.373015	7.142251	5.761449
O	0.391683	6.248016	7.355949
C	0.083561	7.475029	7.979096
H	-0.980845	7.436204	8.246074
H	0.199691	8.306747	7.262384
C	0.962479	7.739200	9.184372
H	2.001506	7.787238	8.832190
H	0.712851	8.737858	9.597365
N	0.908411	6.706109	10.220780
C	2.116417	6.831399	11.047782
H	2.070443	7.733844	11.688488
H	2.976158	6.945794	10.375249
C	-0.281263	6.785961	11.075923
H	-0.563899	7.841235	11.262583
H	-0.025897	6.348713	12.051009
C	-1.515478	6.050310	10.592697

H	-2.302114	6.210016	11.351591
H	-1.911250	6.451009	9.642620
O	-1.261547	4.668032	10.456534
C	-2.465140	3.918499	10.491692
H	-3.133176	4.247572	9.671123
H	-2.989811	4.123163	11.441665
C	-2.240479	2.429550	10.399609
H	-1.502055	2.114440	11.151179
H	-3.206416	1.929771	10.597387
O	-1.776287	2.102722	9.109511
C	-1.239964	0.806793	8.940531
H	-2.060812	0.091284	8.754449
H	-0.721380	0.509765	9.863064
C	-0.301459	0.768439	7.744840
H	-0.180907	-0.295169	7.453830
H	-0.809475	1.260844	6.902420
O	-0.810344	3.933214	7.669314
H	-1.500097	3.338932	8.033918
H	-1.152007	4.762948	7.321168

Nd-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.50064662

E(SCF)+ZPE(0 K)= -1909.833961

H(298 K)= -1909.800097

G(298 K)= -1909.894581

Lowest Frequency = -48.0591cm⁻¹

C	5.858766	1.379640	17.387924
C	5.711695	1.601820	18.782260
C	5.382139	0.467484	19.569125
H	5.272299	0.579501	20.650730
C	5.165583	-0.749293	18.969052
H	4.864487	-1.619607	19.555803
C	5.320817	-0.864483	17.565687
C	4.913422	-2.132193	16.853332
H	5.154952	-3.012817	17.473448
H	3.810105	-2.118974	16.816865
C	4.393843	-2.388189	14.489788
H	3.636073	-3.144862	14.774998
H	4.869711	-2.702386	13.552722
C	3.690964	-1.068256	14.226429
H	2.870225	-1.244137	13.511660
H	3.255577	-0.633218	15.143877
C	4.148886	0.829295	12.768110
H	3.938415	1.761317	13.318473
H	3.227942	0.485366	12.269492
C	5.222070	1.060079	11.724613
H	5.390038	0.148217	11.126837
H	4.908292	1.879284	11.056672
C	7.341046	2.255948	11.745718
H	6.797000	2.979647	11.116086
H	7.995277	1.660087	11.088274
C	6.442566	-3.335570	15.402162
H	6.770728	-3.382968	14.357071
H	6.027620	-4.325488	15.682946
N	5.707453	0.150544	16.825752

N	5.446061	-2.271071	15.501288
O	6.249727	2.198527	15.207265
O	4.619461	-0.157527	13.665290
O	6.411893	1.414456	12.404058
C	7.697275	-2.170652	12.048080
C	8.880383	-1.388662	11.805007
C	9.797574	-1.743028	10.780245
C	10.882061	-0.854807	10.568347
H	11.613205	-1.076024	9.786907
C	10.989673	0.287440	11.322489
H	11.798509	1.000362	11.151767
C	10.033486	0.539833	12.335216
C	10.148972	1.771058	13.195320
H	10.654274	2.577274	12.627974
H	10.828816	1.521790	14.024062
C	9.085536	2.977881	14.988546
H	9.784162	3.827968	14.852035
H	8.116393	3.386042	15.284721
C	9.628122	2.111570	16.110236
H	9.460238	2.621414	17.073895
H	10.714860	1.949548	16.003652
C	9.748727	-0.135115	16.815441
H	10.572806	-0.480448	16.164657
H	10.184814	0.292459	17.733811
C	8.863110	-1.283037	17.209143
H	8.124347	-0.961792	17.966496
H	9.495736	-2.071994	17.649570
C	7.631114	-3.073126	16.301391
H	8.406771	-3.836709	16.125355
H	7.336780	-3.136442	17.363296
C	8.102298	3.040969	12.799341
H	7.351631	3.586284	13.386473
H	8.748598	3.781917	12.288135
N	9.037643	-0.282715	12.583529
N	8.879166	2.231803	13.746893
O	8.987910	0.840137	16.130072
O	8.181629	-1.777516	16.070518
O	6.866780	-1.763717	12.959801
C	7.520750	-3.315943	11.273359
H	6.628587	-3.924052	11.437465
C	8.455592	-3.679453	10.282244
H	8.274841	-4.585225	9.698591
C	9.574893	-2.918789	10.021270
H	10.281403	-3.199662	9.238524
C	6.121868	2.463891	16.471240
C	6.232593	3.739113	17.031041
H	6.387616	4.590025	16.363859
C	6.117470	3.945783	18.421485
H	6.216068	4.963113	18.807976
C	5.869680	2.911670	19.298923
H	5.767390	3.089236	20.370729

Nd-anti-KHQ(1+)

SCF (RwB97XD) = -1944.31022510
 E(SCF)+ZPE(0 K)= -1943.627836
 H(298 K)= -1943.590584

G(298 K)= -1943.693732
Lowest Frequency = 13.3797cm⁻¹

C	5.858766	1.379640	17.387924
C	5.711695	1.601820	18.782260
C	5.382139	0.467484	19.569125
H	5.272299	0.579501	20.650730
C	5.165583	-0.749293	18.969052
H	4.864487	-1.619607	19.555803
C	5.320817	-0.864483	17.565687
C	4.913422	-2.132193	16.853332
H	5.154952	-3.012817	17.473448
H	3.810105	-2.118974	16.816865
C	4.393843	-2.388189	14.489788
H	3.636073	-3.144862	14.774998
H	4.869711	-2.702386	13.552722
C	3.690964	-1.068256	14.226429
H	2.870225	-1.244137	13.511660
H	3.255577	-0.633218	15.143877
C	4.148886	0.829295	12.768110
H	3.938415	1.761317	13.318473
H	3.227942	0.485366	12.269492
C	5.222070	1.060079	11.724613
H	5.390038	0.148217	11.126837
H	4.908292	1.879284	11.056672
C	7.341046	2.255948	11.745718
H	6.797000	2.979647	11.116086
H	7.995277	1.660087	11.088274
C	6.442566	-3.335570	15.402162
H	6.770728	-3.382968	14.357071
H	6.027620	-4.325488	15.682946
N	5.707453	0.150544	16.825752
N	5.446061	-2.271071	15.501288
O	6.249727	2.198527	15.207265
O	4.619461	-0.157527	13.665290
O	6.411893	1.414456	12.404058
C	7.697275	-2.170652	12.048080
C	8.880383	-1.388662	11.805007
C	9.797574	-1.743028	10.780245
C	10.882061	-0.854807	10.568347
H	11.613205	-1.076024	9.786907
C	10.989673	0.287440	11.322489
H	11.798509	1.000362	11.151767
C	10.033486	0.539833	12.335216
C	10.148972	1.771058	13.195320
H	10.654274	2.577274	12.627974
H	10.828816	1.521790	14.024062
C	9.085536	2.977881	14.988546
H	9.784162	3.827968	14.852035
H	8.116393	3.386042	15.284721
C	9.628122	2.111570	16.110236
H	9.460238	2.621414	17.073895
H	10.714860	1.949548	16.003652
C	9.748727	-0.135115	16.815441
H	10.572806	-0.480448	16.164657
H	10.184814	0.292459	17.733811
C	8.863110	-1.283037	17.209143

H	8.124347	-0.961792	17.966496
H	9.495736	-2.071994	17.649570
C	7.631114	-3.073126	16.301391
H	8.406771	-3.836709	16.125355
H	7.336780	-3.136442	17.363296
C	8.102298	3.040969	12.799341
H	7.351631	3.586284	13.386473
H	8.748598	3.781917	12.288135
N	9.037643	-0.282715	12.583529
N	8.879166	2.231803	13.746893
O	8.987910	0.840137	16.130072
O	8.181629	-1.777516	16.070518
O	6.866780	-1.763717	12.959801
C	7.520750	-3.315943	11.273359
H	6.628587	-3.924052	11.437465
C	8.455592	-3.679453	10.282244
H	8.274841	-4.585225	9.698591
C	9.574893	-2.918789	10.021270
H	10.281403	-3.199662	9.238524
C	6.121868	2.463891	16.471240
C	6.232593	3.739113	17.031041
H	6.387616	4.590025	16.363859
C	6.117470	3.945783	18.421485
H	6.216068	4.963113	18.807976
C	5.869680	2.911670	19.298923
H	5.767390	3.089236	20.370729
Nd	7.045009	0.053332	14.476569

Nd3+_lon

SCF (RwB97XD) = -32.0519929666
 E(SCF)+ZPE(0 K)= -32.051993
 H(298 K)= -32.049633
 G(298 K)= -32.069000

Nd	0.887400	3.945900	9.220400
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Nd-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.50951265
 E(SCF)+ZPE(0 K)= -1909.841836
 H(298 K)= -1909.805814
 G(298 K)= -1909.906695
 Lowest Frequency = -31.7202cm-1

N	3.104500	2.604706	9.228479
C	3.127097	1.299426	9.378650
C	4.254313	0.648479	9.929205
H	4.245767	-0.433915	10.066630
C	5.348430	1.400337	10.291200
H	6.224338	0.917925	10.731637
C	5.368076	2.802837	10.068291
C	4.191184	3.360967	9.516340
C	4.068279	4.766379	9.216163
O	2.924798	5.202141	8.763021
C	5.187973	5.553785	9.472419
H	5.150918	6.618601	9.230808

C	6.359489	4.996336	10.033334
H	7.208417	5.656883	10.225608
C	6.466460	3.657521	10.342117
H	7.381097	3.247484	10.773458
N	1.931675	4.422862	11.567586
C	2.557670	5.532216	11.888878
C	3.542036	5.551792	12.903863
H	4.062115	6.481839	13.138735
C	3.836708	4.386624	13.572195
H	4.606312	4.376825	14.347772
C	3.126662	3.191331	13.282868
C	2.158682	3.276186	12.255149
C	1.348536	2.150845	11.866480
O	0.514904	2.310793	10.875023
C	1.549242	0.965650	12.568297
H	0.936765	0.095264	12.321701
C	2.524851	0.879372	13.587193
H	2.653165	-0.073970	14.105465
C	3.311998	1.951784	13.947150
H	4.058257	1.865282	14.738613
C	1.893600	0.552099	8.926969
H	2.188939	-0.425681	8.496603
H	1.269683	0.353186	9.809657
N	1.101892	1.331155	7.967490
C	1.819836	1.462546	6.696998
H	1.823156	0.508370	6.133179
H	2.864398	1.715934	6.917731
C	1.257441	2.547140	5.805399
H	1.923582	2.660877	4.932543
H	0.252014	2.301736	5.417169
O	1.198495	3.761619	6.524423
C	0.946158	4.883655	5.704769
H	-0.064708	4.803673	5.264411
H	1.682624	4.928369	4.883514
C	1.066451	6.130882	6.537464
H	2.091219	6.232355	6.931387
H	0.809625	7.003130	5.913904
O	0.148134	6.019618	7.619193
C	-0.199471	7.241625	8.246338
H	-1.227998	7.120853	8.600993
H	-0.214848	8.051483	7.497941
C	0.764555	7.627797	9.360364
H	1.758958	7.752908	8.909693
H	0.461624	8.618160	9.757845
N	0.895051	6.633393	10.425048
C	2.188782	6.768996	11.106182
H	2.201294	7.650136	11.777838
H	2.961303	6.923226	10.341535
C	-0.179221	6.663602	11.419426
H	-0.309605	7.680092	11.842817
H	0.123832	6.005475	12.243811
C	-1.529779	6.185230	10.922669
H	-2.168586	5.975793	11.798109
H	-2.050032	6.952087	10.323234
O	-1.365377	5.005910	10.158993
C	-2.572869	4.445283	9.673021
H	-2.783814	4.837329	8.661797

H	-3.412592	4.719144	10.332183
C	-2.448698	2.946304	9.663371
H	-2.216492	2.588383	10.681876
H	-3.407465	2.504899	9.337273
O	-1.412813	2.555219	8.784223
C	-1.232455	1.142726	8.810977
H	-2.194272	0.650723	8.583227
H	-0.907862	0.853463	9.822642
C	-0.224272	0.745776	7.761456
H	-0.172821	-0.359558	7.717860
H	-0.609015	1.078391	6.788044

Nd-syn-KHQ(1+)

SCF (RwB97XD) = -1944.32377135
 E(SCF)+ZPE(0 K)= -1943.640223
 H(298 K)= -1943.603651
 G(298 K)= -1943.702707
 Lowest Frequency = 40.4939cm⁻¹

Nd	0.916804	3.972201	9.210283
N	3.104500	2.604706	9.228479
C	3.127097	1.299426	9.378650
C	4.254313	0.648479	9.929205
H	4.245767	-0.433915	10.066630
C	5.348430	1.400337	10.291200
H	6.224338	0.917925	10.731637
C	5.368076	2.802837	10.068291
C	4.191184	3.360967	9.516340
C	4.068279	4.766379	9.216163
O	2.924798	5.202141	8.763021
C	5.187973	5.553785	9.472419
H	5.150918	6.618601	9.230808
C	6.359489	4.996336	10.033334
H	7.208417	5.656883	10.225608
C	6.466460	3.657521	10.342117
H	7.381097	3.247484	10.773458
N	1.931675	4.422862	11.567586
C	2.557670	5.532216	11.888878
C	3.542036	5.551792	12.903863
H	4.062115	6.481839	13.138735
C	3.836708	4.386624	13.572195
H	4.606312	4.376825	14.347772
C	3.126662	3.191331	13.282868
C	2.158682	3.276186	12.255149
C	1.348536	2.150845	11.866480
O	0.514904	2.310793	10.875023
C	1.549242	0.965650	12.568297
H	0.936765	0.095264	12.321701
C	2.524851	0.879372	13.587193
H	2.653165	-0.073970	14.105465
C	3.311998	1.951784	13.947150
H	4.058257	1.865282	14.738613
C	1.893600	0.552099	8.926969
H	2.188939	-0.425681	8.496603
H	1.269683	0.353186	9.809657
N	1.101892	1.331155	7.967490

C	1.819836	1.462546	6.696998
H	1.823156	0.508370	6.133179
H	2.864398	1.715934	6.917731
C	1.257441	2.547140	5.805399
H	1.923582	2.660877	4.932543
H	0.252014	2.301736	5.417169
O	1.198495	3.761619	6.524423
C	0.946158	4.883655	5.704769
H	-0.064708	4.803673	5.264411
H	1.682624	4.928369	4.883514
C	1.066451	6.130882	6.537464
H	2.091219	6.232355	6.931387
H	0.809625	7.003130	5.913904
O	0.148134	6.019618	7.619193
C	-0.199471	7.241625	8.246338
H	-1.227998	7.120853	8.600993
H	-0.214848	8.051483	7.497941
C	0.764555	7.627797	9.360364
H	1.758958	7.752908	8.909693
H	0.461624	8.618160	9.757845
N	0.895051	6.633393	10.425048
C	2.188782	6.768996	11.106182
H	2.201294	7.650136	11.777838
H	2.961303	6.923226	10.341535
C	-0.179221	6.663602	11.419426
H	-0.309605	7.680092	11.842817
H	0.123832	6.005475	12.243811
C	-1.529779	6.185230	10.922669
H	-2.168586	5.975793	11.798109
H	-2.050032	6.952087	10.323234
O	-1.365377	5.005910	10.158993
C	-2.572869	4.445283	9.673021
H	-2.783814	4.837329	8.661797
H	-3.412592	4.719144	10.332183
C	-2.448698	2.946304	9.663371
H	-2.216492	2.588383	10.681876
H	-3.407465	2.504899	9.337273
O	-1.412813	2.555219	8.784223
C	-1.232455	1.142726	8.810977
H	-2.194272	0.650723	8.583227
H	-0.907862	0.853463	9.822642
C	-0.224272	0.745776	7.761456
H	-0.172821	-0.359558	7.717860
H	-0.609015	1.078391	6.788044

Nd-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2020.68624387

E(SCF)+ZPE(0 K)= -2019.977368

H(298 K)= -2019.938279

G(298 K)= -2020.042591

Lowest Frequency = 24.9564cm⁻¹

Nd	0.928096	4.002562	9.077741
N	3.095568	2.592631	9.124547
C	3.105233	1.281198	9.206786
C	4.231707	0.585816	9.702931

H	4.212393	-0.503166	9.770328
C	5.335632	1.300714	10.103796
H	6.211142	0.783558	10.503756
C	5.360320	2.714849	9.983904
C	4.188330	3.318563	9.467867
C	4.081334	4.743660	9.275626
O	2.954911	5.225673	8.828009
C	5.198170	5.503403	9.613810
H	5.166019	6.584672	9.460579
C	6.362399	4.898495	10.138032
H	7.210901	5.537477	10.394223
C	6.461279	3.538174	10.332098
H	7.369401	3.088526	10.736918
N	1.821867	4.479764	11.527437
C	2.356754	5.614503	11.914867
C	3.215302	5.687362	13.037553
H	3.647905	6.646410	13.327495
C	3.502540	4.540592	13.736961
H	4.176161	4.570999	14.596738
C	2.910833	3.307244	13.359206
C	2.053738	3.343956	12.233401
C	1.368810	2.169681	11.761907
O	0.611616	2.286730	10.709171
C	1.586408	0.987656	12.465017
H	1.069753	0.079357	12.145521
C	2.453987	0.952269	13.579245
H	2.599856	0.001505	14.097550
C	3.113566	2.074348	14.030600
H	3.777579	2.030682	14.895470
C	1.853888	0.557764	8.771229
H	2.127630	-0.401609	8.288298
H	1.278486	0.322811	9.675332
N	1.017692	1.368380	7.875973
C	1.691837	1.483878	6.572770
H	1.547331	0.562763	5.974770
H	2.769889	1.586018	6.752954
C	1.258975	2.670577	5.744943
H	1.798760	2.634668	4.782157
H	0.176038	2.655500	5.525807
O	1.577993	3.865299	6.426714
C	1.418823	5.007759	5.613998
H	0.446447	4.956259	5.089577
H	2.217782	5.043572	4.852009
C	1.478675	6.260342	6.449471
H	2.434274	6.312328	6.995235
H	1.371510	7.132790	5.782163
O	0.396326	6.224523	7.374235
C	0.064554	7.452524	7.986633
H	-1.005030	7.401258	8.230663
H	0.185516	8.281077	7.267402
C	0.914296	7.739071	9.209846
H	1.958465	7.799076	8.874703
H	0.642075	8.738569	9.606202
N	0.858697	6.715575	10.257576
C	2.072761	6.831809	11.077506
H	2.030846	7.730602	11.724206
H	2.925120	6.953656	10.396549

C	-0.322024	6.801811	11.122762
H	-0.564175	7.856908	11.362417
H	-0.072694	6.306796	12.071431
C	-1.588510	6.138396	10.615162
H	-2.350145	6.244953	11.407181
H	-2.001397	6.622837	9.713477
O	-1.364467	4.764666	10.358399
C	-2.556218	3.997876	10.378254
H	-3.213575	4.306726	9.541946
H	-3.102867	4.192427	11.317183
C	-2.260301	2.520812	10.307572
H	-1.586398	2.229811	11.128176
H	-3.215336	1.971091	10.393635
O	-1.634166	2.233383	9.075716
C	-1.238125	0.884419	8.909556
H	-2.129251	0.256986	8.727678
H	-0.748913	0.545606	9.834272
C	-0.311404	0.764839	7.713607
H	-0.217065	-0.311556	7.465015
H	-0.802456	1.240504	6.851750
O	-1.080719	3.990257	7.324323
H	-1.755255	3.421999	7.732272
H	-1.458394	4.824947	7.032941

Pr-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.50408090
 E(SCF)+ZPE(0 K)= -1909.837596
 H(298 K)= -1909.802673
 G(298 K)= -1909.901681
 Lowest Frequency = -47.9884cm⁻¹

C	5.846347	1.384091	17.388088
C	5.689097	1.613240	18.780559
C	5.335644	0.486583	19.567887
H	5.216757	0.604109	20.647956
C	5.108784	-0.729798	18.970208
H	4.791080	-1.593859	19.557416
C	5.276530	-0.852182	17.569140
C	4.862601	-2.116113	16.854040
H	5.052091	-2.997124	17.492143
H	3.763236	-2.070191	16.769436
C	4.434899	-2.438880	14.480616
H	3.678041	-3.200899	14.753706
H	4.950227	-2.764655	13.568450
C	3.722610	-1.136077	14.164567
H	2.930945	-1.339882	13.424505
H	3.247529	-0.688662	15.056274
C	4.178021	0.790549	12.753485
H	3.965824	1.704062	13.333713
H	3.256445	0.458956	12.247535
C	5.246578	1.056917	11.714632
H	5.412596	0.165653	11.085664
H	4.927740	1.895771	11.074041
C	7.359355	2.257060	11.757521
H	6.807011	2.989925	11.146020
H	8.015812	1.682085	11.083966

C	6.453756	-3.344827	15.495688
H	6.828817	-3.411827	14.466968
H	6.030681	-4.330155	15.780443
N	5.682720	0.155471	16.829268
N	5.447546	-2.284484	15.526949
O	6.270823	2.190519	15.208441
O	4.656547	-0.222845	13.616286
O	6.439147	1.392004	12.398589
C	7.737879	-2.206899	12.042947
C	8.882989	-1.384307	11.753620
C	9.749632	-1.687576	10.669460
C	10.805171	-0.772682	10.428746
H	11.496955	-0.955620	9.602834
C	10.935655	0.345785	11.214664
H	11.724292	1.076739	11.026866
C	10.028806	0.549461	12.281752
C	10.167010	1.752465	13.177577
H	10.675362	2.571511	12.631837
H	10.849187	1.468734	13.993121
C	9.131208	2.948308	14.995741
H	9.825237	3.800721	14.850401
H	8.165922	3.353001	15.310291
C	9.692726	2.082752	16.106523
H	9.568874	2.608940	17.068271
H	10.771723	1.893162	15.968006
C	9.742829	-0.130823	16.910449
H	10.578906	-0.518043	16.299902
H	10.160244	0.327368	17.822823
C	8.822746	-1.244752	17.322945
H	8.066031	-0.879139	18.041512
H	9.425310	-2.025822	17.816370
C	7.599717	-3.055098	16.440068
H	8.376686	-3.829808	16.330187
H	7.255824	-3.074688	17.488860
C	8.117562	3.027440	12.823844
H	7.364835	3.554744	13.424577
H	8.756530	3.782521	12.324010
N	9.058569	-0.296600	12.553167
N	8.905584	2.207784	13.753527
O	9.022036	0.829373	16.163089
O	8.170293	-1.773551	16.182882
O	6.956275	-1.853308	13.018020
C	7.542593	-3.330887	11.242250
H	6.679205	-3.969103	11.441742
C	8.424753	-3.639427	10.186440
H	8.231140	-4.531187	9.585585
C	9.509647	-2.844164	9.886649
H	10.176872	-3.084292	9.057261
C	6.135300	2.461443	16.470227
C	6.260690	3.736364	17.027800
H	6.435652	4.582816	16.359839
C	6.134838	3.949311	18.416370
H	6.245504	4.966266	18.800609
C	5.862114	2.922245	19.294630
H	5.752031	3.104958	20.364796

Pr-anti-KHQ(1+)

SCF (RwB97XD) = -1943.69177634
 E(SCF)+ZPE(0 K)= -1943.009540
 H(298 K)= -1942.972233
 G(298 K)= -1943.075528
 Lowest Frequency = 15.0646cm⁻¹

C	5.846347	1.384091	17.388088
C	5.689097	1.613240	18.780559
C	5.335644	0.486583	19.567887
H	5.216757	0.604109	20.647956
C	5.108784	-0.729798	18.970208
H	4.791080	-1.593859	19.557416
C	5.276530	-0.852182	17.569140
C	4.862601	-2.116113	16.854040
H	5.052091	-2.997124	17.492143
H	3.763236	-2.070191	16.769436
C	4.434899	-2.438880	14.480616
H	3.678041	-3.200899	14.753706
H	4.950227	-2.764655	13.568450
C	3.722610	-1.136077	14.164567
H	2.930945	-1.339882	13.424505
H	3.247529	-0.688662	15.056274
C	4.178021	0.790549	12.753485
H	3.965824	1.704062	13.333713
H	3.256445	0.458956	12.247535
C	5.246578	1.056917	11.714632
H	5.412596	0.165653	11.085664
H	4.927740	1.895771	11.074041
C	7.359355	2.257060	11.757521
H	6.807011	2.989925	11.146020
H	8.015812	1.682085	11.083966
C	6.453756	-3.344827	15.495688
H	6.828817	-3.411827	14.466968
H	6.030681	-4.330155	15.780443
N	5.682720	0.155471	16.829268
N	5.447546	-2.284484	15.526949
O	6.270823	2.190519	15.208441
O	4.656547	-0.222845	13.616286
O	6.439147	1.392004	12.398589
C	7.737879	-2.206899	12.042947
C	8.882989	-1.384307	11.753620
C	9.749632	-1.687576	10.669460
C	10.805171	-0.772682	10.428746
H	11.496955	-0.955620	9.602834
C	10.935655	0.345785	11.214664
H	11.724292	1.076739	11.026866
C	10.028806	0.549461	12.281752
C	10.167010	1.752465	13.177577
H	10.675362	2.571511	12.631837
H	10.849187	1.468734	13.993121
C	9.131208	2.948308	14.995741
H	9.825237	3.800721	14.850401
H	8.165922	3.353001	15.310291
C	9.692726	2.082752	16.106523
H	9.568874	2.608940	17.068271
H	10.771723	1.893162	15.968006

C	9.742829	-0.130823	16.910449
H	10.578906	-0.518043	16.299902
H	10.160244	0.327368	17.822823
C	8.822746	-1.244752	17.322945
H	8.066031	-0.879139	18.041512
H	9.425310	-2.025822	17.816370
C	7.599717	-3.055098	16.440068
H	8.376686	-3.829808	16.330187
H	7.255824	-3.074688	17.488860
C	8.117562	3.027440	12.823844
H	7.364835	3.554744	13.424577
H	8.756530	3.782521	12.324010
N	9.058569	-0.296600	12.553167
N	8.905584	2.207784	13.753527
O	9.022036	0.829373	16.163089
O	8.170293	-1.773551	16.182882
O	6.956275	-1.853308	13.018020
C	7.542593	-3.330887	11.242250
H	6.679205	-3.969103	11.441742
C	8.424753	-3.639427	10.186440
H	8.231140	-4.531187	9.585585
C	9.509647	-2.844164	9.886649
H	10.176872	-3.084292	9.057261
C	6.135300	2.461443	16.470227
C	6.260690	3.736364	17.027800
H	6.435652	4.582816	16.359839
C	6.134838	3.949311	18.416370
H	6.245504	4.966266	18.800609
C	5.862114	2.922245	19.294630
H	5.752031	3.104958	20.364796
Pr	7.077519	0.022200	14.492220

Pr3+_Ion

SCF (RwB97XD) = -31.4459258508
 E(SCF)+ZPE(0 K)= -31.445926
 H(298 K)= -31.443565
 G(298 K)= -31.462922

Pr 0.887400 3.945900 9.220400

Pr-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.51139089
 E(SCF)+ZPE(0 K)= -1909.843980
 H(298 K)= -1909.808788
 G(298 K)= -1909.906538
 Lowest Frequency = -31.1384cm⁻¹

N	3.113140	2.599151	9.226567
C	3.130648	1.293714	9.375076
C	4.251723	0.638587	9.933310
H	4.239718	-0.444094	10.068261
C	5.343806	1.387415	10.307263
H	6.214772	0.902111	10.754278
C	5.367800	2.790854	10.090445
C	4.197672	3.353500	9.528108

C	4.080720	4.761278	9.233789
O	2.944530	5.203491	8.768890
C	5.198930	5.545006	9.508360
H	5.166028	6.611315	9.272764
C	6.363059	4.982715	10.079228
H	7.210662	5.640854	10.285167
C	6.464508	3.641893	10.381187
H	7.373455	3.227772	10.820582
N	1.917814	4.429488	11.575852
C	2.537631	5.542702	11.895592
C	3.518779	5.570170	12.913604
H	4.033082	6.503533	13.148085
C	3.818726	4.407822	13.584233
H	4.586355	4.403759	14.361818
C	3.118245	3.207163	13.293701
C	2.151110	3.284149	12.264167
C	1.351522	2.150948	11.874289
O	0.516534	2.301103	10.882627
C	1.563317	0.967420	12.576163
H	0.959728	0.091366	12.327698
C	2.537653	0.889746	13.596617
H	2.674185	-0.062611	14.114620
C	3.313793	1.969572	13.958396
H	4.059580	1.890062	14.751039
C	1.896092	0.549699	8.919704
H	2.189575	-0.428343	8.488703
H	1.271747	0.351725	9.802479
N	1.104384	1.329947	7.960351
C	1.822844	1.460710	6.689586
H	1.825896	0.505897	6.126848
H	2.867409	1.713437	6.911329
C	1.263287	2.544727	5.794807
H	1.929360	2.652596	4.921167
H	0.256654	2.301806	5.408138
O	1.209732	3.762011	6.509773
C	0.969739	4.885877	5.688536
H	-0.037611	4.811183	5.239354
H	1.713672	4.927544	4.873878
C	1.088704	6.132645	6.523102
H	2.110033	6.227579	6.927959
H	0.844778	7.006680	5.896787
O	0.157578	6.027599	7.594616
C	-0.190057	7.249752	8.221403
H	-1.221592	7.130872	8.568262
H	-0.197364	8.061190	7.474497
C	0.766275	7.631624	9.343768
H	1.765173	7.751740	8.901622
H	0.464605	8.623811	9.737583
N	0.883891	6.638504	10.411997
C	2.172148	6.775416	11.104532
H	2.179221	7.660038	11.771642
H	2.950975	6.925279	10.345218
C	-0.199264	6.674626	11.397109
H	-0.331342	7.693490	11.814226
H	0.096800	6.020417	12.227210
C	-1.547842	6.195546	10.894776
H	-2.194002	6.001286	11.768370

H	-2.060531	6.955960	10.280872
O	-1.382554	5.004616	10.149655
C	-2.588625	4.430091	9.676311
H	-2.813059	4.816185	8.665685
H	-3.424934	4.698303	10.342274
C	-2.451150	2.931680	9.671257
H	-2.206312	2.579433	10.688767
H	-3.409559	2.481567	9.356212
O	-1.420851	2.544839	8.783178
C	-1.230371	1.133454	8.807758
H	-2.189308	0.634914	8.582063
H	-0.900770	0.845220	9.818174
C	-0.222235	0.744248	7.754543
H	-0.169111	-0.360796	7.705476
H	-0.609182	1.081043	6.783356

Pr-syn-KHQ(1+)

SCF (RwB97XD) = -1943.70512542
 E(SCF)+ZPE(0 K)= -1943.021909
 H(298 K)= -1942.985234
 G(298 K)= -1943.084591
 Lowest Frequency = 41.2453cm⁻¹

Pr	0.912933	3.972685	9.201510
N	3.113140	2.599151	9.226567
C	3.130648	1.293714	9.375076
C	4.251723	0.638587	9.933310
H	4.239718	-0.444094	10.068261
C	5.343806	1.387415	10.307263
H	6.214772	0.902111	10.754278
C	5.367800	2.790854	10.090445
C	4.197672	3.353500	9.528108
C	4.080720	4.761278	9.233789
O	2.944530	5.203491	8.768890
C	5.198930	5.545006	9.508360
H	5.166028	6.611315	9.272764
C	6.363059	4.982715	10.079228
H	7.210662	5.640854	10.285167
C	6.464508	3.641893	10.381187
H	7.373455	3.227772	10.820582
N	1.917814	4.429488	11.575852
C	2.537631	5.542702	11.895592
C	3.518779	5.570170	12.913604
H	4.033082	6.503533	13.148085
C	3.818726	4.407822	13.584233
H	4.586355	4.403759	14.361818
C	3.118245	3.207163	13.293701
C	2.151110	3.284149	12.264167
C	1.351522	2.150948	11.874289
O	0.516534	2.301103	10.882627
C	1.563317	0.967420	12.576163
H	0.959728	0.091366	12.327698
C	2.537653	0.889746	13.596617
H	2.674185	-0.062611	14.114620
C	3.313793	1.969572	13.958396
H	4.059580	1.890062	14.751039

C	1.896092	0.549699	8.919704
H	2.189575	-0.428343	8.488703
H	1.271747	0.351725	9.802479
N	1.104384	1.329947	7.960351
C	1.822844	1.460710	6.689586
H	1.825896	0.505897	6.126848
H	2.867409	1.713437	6.911329
C	1.263287	2.544727	5.794807
H	1.929360	2.652596	4.921167
H	0.256654	2.301806	5.408138
O	1.209732	3.762011	6.509773
C	0.969739	4.885877	5.688536
H	-0.037611	4.811183	5.239354
H	1.713672	4.927544	4.873878
C	1.088704	6.132645	6.523102
H	2.110033	6.227579	6.927959
H	0.844778	7.006680	5.896787
O	0.157578	6.027599	7.594616
C	-0.190057	7.249752	8.221403
H	-1.221592	7.130872	8.568262
H	-0.197364	8.061190	7.474497
C	0.766275	7.631624	9.343768
H	1.765173	7.751740	8.901622
H	0.464605	8.623811	9.737583
N	0.883891	6.638504	10.411997
C	2.172148	6.775416	11.104532
H	2.179221	7.660038	11.771642
H	2.950975	6.925279	10.345218
C	-0.199264	6.674626	11.397109
H	-0.331342	7.693490	11.814226
H	0.096800	6.020417	12.227210
C	-1.547842	6.195546	10.894776
H	-2.194002	6.001286	11.768370
H	-2.060531	6.955960	10.280872
O	-1.382554	5.004616	10.149655
C	-2.588625	4.430091	9.676311
H	-2.813059	4.816185	8.665685
H	-3.424934	4.698303	10.342274
C	-2.451150	2.931680	9.671257
H	-2.206312	2.579433	10.688767
H	-3.409559	2.481567	9.356212
O	-1.420851	2.544839	8.783178
C	-1.230371	1.133454	8.807758
H	-2.189308	0.634914	8.582063
H	-0.900770	0.845220	9.818174
C	-0.222235	0.744248	7.754543
H	-0.169111	-0.360796	7.705476
H	-0.609182	1.081043	6.783356

Pr-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2020.06803374

E(SCF)+ZPE(0 K)= -2019.359614

H(298 K)= -2019.320362

G(298 K)= -2019.424800

Lowest Frequency = 31.3267cm⁻¹

Pr	0.915427	4.003331	9.073081
N	3.098778	2.588868	9.121713
C	3.105337	1.277608	9.204930
C	4.227492	0.580167	9.707989
H	4.206074	-0.508754	9.775817
C	5.329560	1.293674	10.116168
H	6.201649	0.775369	10.522071
C	5.356870	2.707954	9.997751
C	4.189581	3.314034	9.473230
C	4.086056	4.740345	9.283264
O	2.964795	5.227116	8.828489
C	5.201871	5.497112	9.632535
H	5.172286	6.578824	9.481846
C	6.360903	4.889589	10.164637
H	7.208178	5.526834	10.429142
C	6.456264	3.528668	10.356464
H	7.360329	3.076687	10.767719
N	1.819028	4.480068	11.535042
C	2.355284	5.615840	11.917401
C	3.223083	5.690904	13.032869
H	3.656308	6.650827	13.318977
C	3.519457	4.544625	13.728964
H	4.200805	4.576277	14.582587
C	2.928664	3.309522	13.355409
C	2.060496	3.343791	12.237680
C	1.377502	2.165678	11.771106
O	0.609906	2.276938	10.725415
C	1.609088	0.984193	12.471182
H	1.094840	0.073467	12.154717
C	2.486916	0.951998	13.577111
H	2.642976	0.001367	14.092711
C	3.144369	2.077274	14.023654
H	3.816856	2.036500	14.882099
C	1.853390	0.556027	8.766889
H	2.125852	-0.403808	8.284196
H	1.276958	0.322499	9.670879
N	1.018048	1.367520	7.871065
C	1.692362	1.482811	6.567730
H	1.550125	0.560397	5.971156
H	2.769983	1.587500	6.749036
C	1.258161	2.667273	5.736518
H	1.801948	2.631647	4.775966
H	0.176327	2.648158	5.512222
O	1.570754	3.863657	6.418182
C	1.413001	5.007579	5.607197
H	0.439535	4.959583	5.084549
H	2.210964	5.042595	4.844138
C	1.478780	6.258049	6.446178
H	2.436015	6.305559	6.989839
H	1.372694	7.132807	5.781790
O	0.398617	6.222557	7.373672
C	0.063253	7.449993	7.985516
H	-1.006833	7.396154	8.227143
H	0.183997	8.278799	7.266549
C	0.909490	7.739177	9.210932
H	1.954367	7.800170	8.878047
H	0.634821	8.738894	9.605020

N	0.853283	6.717178	10.260509
C	2.067994	6.832748	11.080017
H	2.026793	7.731840	11.726363
H	2.919730	6.954007	10.398061
C	-0.326976	6.804884	11.126559
H	-0.565502	7.860185	11.368991
H	-0.077955	6.306639	12.073637
C	-1.596710	6.146880	10.618954
H	-2.356604	6.252341	11.412800
H	-2.009794	6.635546	9.719598
O	-1.375850	4.773574	10.357082
C	-2.565813	4.004561	10.372002
H	-3.221081	4.312080	9.533608
H	-3.116435	4.196133	11.309234
C	-2.262535	2.528686	10.301778
H	-1.592043	2.239944	11.126120
H	-3.215121	1.973843	10.380578
O	-1.626101	2.244095	9.073455
C	-1.237753	0.892071	8.906526
H	-2.133046	0.270528	8.725206
H	-0.749986	0.550698	9.831015
C	-0.312760	0.767479	7.709703
H	-0.222363	-0.309547	7.462522
H	-0.802795	1.244090	6.847662
O	-1.111290	3.996992	7.300528
H	-1.778374	3.422512	7.711213
H	-1.505246	4.820915	7.000835

Sm-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.49519680
 E(SCF)+ZPE(0 K)= -1909.828907
 H(298 K)= -1909.794829
 G(298 K)= -1909.890384
 Lowest Frequency = -63.3831cm-1

C	5.884247	1.360286	17.383169
C	5.759406	1.558673	18.782506
C	5.473532	0.405109	19.558857
H	5.382692	0.498428	20.643979
C	5.273203	-0.806777	18.944467
H	5.003084	-1.692521	19.523182
C	5.402540	-0.897909	17.536291
C	5.008229	-2.166945	16.818481
H	5.341890	-3.046164	17.395294
H	3.905461	-2.214495	16.864020
C	4.331221	-2.301149	14.482774
H	3.577369	-3.055171	14.784699
H	4.739807	-2.583948	13.504851
C	3.642324	-0.957887	14.317495
H	2.774948	-1.086077	13.649686
H	3.276102	-0.553040	15.277665
C	4.078047	0.940748	12.841916
H	3.896862	1.880212	13.389531
H	3.139954	0.605894	12.370300
C	5.128390	1.146222	11.769324
H	5.269613	0.225609	11.178827

H	4.811645	1.965576	11.102819
C	7.294064	2.261136	11.716300
H	6.774855	2.961903	11.041546
H	7.933716	1.606423	11.101744
C	6.421573	-3.313046	15.211992
H	6.661799	-3.332969	14.143771
H	6.023929	-4.310158	15.492049
N	5.752311	0.135810	16.804550
N	5.447443	-2.246710	15.428911
O	6.210623	2.216903	15.208194
O	4.556157	-0.044303	13.737676
O	6.337992	1.489154	12.419326
C	7.632739	-2.113557	12.078817
C	8.878730	-1.409167	11.934221
C	9.890754	-1.875230	11.055374
C	11.030132	-1.043286	10.907706
H	11.836497	-1.350305	10.237116
C	11.095915	0.153253	11.576754
H	11.945384	0.826113	11.444282
C	10.042823	0.516749	12.451476
C	10.112644	1.817716	13.208976
H	10.601263	2.584296	12.575815
H	10.798132	1.662933	14.056063
C	8.996023	3.043442	14.956204
H	9.704137	3.888956	14.842514
H	8.019349	3.457223	15.215837
C	9.496361	2.170535	16.097736
H	9.236191	2.642757	17.059494
H	10.593557	2.063737	16.062176
C	9.766423	-0.131803	16.581672
H	10.542661	-0.395370	15.839873
H	10.263947	0.233849	17.495125
C	8.950139	-1.337965	16.949477
H	8.263631	-1.099597	17.782924
H	9.638230	-2.135135	17.277582
C	7.682787	-3.088545	16.018772
H	8.449732	-3.823881	15.724613
H	7.483009	-3.227377	17.095290
C	8.074536	3.077964	12.731391
H	7.336809	3.669682	13.289521
H	8.737420	3.780000	12.188046
N	8.997235	-0.255049	12.648274
N	8.829218	2.291474	13.713647
O	8.921896	0.866378	16.043411
O	8.194791	-1.770004	15.832184
O	6.719187	-1.600330	12.845746
C	7.493316	-3.308441	11.373475
H	6.553931	-3.858818	11.460017
C	8.522597	-3.787734	10.537068
H	8.367343	-4.727146	10.001215
C	9.702659	-3.097015	10.362763
H	10.481814	-3.465905	9.693753
C	6.100093	2.463098	16.477966
C	6.187352	3.733500	17.052122
H	6.306346	4.596883	16.393716
C	6.095367	3.917757	18.447477
H	6.174648	4.931852	18.846638

C	5.893368	2.865009	19.314595
H	5.808203	3.024897	20.390674

Sm-anti-KHQ(1+)₂

SCF (RwB97XD) = -1945.53099151
 E(SCF)+ZPE(0 K)= -1944.848587
 H(298 K)= -1944.811315
 G(298 K)= -1944.914932
 Lowest Frequency = 12.4938cm⁻¹

C	5.884247	1.360286	17.383169
C	5.759406	1.558673	18.782506
C	5.473532	0.405109	19.558857
H	5.382692	0.498428	20.643979
C	5.273203	-0.806777	18.944467
H	5.003084	-1.692521	19.523182
C	5.402540	-0.897909	17.536291
C	5.008229	-2.166945	16.818481
H	5.341890	-3.046164	17.395294
H	3.905461	-2.214495	16.864020
C	4.331221	-2.301149	14.482774
H	3.577369	-3.055171	14.784699
H	4.739807	-2.583948	13.504851
C	3.642324	-0.957887	14.317495
H	2.774948	-1.086077	13.649686
H	3.276102	-0.553040	15.277665
C	4.078047	0.940748	12.841916
H	3.896862	1.880212	13.389531
H	3.139954	0.605894	12.370300
C	5.128390	1.146222	11.769324
H	5.269613	0.225609	11.178827
H	4.811645	1.965576	11.102819
C	7.294064	2.261136	11.716300
H	6.774855	2.961903	11.041546
H	7.933716	1.606423	11.101744
C	6.421573	-3.313046	15.211992
H	6.661799	-3.332969	14.143771
H	6.023929	-4.310158	15.492049
N	5.752311	0.135810	16.804550
N	5.447443	-2.246710	15.428911
O	6.210623	2.216903	15.208194
O	4.556157	-0.044303	13.737676
O	6.337992	1.489154	12.419326
C	7.632739	-2.113557	12.078817
C	8.878730	-1.409167	11.934221
C	9.890754	-1.875230	11.055374
C	11.030132	-1.043286	10.907706
H	11.836497	-1.350305	10.237116
C	11.095915	0.153253	11.576754
H	11.945384	0.826113	11.444282
C	10.042823	0.516749	12.451476
C	10.112644	1.817716	13.208976
H	10.601263	2.584296	12.575815
H	10.798132	1.662933	14.056063
C	8.996023	3.043442	14.956204
H	9.704137	3.888956	14.842514

H	8.019349	3.457223	15.215837
C	9.496361	2.170535	16.097736
H	9.236191	2.642757	17.059494
H	10.593557	2.063737	16.062176
C	9.766423	-0.131803	16.581672
H	10.542661	-0.395370	15.839873
H	10.263947	0.233849	17.495125
C	8.950139	-1.337965	16.949477
H	8.263631	-1.099597	17.782924
H	9.638230	-2.135135	17.277582
C	7.682787	-3.088545	16.018772
H	8.449732	-3.823881	15.724613
H	7.483009	-3.227377	17.095290
C	8.074536	3.077964	12.731391
H	7.336809	3.669682	13.289521
H	8.737420	3.780000	12.188046
N	8.997235	-0.255049	12.648274
N	8.829218	2.291474	13.713647
O	8.921896	0.866378	16.043411
O	8.194791	-1.770004	15.832184
O	6.719187	-1.600330	12.845746
C	7.493316	-3.308441	11.373475
H	6.553931	-3.858818	11.460017
C	8.522597	-3.787734	10.537068
H	8.367343	-4.727146	10.001215
C	9.702659	-3.097015	10.362763
H	10.481814	-3.465905	9.693753
C	6.100093	2.463098	16.477966
C	6.187352	3.733500	17.052122
H	6.306346	4.596883	16.393716
C	6.095367	3.917757	18.447477
H	6.174648	4.931852	18.846638
C	5.893368	2.865009	19.314595
H	5.808203	3.024897	20.390674
Sm	6.977950	0.115972	14.433727

Sm3+_lon

SCF (RwB97XD) = -33.2499966812
 E(SCF)+ZPE(0 K)= -33.249997
 H(298 K)= -33.247636
 G(298 K)= -33.267100

Sm 0.887400 3.945900 9.220400

Sm-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.50576787
 E(SCF)+ZPE(0 K)= -1909.837807
 H(298 K)= -1909.801843
 G(298 K)= -1909.902823
 Lowest Frequency = -35.9308cm-1

N	3.094179	2.614824	9.246232
C	3.125477	1.310656	9.405856
C	4.259950	0.670463	9.953853
H	4.257171	-0.410658	10.101002

C	5.354658	1.429935	10.298177
H	6.236451	0.955284	10.735295
C	5.367353	2.829493	10.057501
C	4.182118	3.376315	9.513364
C	4.049715	4.775903	9.195372
O	2.896420	5.197740	8.753969
C	5.169468	5.571331	9.422965
H	5.125757	6.632187	9.165653
C	6.350452	5.025760	9.976489
H	7.199766	5.691748	10.146999
C	6.466055	3.692263	10.304477
H	7.387944	3.291967	10.729479
N	1.944449	4.415654	11.553527
C	2.580225	5.518571	11.878000
C	3.564760	5.526216	12.892752
H	4.094530	6.450526	13.128521
C	3.845307	4.357798	13.562020
H	4.614161	4.339395	14.338191
C	3.118502	3.172131	13.274910
C	2.154992	3.268795	12.244776
C	1.326657	2.157634	11.857232
O	0.502103	2.332651	10.860665
C	1.502056	0.971935	12.564222
H	0.874011	0.111910	12.320501
C	2.473925	0.872442	13.586089
H	2.583272	-0.080843	14.108780
C	3.280183	1.931361	13.943611
H	4.022540	1.833996	14.737476
C	1.897578	0.554394	8.955429
H	2.200154	-0.424569	8.532780
H	1.268327	0.357202	9.834475
N	1.112026	1.326349	7.986836
C	1.837722	1.455872	6.721628
H	1.846337	0.501448	6.158295
H	2.880469	1.711998	6.947077
C	1.275236	2.538545	5.829002
H	1.947486	2.661666	4.962113
H	0.275208	2.286272	5.431351
O	1.199389	3.749971	6.551324
C	0.925763	4.864667	5.729149
H	-0.089474	4.771408	5.301540
H	1.651463	4.912724	4.898580
C	1.042758	6.116579	6.553478
H	2.071874	6.235140	6.929744
H	0.761589	6.981784	5.930829
O	0.145209	5.996304	7.651366
C	-0.209012	7.219616	8.272774
H	-1.234000	7.094293	8.635389
H	-0.235527	8.023855	7.518955
C	0.760410	7.618728	9.377044
H	1.749250	7.753705	8.917361
H	0.450407	8.606100	9.776582
N	0.909122	6.624993	10.438475
C	2.209034	6.760641	11.105455
H	2.227610	7.637070	11.783114
H	2.973964	6.921161	10.334752
C	-0.155113	6.644855	11.442740

H	-0.286713	7.657631	11.874510
H	0.156180	5.981967	12.259951
C	-1.505345	6.164674	10.948008
H	-2.136298	5.927461	11.821940
H	-2.036194	6.941430	10.370867
O	-1.336258	5.006738	10.152820
C	-2.540843	4.477472	9.626700
H	-2.710415	4.881122	8.612256
H	-3.394424	4.765637	10.261137
C	-2.447771	2.977301	9.609116
H	-2.260734	2.607766	10.632649
H	-3.402285	2.556896	9.244929
O	-1.388199	2.573340	8.765750
C	-1.228192	1.158731	8.805530
H	-2.193674	0.678755	8.568099
H	-0.921940	0.873028	9.823708
C	-0.211654	0.740389	7.773723
H	-0.163481	-0.365599	7.748053
H	-0.584470	1.058607	6.791060

Sm-syn-KHQ(1+)

SCF (RWB97XD) = -1945.54409397

E(SCF)+ZPE(0 K)= -1944.860709

H(298 K)= -1944.824024

G(298 K)= -1944.923704

Lowest Frequency = 39.3530cm⁻¹

Sm	0.927939	3.970804	9.221802
N	3.094179	2.614824	9.246232
C	3.125477	1.310656	9.405856
C	4.259950	0.670463	9.953853
H	4.257171	-0.410658	10.101002
C	5.354658	1.429935	10.298177
H	6.236451	0.955284	10.735295
C	5.367353	2.829493	10.057501
C	4.182118	3.376315	9.513364
C	4.049715	4.775903	9.195372
O	2.896420	5.197740	8.753969
C	5.169468	5.571331	9.422965
H	5.125757	6.632187	9.165653
C	6.350452	5.025760	9.976489
H	7.199766	5.691748	10.146999
C	6.466055	3.692263	10.304477
H	7.387944	3.291967	10.729479
N	1.944449	4.415654	11.553527
C	2.580225	5.518571	11.878000
C	3.564760	5.526216	12.892752
H	4.094530	6.450526	13.128521
C	3.845307	4.357798	13.562020
H	4.614161	4.339395	14.338191
C	3.118502	3.172131	13.274910
C	2.154992	3.268795	12.244776
C	1.326657	2.157634	11.857232
O	0.502103	2.332651	10.860665
C	1.502056	0.971935	12.564222
H	0.874011	0.111910	12.320501

C	2.473925	0.872442	13.586089
H	2.583272	-0.080843	14.108780
C	3.280183	1.931361	13.943611
H	4.022540	1.833996	14.737476
C	1.897578	0.554394	8.955429
H	2.200154	-0.424569	8.532780
H	1.268327	0.357202	9.834475
N	1.112026	1.326349	7.986836
C	1.837722	1.455872	6.721628
H	1.846337	0.501448	6.158295
H	2.880469	1.711998	6.947077
C	1.275236	2.538545	5.829002
H	1.947486	2.661666	4.962113
H	0.275208	2.286272	5.431351
O	1.199389	3.749971	6.551324
C	0.925763	4.864667	5.729149
H	-0.089474	4.771408	5.301540
H	1.651463	4.912724	4.898580
C	1.042758	6.116579	6.553478
H	2.071874	6.235140	6.929744
H	0.761589	6.981784	5.930829
O	0.145209	5.996304	7.651366
C	-0.209012	7.219616	8.272774
H	-1.234000	7.094293	8.635389
H	-0.235527	8.023855	7.518955
C	0.760410	7.618728	9.377044
H	1.749250	7.753705	8.917361
H	0.450407	8.606100	9.776582
N	0.909122	6.624993	10.438475
C	2.209034	6.760641	11.105455
H	2.227610	7.637070	11.783114
H	2.973964	6.921161	10.334752
C	-0.155113	6.644855	11.442740
H	-0.286713	7.657631	11.874510
H	0.156180	5.981967	12.259951
C	-1.505345	6.164674	10.948008
H	-2.136298	5.927461	11.821940
H	-2.036194	6.941430	10.370867
O	-1.336258	5.006738	10.152820
C	-2.540843	4.477472	9.626700
H	-2.710415	4.881122	8.612256
H	-3.394424	4.765637	10.261137
C	-2.447771	2.977301	9.609116
H	-2.260734	2.607766	10.632649
H	-3.402285	2.556896	9.244929
O	-1.388199	2.573340	8.765750
C	-1.228192	1.158731	8.805530
H	-2.193674	0.678755	8.568099
H	-0.921940	0.873028	9.823708
C	-0.211654	0.740389	7.773723
H	-0.163481	-0.365599	7.748053
H	-0.584470	1.058607	6.791060

Sm-syn-H2O-KHQ(1+)

SCF (RwB97XD) = -2021.90572700

E(SCF)+ZPE(0 K)= -2021.196321

H(298 K)= -2021.157448

G(298 K)= -2021.261151

Lowest Frequency = 24.7545cm⁻¹

Sm	0.958098	4.012483	9.081065
N	3.092713	2.605159	9.126776
C	3.104391	1.293492	9.209658
C	4.236686	0.599725	9.694662
H	4.218335	-0.489203	9.762910
C	5.345615	1.314833	10.081272
H	6.225840	0.798076	10.471284
C	5.369027	2.728515	9.957284
C	4.190527	3.330436	9.455179
C	4.081339	4.753655	9.257559
O	2.948011	5.230593	8.821291
C	5.201360	5.515939	9.577054
H	5.167001	6.596415	9.418986
C	6.372777	4.913191	10.088278
H	7.224631	5.553282	10.330077
C	6.474447	3.553769	10.286895
H	7.388237	3.106100	10.681002
N	1.830680	4.482915	11.509648
C	2.364622	5.614338	11.907977
C	3.205073	5.680331	13.044483
H	3.638708	6.636396	13.342573
C	3.471074	4.531488	13.749530
H	4.129361	4.557342	14.621253
C	2.873568	3.303489	13.363627
C	2.039358	3.347313	12.221653
C	1.345332	2.183307	11.740906
O	0.609867	2.313374	10.674456
C	1.529833	1.000479	12.451444
H	1.004267	0.098970	12.127243
C	2.376500	0.956323	13.581958
H	2.497616	0.005438	14.106350
C	3.045175	2.069410	14.042018
H	3.691657	2.018151	14.919652
C	1.852662	0.567861	8.780377
H	2.127658	-0.391880	8.298745
H	1.279615	0.332455	9.685475
N	1.014849	1.375495	7.884974
C	1.689884	1.489068	6.582437
H	1.542095	0.569312	5.983205
H	2.768457	1.587306	6.761361
C	1.260735	2.678342	5.758232
H	1.795148	2.640840	4.792543
H	0.176548	2.669368	5.545251
O	1.590045	3.870751	6.439141
C	1.429810	5.010101	5.622415
H	0.457413	4.954831	5.098281
H	2.228396	5.044196	4.859968
C	1.484582	6.265948	6.451891
H	2.441405	6.327914	6.993725
H	1.368056	7.134534	5.781121
O	0.405848	6.225005	7.380014
C	0.071052	7.453794	7.988681
H	-0.997778	7.400927	8.235282

H	0.188696	8.280538	7.266944
C	0.922971	7.742656	9.209099
H	1.966043	7.807004	8.871551
H	0.648168	8.739918	9.609145
N	0.872425	6.715298	10.252591
C	2.086255	6.833465	11.072275
H	2.042711	7.730895	11.720639
H	2.938896	6.957661	10.392179
C	-0.309265	6.793753	11.117001
H	-0.561733	7.847446	11.351796
H	-0.057136	6.305430	12.068298
C	-1.568304	6.116304	10.610573
H	-2.333961	6.227366	11.398095
H	-1.980317	6.589475	9.702523
O	-1.337552	4.741118	10.368384
C	-2.533430	3.979321	10.397593
H	-3.195326	4.293061	9.566670
H	-3.070753	4.179362	11.340755
C	-2.257290	2.498766	10.324022
H	-1.567465	2.203144	11.129263
H	-3.217611	1.962985	10.436988
O	-1.668198	2.200789	9.078124
C	-1.241927	0.862800	8.913360
H	-2.117456	0.214249	8.729389
H	-0.746919	0.533204	9.838223
C	-0.310210	0.763291	7.718990
H	-0.205486	-0.310011	7.460992
H	-0.804986	1.241511	6.860659
O	-1.030384	3.978438	7.389114
H	-1.705434	3.401534	7.787551
H	-1.407916	4.810734	7.090827

Tb-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.48877346
 E(SCF)+ZPE(0 K)= -1909.822433
 H(298 K)= -1909.788357
 G(298 K)= -1909.883823
 Lowest Frequency = -83.3634cm⁻¹

C	5.882564	1.363434	17.362377
C	5.725195	1.567149	18.756586
C	5.459984	0.410525	19.536279
H	5.344506	0.507792	20.618661
C	5.307688	-0.808768	18.925450
H	5.051186	-1.699175	19.503279
C	5.467883	-0.905550	17.519978
C	5.137457	-2.201188	16.818317
H	5.614091	-3.039203	17.352453
H	4.053558	-2.368703	16.960744
C	4.285050	-2.221573	14.533525
H	3.527169	-2.956273	14.871001
H	4.612498	-2.495941	13.522976
C	3.635093	-0.852315	14.440741
H	2.720710	-0.934862	13.831471
H	3.351018	-0.453787	15.430357
C	4.060024	1.011461	12.910500

H	3.897199	1.961353	13.445317
H	3.111864	0.676582	12.459755
C	5.096308	1.187672	11.818476
H	5.217347	0.256425	11.240835
H	4.781281	2.003109	11.146560
C	7.282961	2.263783	11.722574
H	6.770890	2.946405	11.024397
H	7.919132	1.584131	11.131795
C	6.390371	-3.312166	15.064580
H	6.517004	-3.321559	13.978762
H	6.005726	-4.307495	15.367411
N	5.802088	0.131296	16.786589
N	5.466540	-2.232793	15.397771
O	6.210157	2.212933	15.189245
O	4.543011	0.037164	13.816028
O	6.319614	1.521771	12.447145
C	7.586644	-2.060383	12.126224
C	8.870703	-1.415487	12.060088
C	9.931331	-1.958484	11.290868
C	11.112562	-1.176661	11.205551
H	11.960526	-1.545582	10.623275
C	11.166546	0.050579	11.816779
H	12.047940	0.688090	11.722612
C	10.056870	0.496799	12.576961
C	10.102239	1.849654	13.240948
H	10.569572	2.573822	12.544772
H	10.801681	1.780845	14.088716
C	8.951177	3.073911	14.965557
H	9.683015	3.902772	14.884755
H	7.976814	3.510520	15.192581
C	9.387193	2.173956	16.120401
H	9.020879	2.594420	17.070427
H	10.485678	2.116332	16.178560
C	9.818165	-0.166499	16.297864
H	10.490853	-0.335941	15.437081
H	10.425897	0.129114	17.168176
C	9.085159	-1.429049	16.650849
H	8.500805	-1.286711	17.578763
H	9.826846	-2.228078	16.818679
C	7.735467	-3.123932	15.736815
H	8.471245	-3.818766	15.299317
H	7.664292	-3.347989	16.815149
C	8.069375	3.102919	12.715278
H	7.336534	3.716819	13.255292
H	8.738335	3.784279	12.153441
N	8.975027	-0.232975	12.728728
N	8.812833	2.332484	13.716105
O	8.881767	0.844588	15.978185
O	8.208149	-1.785343	15.598798
O	6.639490	-1.483301	12.800869
C	7.452569	-3.274626	11.452295
H	6.483293	-3.777781	11.470811
C	8.526954	-3.831357	10.728025
H	8.374450	-4.783426	10.214171
C	9.749045	-3.200525	10.633834
H	10.564691	-3.629503	10.049517
C	6.072693	2.466374	16.454978

C	6.105827	3.743873	17.018006
H	6.205910	4.605159	16.353829
C	5.984594	3.934841	18.410087
H	6.022062	4.953622	18.803236
C	5.804249	2.881022	19.280810
H	5.694534	3.044889	20.354059

Tb-anti-KHQ(1+)

SCF (RwB97XD) = -1947.31128663

E(SCF)+ZPE(0 K)= -1946.628546

H(298 K)= -1946.591406

G(298 K)= -1946.694192

Lowest Frequency = 16.9225cm⁻¹

C	5.882564	1.363434	17.362377
C	5.725195	1.567149	18.756586
C	5.459984	0.410525	19.536279
H	5.344506	0.507792	20.618661
C	5.307688	-0.808768	18.925450
H	5.051186	-1.699175	19.503279
C	5.467883	-0.905550	17.519978
C	5.137457	-2.201188	16.818317
H	5.614091	-3.039203	17.352453
H	4.053558	-2.368703	16.960744
C	4.285050	-2.221573	14.533525
H	3.527169	-2.956273	14.871001
H	4.612498	-2.495941	13.522976
C	3.635093	-0.852315	14.440741
H	2.720710	-0.934862	13.831471
H	3.351018	-0.453787	15.430357
C	4.060024	1.011461	12.910500
H	3.897199	1.961353	13.445317
H	3.111864	0.676582	12.459755
C	5.096308	1.187672	11.818476
H	5.217347	0.256425	11.240835
H	4.781281	2.003109	11.146560
C	7.282961	2.263783	11.722574
H	6.770890	2.946405	11.024397
H	7.919132	1.584131	11.131795
C	6.390371	-3.312166	15.064580
H	6.517004	-3.321559	13.978762
H	6.005726	-4.307495	15.367411
N	5.802088	0.131296	16.786589
N	5.466540	-2.232793	15.397771
O	6.210157	2.212933	15.189245
O	4.543011	0.037164	13.816028
O	6.319614	1.521771	12.447145
C	7.586644	-2.060383	12.126224
C	8.870703	-1.415487	12.060088
C	9.931331	-1.958484	11.290868
C	11.112562	-1.176661	11.205551
H	11.960526	-1.545582	10.623275
C	11.166546	0.050579	11.816779
H	12.047940	0.688090	11.722612
C	10.056870	0.496799	12.576961
C	10.102239	1.849654	13.240948

H	10.569572	2.573822	12.544772
H	10.801681	1.780845	14.088716
C	8.951177	3.073911	14.965557
H	9.683015	3.902772	14.884755
H	7.976814	3.510520	15.192581
C	9.387193	2.173956	16.120401
H	9.020879	2.594420	17.070427
H	10.485678	2.116332	16.178560
C	9.818165	-0.166499	16.297864
H	10.490853	-0.335941	15.437081
H	10.425897	0.129114	17.168176
C	9.085159	-1.429049	16.650849
H	8.500805	-1.286711	17.578763
H	9.826846	-2.228078	16.818679
C	7.735467	-3.123932	15.736815
H	8.471245	-3.818766	15.299317
H	7.664292	-3.347989	16.815149
C	8.069375	3.102919	12.715278
H	7.336534	3.716819	13.255292
H	8.738335	3.784279	12.153441
N	8.975027	-0.232975	12.728728
N	8.812833	2.332484	13.716105
O	8.881767	0.844588	15.978185
O	8.208149	-1.785343	15.598798
O	6.639490	-1.483301	12.800869
C	7.452569	-3.274626	11.452295
H	6.483293	-3.777781	11.470811
C	8.526954	-3.831357	10.728025
H	8.374450	-4.783426	10.214171
C	9.749045	-3.200525	10.633834
H	10.564691	-3.629503	10.049517
C	6.072693	2.466374	16.454978
C	6.105827	3.743873	17.018006
H	6.205910	4.605159	16.353829
C	5.984594	3.934841	18.410087
H	6.022062	4.953622	18.803236
C	5.804249	2.881022	19.280810
H	5.694534	3.044889	20.354059
Tb	6.942652	0.152257	14.415454

Tb3+_lon

SCF (RwB97XD) = -34.9986652250
 E(SCF)+ZPE(0 K)= -34.998665
 H(298 K)= -34.996305
 G(298 K)= -35.015832

Tb 0.887400 3.945900 9.220400

Tb-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.50037905
 E(SCF)+ZPE(0 K)= -1909.832513
 H(298 K)= -1909.797441
 G(298 K)= -1909.894619
 Lowest Frequency = -36.3692cm-1

N	3.082009	2.630046	9.268686
C	3.128966	1.327598	9.440420
C	4.275742	0.704893	9.982655
H	4.284175	-0.374418	10.142172
C	5.369129	1.477310	10.301927
H	6.260762	1.015476	10.732776
C	5.367613	2.872698	10.038607
C	4.169246	3.401425	9.506946
C	4.020064	4.792451	9.165569
O	2.853115	5.193456	8.740779
C	5.137393	5.600642	9.353604
H	5.081462	6.655607	9.075360
C	6.332689	5.074046	9.895683
H	7.180411	5.748990	10.036129
C	6.464046	3.748438	10.248557
H	7.396884	3.363362	10.663595
N	1.963565	4.406659	11.534692
C	2.609819	5.502003	11.864416
C	3.593729	5.495408	12.879558
H	4.134137	6.413020	13.117254
C	3.857291	4.323359	13.549941
H	4.624393	4.294799	14.327540
C	3.110837	3.149569	13.264807
C	2.153926	3.260227	12.230883
C	1.302944	2.167338	11.845276
O	0.490253	2.360835	10.842287
C	1.445837	0.982299	12.559653
H	0.798103	0.135818	12.320137
C	2.412495	0.866728	13.585547
H	2.497563	-0.085569	14.114485
C	3.242419	1.908308	13.939768
H	3.979160	1.797895	14.737146
C	1.909753	0.555359	8.995372
H	2.224025	-0.424995	8.584412
H	1.276260	0.360082	9.871419
N	1.127745	1.313363	8.015567
C	1.859712	1.443384	6.755729
H	1.877687	0.489078	6.192325
H	2.899649	1.707115	6.984837
C	1.290745	2.521762	5.863482
H	1.967531	2.659255	5.002300
H	0.297545	2.257183	5.456921
O	1.190982	3.729439	6.589388
C	0.880342	4.831391	5.763852
H	-0.143455	4.717815	5.362208
H	1.584314	4.882113	4.915014
C	0.997923	6.092590	6.571377
H	2.034079	6.234480	6.917664
H	0.682776	6.945358	5.948071
O	0.134214	5.967802	7.695185
C	-0.219462	7.196290	8.307879
H	-1.241043	7.074741	8.680348
H	-0.254057	7.992186	7.546017
C	0.758877	7.608004	9.398774
H	1.740755	7.750389	8.926917
H	0.444224	8.593407	9.799804
N	0.927716	6.616391	10.456900

C	2.234755	6.751355	11.106429
H	2.260953	7.620744	11.792916
H	2.990261	6.921550	10.328879
C	-0.125013	6.621112	11.471615
H	-0.263055	7.629362	11.911946
H	0.198964	5.955472	12.281284
C	-1.472828	6.131841	10.979338
H	-2.092439	5.857598	11.850361
H	-2.019921	6.917645	10.430377
O	-1.294798	5.002430	10.144987
C	-2.492171	4.515623	9.564221
H	-2.603206	4.932179	8.546906
H	-3.363118	4.825365	10.163369
C	-2.442035	3.014794	9.536136
H	-2.315342	2.632771	10.564211
H	-3.388845	2.623098	9.122996
O	-1.354144	2.590426	8.741530
C	-1.219433	1.173915	8.804071
H	-2.188773	0.707549	8.555834
H	-0.936768	0.898358	9.831537
C	-0.192066	0.723627	7.797918
H	-0.147324	-0.382711	7.802347
H	-0.550218	1.015881	6.801989

Tb-syn-KHQ(1+)

SCF (RwB97XD) = -1947.32290624
 E(SCF)+ZPE(0 K)= -1946.638977
 H(298 K)= -1946.602395
 G(298 K)= -1946.701882
 Lowest Frequency = 39.1863cm⁻¹

Tb	0.942653	3.967616	9.238382
N	3.082009	2.630046	9.268686
C	3.128966	1.327598	9.440420
C	4.275742	0.704893	9.982655
H	4.284175	-0.374418	10.142172
C	5.369129	1.477310	10.301927
H	6.260762	1.015476	10.732776
C	5.367613	2.872698	10.038607
C	4.169246	3.401425	9.506946
C	4.020064	4.792451	9.165569
O	2.853115	5.193456	8.740779
C	5.137393	5.600642	9.353604
H	5.081462	6.655607	9.075360
C	6.332689	5.074046	9.895683
H	7.180411	5.748990	10.036129
C	6.464046	3.748438	10.248557
H	7.396884	3.363362	10.663595
N	1.963565	4.406659	11.534692
C	2.609819	5.502003	11.864416
C	3.593729	5.495408	12.879558
H	4.134137	6.413020	13.117254
C	3.857291	4.323359	13.549941
H	4.624393	4.294799	14.327540
C	3.110837	3.149569	13.264807
C	2.153926	3.260227	12.230883

C	1.302944	2.167338	11.845276
O	0.490253	2.360835	10.842287
C	1.445837	0.982299	12.559653
H	0.798103	0.135818	12.320137
C	2.412495	0.866728	13.585547
H	2.497563	-0.085569	14.114485
C	3.242419	1.908308	13.939768
H	3.979160	1.797895	14.737146
C	1.909753	0.555359	8.995372
H	2.224025	-0.424995	8.584412
H	1.276260	0.360082	9.871419
N	1.127745	1.313363	8.015567
C	1.859712	1.443384	6.755729
H	1.877687	0.489078	6.192325
H	2.899649	1.707115	6.984837
C	1.290745	2.521762	5.863482
H	1.967531	2.659255	5.002300
H	0.297545	2.257183	5.456921
O	1.190982	3.729439	6.589388
C	0.880342	4.831391	5.763852
H	-0.143455	4.717815	5.362208
H	1.584314	4.882113	4.915014
C	0.997923	6.092590	6.571377
H	2.034079	6.234480	6.917664
H	0.682776	6.945358	5.948071
O	0.134214	5.967802	7.695185
C	-0.219462	7.196290	8.307879
H	-1.241043	7.074741	8.680348
H	-0.254057	7.992186	7.546017
C	0.758877	7.608004	9.398774
H	1.740755	7.750389	8.926917
H	0.444224	8.593407	9.799804
N	0.927716	6.616391	10.456900
C	2.234755	6.751355	11.106429
H	2.260953	7.620744	11.792916
H	2.990261	6.921550	10.328879
C	-0.125013	6.621112	11.471615
H	-0.263055	7.629362	11.911946
H	0.198964	5.955472	12.281284
C	-1.472828	6.131841	10.979338
H	-2.092439	5.857598	11.850361
H	-2.019921	6.917645	10.430377
O	-1.294798	5.002430	10.144987
C	-2.492171	4.515623	9.564221
H	-2.603206	4.932179	8.546906
H	-3.363118	4.825365	10.163369
C	-2.442035	3.014794	9.536136
H	-2.315342	2.632771	10.564211
H	-3.388845	2.623098	9.122996
O	-1.354144	2.590426	8.741530
C	-1.219433	1.173915	8.804071
H	-2.188773	0.707549	8.555834
H	-0.936768	0.898358	9.831537
C	-0.192066	0.723627	7.797918
H	-0.147324	-0.382711	7.802347
H	-0.550218	1.015881	6.801989

Tb-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2023.68386261

E(SCF)+ZPE(0 K)= -2022.974169

H(298 K)= -2022.935391

G(298 K)= -2023.039301

Lowest Frequency = 21.7781cm⁻¹

Tb	1.002431	4.020350	9.088277
N	3.092913	2.617820	9.133590
C	3.107400	1.306076	9.220508
C	4.247345	0.616013	9.692626
H	4.230769	-0.472682	9.764687
C	5.362197	1.332825	10.058926
H	6.248556	0.817843	10.437231
C	5.383375	2.745610	9.926215
C	4.196489	3.343564	9.440725
C	4.083325	4.763904	9.233075
O	2.941005	5.232659	8.810192
C	5.206622	5.530581	9.526710
H	5.168763	6.609611	9.360050
C	6.387423	4.932303	10.022356
H	7.242934	5.574754	10.244003
C	6.493702	3.574587	10.229757
H	7.414895	3.130864	10.610861
N	1.839918	4.489897	11.485464
C	2.370051	5.618967	11.895742
C	3.182408	5.680568	13.052453
H	3.615374	6.634061	13.359545
C	3.418970	4.531808	13.768910
H	4.053908	4.555356	14.657854
C	2.816687	3.309048	13.374088
C	2.016459	3.357294	12.209041
C	1.313825	2.204537	11.717079
O	0.610801	2.346610	10.630421
C	1.453677	1.023974	12.440577
H	0.918826	0.129926	12.110887
C	2.268949	0.973147	13.594452
H	2.356838	0.024413	14.129202
C	2.946486	2.076416	14.064939
H	3.566847	2.019042	14.960840
C	1.855072	0.576682	8.800848
H	2.131473	-0.384535	8.322757
H	1.284928	0.342740	9.707723
N	1.015659	1.379342	7.903871
C	1.691890	1.486924	6.601794
H	1.539445	0.567475	6.003250
H	2.771175	1.579537	6.779121
C	1.269119	2.677364	5.777985
H	1.798419	2.634394	4.809702
H	0.183925	2.675135	5.570233
O	1.610246	3.869092	6.454102
C	1.447000	5.002163	5.629371
H	0.476004	4.938296	5.103366
H	2.246553	5.034598	4.867873
C	1.490427	6.264711	6.447553
H	2.446409	6.341383	6.988181

H	1.365014	7.126062	5.769019
O	0.412273	6.220745	7.375512
C	0.077725	7.451700	7.979496
H	-0.989937	7.399541	8.230766
H	0.192091	8.275477	7.253909
C	0.934731	7.743368	9.194934
H	1.976407	7.808957	8.853454
H	0.660330	8.739933	9.596873
N	0.888318	6.714874	10.236704
C	2.101294	6.837378	11.056840
H	2.056191	7.735768	11.703586
H	2.955148	6.960388	10.378177
C	-0.294815	6.789436	11.099571
H	-0.558143	7.842740	11.323458
H	-0.040121	6.313562	12.056412
C	-1.545559	6.094089	10.598192
H	-2.316046	6.215130	11.379666
H	-1.955978	6.549650	9.680325
O	-1.307058	4.716734	10.380577
C	-2.507688	3.961237	10.417345
H	-3.172303	4.279349	9.590131
H	-3.037609	4.169111	11.363105
C	-2.256723	2.476054	10.344291
H	-1.549057	2.175111	11.131331
H	-3.222763	1.959185	10.492302
O	-1.715157	2.159162	9.082867
C	-1.245453	0.836302	8.924950
H	-2.098678	0.159212	8.739118
H	-0.744677	0.523344	9.852329
C	-0.305215	0.757670	7.734749
H	-0.188586	-0.312860	7.469789
H	-0.802918	1.235104	6.877686
O	-0.953117	3.955935	7.480708
H	-1.631162	3.370277	7.867536
H	-1.323364	4.786421	7.168012

Tm-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.47850265
 E(SCF)+ZPE(0 K)= -1909.812747
 H(298 K)= -1909.778336
 G(298 K)= -1909.876253
 Lowest Frequency = -98.6645cm-1

C	5.812841	1.411676	17.306359
C	5.474877	1.670067	18.658882
C	5.172234	0.538118	19.459976
H	4.903947	0.678735	20.509936
C	5.176064	-0.715359	18.902091
H	4.898106	-1.593517	19.488326
C	5.539287	-0.868106	17.540838
C	5.528252	-2.235988	16.907980
H	6.389457	-2.796182	17.305380
H	4.637668	-2.790028	17.265176
C	4.284472	-2.132485	14.802705
H	3.537501	-2.773934	15.310792
H	4.407958	-2.502144	13.776773

C	3.720544	-0.724344	14.691946
H	2.754296	-0.781857	14.164672
H	3.545858	-0.251587	15.672195
C	4.132557	1.061905	13.070117
H	4.034161	2.009366	13.624490
H	3.151464	0.765455	12.664647
C	5.119823	1.211041	11.927981
H	5.163077	0.286927	11.328986
H	4.809529	2.053499	11.288607
C	7.336972	2.235873	11.768540
H	6.809757	2.922514	11.086276
H	7.971311	1.571280	11.159590
C	6.382891	-3.334942	14.946899
H	6.265203	-3.353751	13.862115
H	6.033266	-4.310501	15.340387
N	5.890678	0.152753	16.792988
N	5.594014	-2.218351	15.454329
O	6.296859	2.174993	15.136861
O	4.626121	0.055808	13.934447
O	6.391599	1.470642	12.491843
C	7.557767	-2.037314	12.139855
C	8.857019	-1.422828	12.078286
C	9.903566	-1.979667	11.300571
C	11.103783	-1.225544	11.227441
H	11.943390	-1.606523	10.640858
C	11.185900	-0.008266	11.855131
H	12.082039	0.609688	11.770374
C	10.085261	0.455042	12.618201
C	10.152767	1.799581	13.296088
H	10.639386	2.522533	12.611799
H	10.841876	1.710155	14.150835
C	9.003875	3.019940	15.020908
H	9.768181	3.820787	14.963848
H	8.043690	3.492876	15.233666
C	9.380785	2.089959	16.176949
H	8.970784	2.488384	17.118291
H	10.474949	2.028548	16.286820
C	9.820816	-0.252099	16.288094
H	10.539261	-0.354324	15.454326
H	10.376939	-0.004369	17.206711
C	9.095335	-1.549368	16.513802
H	8.481793	-1.491570	17.431423
H	9.846150	-2.346320	16.639249
C	7.866209	-3.190377	15.295706
H	8.476120	-3.675302	14.517282
H	8.091052	-3.683718	16.254458
C	8.131509	3.070824	12.760813
H	7.405321	3.692350	13.299983
H	8.806638	3.743860	12.196162
N	8.987395	-0.251632	12.760673
N	8.866568	2.294953	13.763157
O	8.883324	0.763051	15.984812
O	8.262554	-1.820626	15.402906
O	6.633220	-1.453215	12.836768
C	7.389173	-3.232089	11.438352
H	6.405961	-3.707734	11.443671
C	8.449011	-3.803122	10.703485

H	8.270667	-4.739859	10.170096
C	9.688721	-3.205228	10.622635
H	10.492714	-3.645874	10.030917
C	6.031978	2.480798	16.369004
C	5.944764	3.783152	16.863415
H	6.079177	4.616136	16.169835
C	5.652488	4.030958	18.220802
H	5.594605	5.067047	18.562785
C	5.418332	3.009731	19.116979
H	5.169672	3.216454	20.159161

Tm-anti-KHQ(1+)

SCF (RwB97XD) = -1949.64330447
 E(SCF)+ZPE(0 K)= -1948.960766
 H(298 K)= -1948.923478
 G(298 K)= -1949.026583
 Lowest Frequency = 21.1575cm⁻¹

C	5.812841	1.411676	17.306359
C	5.474877	1.670067	18.658882
C	5.172234	0.538118	19.459976
H	4.903947	0.678735	20.509936
C	5.176064	-0.715359	18.902091
H	4.898106	-1.593517	19.488326
C	5.539287	-0.868106	17.540838
C	5.528252	-2.235988	16.907980
H	6.389457	-2.796182	17.305380
H	4.637668	-2.790028	17.265176
C	4.284472	-2.132485	14.802705
H	3.537501	-2.773934	15.310792
H	4.407958	-2.502144	13.776773
C	3.720544	-0.724344	14.691946
H	2.754296	-0.781857	14.164672
H	3.545858	-0.251587	15.672195
C	4.132557	1.061905	13.070117
H	4.034161	2.009366	13.624490
H	3.151464	0.765455	12.664647
C	5.119823	1.211041	11.927981
H	5.163077	0.286927	11.328986
H	4.809529	2.053499	11.288607
C	7.336972	2.235873	11.768540
H	6.809757	2.922514	11.086276
H	7.971311	1.571280	11.159590
C	6.382891	-3.334942	14.946899
H	6.265203	-3.353751	13.862115
H	6.033266	-4.310501	15.340387
N	5.890678	0.152753	16.792988
N	5.594014	-2.218351	15.454329
O	6.296859	2.174993	15.136861
O	4.626121	0.055808	13.934447
O	6.391599	1.470642	12.491843
C	7.557767	-2.037314	12.139855
C	8.857019	-1.422828	12.078286
C	9.903566	-1.979667	11.300571
C	11.103783	-1.225544	11.227441
H	11.943390	-1.606523	10.640858

C	11.185900	-0.008266	11.855131
H	12.082039	0.609688	11.770374
C	10.085261	0.455042	12.618201
C	10.152767	1.799581	13.296088
H	10.639386	2.522533	12.611799
H	10.841876	1.710155	14.150835
C	9.003875	3.019940	15.020908
H	9.768181	3.820787	14.963848
H	8.043690	3.492876	15.233666
C	9.380785	2.089959	16.176949
H	8.970784	2.488384	17.118291
H	10.474949	2.028548	16.286820
C	9.820816	-0.252099	16.288094
H	10.539261	-0.354324	15.454326
H	10.376939	-0.004369	17.206711
C	9.095335	-1.549368	16.513802
H	8.481793	-1.491570	17.431423
H	9.846150	-2.346320	16.639249
C	7.866209	-3.190377	15.295706
H	8.476120	-3.675302	14.517282
H	8.091052	-3.683718	16.254458
C	8.131509	3.070824	12.760813
H	7.405321	3.692350	13.299983
H	8.806638	3.743860	12.196162
N	8.987395	-0.251632	12.760673
N	8.866568	2.294953	13.763157
O	8.883324	0.763051	15.984812
O	8.262554	-1.820626	15.402906
O	6.633220	-1.453215	12.836768
C	7.389173	-3.232089	11.438352
H	6.405961	-3.707734	11.443671
C	8.449011	-3.803122	10.703485
H	8.270667	-4.739859	10.170096
C	9.688721	-3.205228	10.622635
H	10.492714	-3.645874	10.030917
C	6.031978	2.480798	16.369004
C	5.944764	3.783152	16.863415
H	6.079177	4.616136	16.169835
C	5.652488	4.030958	18.220802
H	5.594605	5.067047	18.562785
C	5.418332	3.009731	19.116979
H	5.169672	3.216454	20.159161
Tm	6.997165	0.135760	14.418995

Tm3+_lon

SCF (RwB97XD) = -37.2924025798
E(SCF)+ZPE(0 K)= -37.292403
H(298 K)= -37.290042
G(298 K)= -37.309656

Tm 0.887400 3.945900 9.220400

Tm-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.49371273
E(SCF)+ZPE(0 K)= -1909.825592

H(298 K)= -1909.790583
 G(298 K)= -1909.887883
 Lowest Frequency = -38.9870cm⁻¹

N	3.065973	2.635677	9.314922
C	3.128018	1.336781	9.511663
C	4.286501	0.736069	10.053366
H	4.305098	-0.339561	10.235203
C	5.379185	1.522480	10.339487
H	6.280131	1.076706	10.767876
C	5.364472	2.910013	10.039343
C	4.153782	3.416652	9.515546
C	3.990221	4.794448	9.135505
O	2.810887	5.171569	8.722994
C	5.105110	5.614758	9.274476
H	5.037984	6.659908	8.963665
C	6.313680	5.111320	9.810164
H	7.160166	5.794526	9.912804
C	6.459215	3.798267	10.201850
H	7.402176	3.431311	10.610346
N	1.976011	4.425462	11.509260
C	2.629446	5.517453	11.836990
C	3.600265	5.510508	12.864441
H	4.148201	6.424720	13.097949
C	3.838482	4.344811	13.555559
H	4.594037	4.317087	14.344417
C	3.075258	3.179840	13.279675
C	2.137669	3.290116	12.229073
C	1.267249	2.211751	11.851985
O	0.477609	2.410589	10.831442
C	1.367235	1.038894	12.591958
H	0.701216	0.204205	12.361517
C	2.316578	0.921138	13.634465
H	2.369871	-0.021620	14.184181
C	3.167070	1.948829	13.980090
H	3.888473	1.836489	14.791103
C	1.918166	0.543696	9.079871
H	2.244184	-0.445192	8.699241
H	1.275614	0.366448	9.952867
N	1.146975	1.273014	8.073685
C	1.890869	1.384347	6.821396
H	1.916634	0.423377	6.269506
H	2.928359	1.653932	7.054437
C	1.323527	2.449967	5.914544
H	2.008154	2.588738	5.059733
H	0.337815	2.171900	5.498844
O	1.201977	3.662748	6.628554
C	0.855856	4.739318	5.784886
H	-0.175269	4.600754	5.410437
H	1.538367	4.779502	4.918149
C	0.972985	6.020950	6.556660
H	2.014281	6.189148	6.872946
H	0.627917	6.851667	5.919753
O	0.140086	5.911897	7.704345
C	-0.211733	7.156088	8.287283
H	-1.232281	7.048499	8.666488
H	-0.248306	7.931175	7.504789

C	0.771862	7.595147	9.361812
H	1.749686	7.730913	8.879942
H	0.455245	8.587389	9.744466
N	0.950768	6.624661	10.434926
C	2.260576	6.764344	11.072874
H	2.293844	7.636585	11.755551
H	3.012309	6.929791	10.290941
C	-0.097174	6.633290	11.452268
H	-0.246187	7.645361	11.880322
H	0.234331	5.982120	12.270301
C	-1.438691	6.123248	10.963249
H	-2.050925	5.826855	11.832061
H	-2.000076	6.906779	10.425819
O	-1.246798	5.008805	10.111025
C	-2.432325	4.556735	9.480012
H	-2.482545	4.970956	8.456968
H	-3.319170	4.896300	10.037698
C	-2.425440	3.056457	9.458604
H	-2.361817	2.676505	10.493203
H	-3.361076	2.688787	9.000264
O	-1.311397	2.599807	8.721578
C	-1.208004	1.183071	8.825784
H	-2.181950	0.730467	8.570510
H	-0.952656	0.931493	9.866264
C	-0.170348	0.682480	7.855775
H	-0.135211	-0.423063	7.906260
H	-0.509502	0.935385	6.842680

Tm-syn-KHQ(1+)

SCF (RwB97XD) = -1949.65187867
 E(SCF)+ZPE(0 K)= -1948.967705
 H(298 K)= -1948.931128
 G(298 K)= -1949.030731
 Lowest Frequency = 35.7590cm⁻¹

Tm	0.966323	3.958461	9.255314
N	3.065973	2.635677	9.314922
C	3.128018	1.336781	9.511663
C	4.286501	0.736069	10.053366
H	4.305098	-0.339561	10.235203
C	5.379185	1.522480	10.339487
H	6.280131	1.076706	10.767876
C	5.364472	2.910013	10.039343
C	4.153782	3.416652	9.515546
C	3.990221	4.794448	9.135505
O	2.810887	5.171569	8.722994
C	5.105110	5.614758	9.274476
H	5.037984	6.659908	8.963665
C	6.313680	5.111320	9.810164
H	7.160166	5.794526	9.912804
C	6.459215	3.798267	10.201850
H	7.402176	3.431311	10.610346
N	1.976011	4.425462	11.509260
C	2.629446	5.517453	11.836990
C	3.600265	5.510508	12.864441
H	4.148201	6.424720	13.097949

C	3.838482	4.344811	13.555559
H	4.594037	4.317087	14.344417
C	3.075258	3.179840	13.279675
C	2.137669	3.290116	12.229073
C	1.267249	2.211751	11.851985
O	0.477609	2.410589	10.831442
C	1.367235	1.038894	12.591958
H	0.701216	0.204205	12.361517
C	2.316578	0.921138	13.634465
H	2.369871	-0.021620	14.184181
C	3.167070	1.948829	13.980090
H	3.888473	1.836489	14.791103
C	1.918166	0.543696	9.079871
H	2.244184	-0.445192	8.699241
H	1.275614	0.366448	9.952867
N	1.146975	1.273014	8.073685
C	1.890869	1.384347	6.821396
H	1.916634	0.423377	6.269506
H	2.928359	1.653932	7.054437
C	1.323527	2.449967	5.914544
H	2.008154	2.588738	5.059733
H	0.337815	2.171900	5.498844
O	1.201977	3.662748	6.628554
C	0.855856	4.739318	5.784886
H	-0.175269	4.600754	5.410437
H	1.538367	4.779502	4.918149
C	0.972985	6.020950	6.556660
H	2.014281	6.189148	6.872946
H	0.627917	6.851667	5.919753
O	0.140086	5.911897	7.704345
C	-0.211733	7.156088	8.287283
H	-1.232281	7.048499	8.666488
H	-0.248306	7.931175	7.504789
C	0.771862	7.595147	9.361812
H	1.749686	7.730913	8.879942
H	0.455245	8.587389	9.744466
N	0.950768	6.624661	10.434926
C	2.260576	6.764344	11.072874
H	2.293844	7.636585	11.755551
H	3.012309	6.929791	10.290941
C	-0.097174	6.633290	11.452268
H	-0.246187	7.645361	11.880322
H	0.234331	5.982120	12.270301
C	-1.438691	6.123248	10.963249
H	-2.050925	5.826855	11.832061
H	-2.000076	6.906779	10.425819
O	-1.246798	5.008805	10.111025
C	-2.432325	4.556735	9.480012
H	-2.482545	4.970956	8.456968
H	-3.319170	4.896300	10.037698
C	-2.425440	3.056457	9.458604
H	-2.361817	2.676505	10.493203
H	-3.361076	2.688787	9.000264
O	-1.311397	2.599807	8.721578
C	-1.208004	1.183071	8.825784
H	-2.181950	0.730467	8.570510
H	-0.952656	0.931493	9.866264

C	-0.170348	0.682480	7.855775
H	-0.135211	-0.423063	7.906260
H	-0.509502	0.935385	6.842680

Tm-syn-H2O-KHQ(1+)

SCF (RwB97XD) = -2026.01309233
 E(SCF)+ZPE(0 K)= -2025.303178
 H(298 K)= -2025.264507
 G(298 K)= -2025.368266
 Lowest Frequency = 23.4511cm⁻¹

Tm	1.067016	4.021124	9.107353
N	3.099698	2.629457	9.128138
C	3.119059	1.316443	9.205935
C	4.271994	0.627220	9.646406
H	4.259274	-0.461984	9.711093
C	5.395483	1.343214	9.987836
H	6.291960	0.827106	10.339864
C	5.411723	2.756248	9.859687
C	4.211566	3.353549	9.408791
C	4.091602	4.772381	9.203146
O	2.936157	5.234358	8.807073
C	5.219367	5.542058	9.466189
H	5.175353	6.620874	9.300078
C	6.414412	4.944991	9.929358
H	7.274736	5.588570	10.127634
C	6.528618	3.587362	10.132683
H	7.461043	3.145138	10.487243
N	1.852788	4.488863	11.464917
C	2.369446	5.617006	11.895620
C	3.135304	5.675306	13.083465
H	3.559427	6.627319	13.406972
C	3.334541	4.526938	13.812787
H	3.931851	4.549546	14.727464
C	2.736554	3.308445	13.399226
C	1.988345	3.359750	12.201131
C	1.284481	2.218385	11.688539
O	0.625846	2.373776	10.575854
C	1.370985	1.040469	12.423258
H	0.832540	0.153790	12.079824
C	2.138143	0.983794	13.610329
H	2.186225	0.037655	14.154557
C	2.815532	2.077791	14.101919
H	3.395963	2.015181	15.023823
C	1.863974	0.584667	8.799393
H	2.140226	-0.375757	8.319260
H	1.301903	0.347014	9.709957
N	1.018330	1.386356	7.909725
C	1.686658	1.497398	6.604792
H	1.523895	0.583594	6.000176
H	2.768153	1.580720	6.773523
C	1.266606	2.696445	5.793747
H	1.781463	2.652578	4.817705
H	0.178520	2.705355	5.601742
O	1.628591	3.882763	6.468735
C	1.459350	5.013529	5.641729

H	0.489853	4.941544	5.113790
H	2.259456	5.049605	4.880924
C	1.488115	6.279958	6.452534
H	2.440239	6.366816	6.997902
H	1.362146	7.136156	5.767271
O	0.404199	6.234761	7.372240
C	0.082650	7.464547	7.984172
H	-0.982806	7.419160	8.245586
H	0.195931	8.291190	7.261475
C	0.953342	7.743542	9.192174
H	1.992927	7.801645	8.843115
H	0.691121	8.740379	9.601586
N	0.905874	6.710947	10.229177
C	2.116690	6.834855	11.052140
H	2.071628	7.734766	11.696555
H	2.973423	6.953366	10.376412
C	-0.280622	6.784440	11.088366
H	-0.557479	7.838082	11.292710
H	-0.024206	6.329776	12.055056
C	-1.520615	6.063855	10.596763
H	-2.299843	6.204854	11.366596
H	-1.924629	6.489157	9.661327
O	-1.271449	4.683736	10.423227
C	-2.474837	3.932650	10.460645
H	-3.141807	4.257519	9.637682
H	-3.000224	4.141653	11.409044
C	-2.246260	2.443738	10.379641
H	-1.514025	2.135143	11.140114
H	-3.213309	1.943028	10.569927
O	-1.766349	2.111426	9.097160
C	-1.241780	0.809658	8.937159
H	-2.068026	0.099705	8.753359
H	-0.727119	0.514589	9.862530
C	-0.301305	0.760068	7.743883
H	-0.177334	-0.306013	7.463797
H	-0.807502	1.243136	6.895027
O	-0.857539	3.929837	7.602395
H	-1.536264	3.333685	7.981556
H	-1.221664	4.759449	7.279042

Yb-anti-KHQ-Ligand(2-)

SCF (RwB97XD) = -1910.47711962
 E(SCF)+ZPE(0 K)= -1909.810950
 H(298 K)= -1909.776767
 G(298 K)= -1909.873267
 Lowest Frequency = -68.0613cm⁻¹

C	5.821005	1.407045	17.300756
C	5.486098	1.666717	18.653693
C	5.187407	0.535342	19.457056
H	4.922389	0.676639	20.507749
C	5.190126	-0.718430	18.899960
H	4.914219	-1.596342	19.487533
C	5.548413	-0.872179	17.537477
C	5.531186	-2.240067	16.904891
H	6.392422	-2.803188	17.298218

H	4.640463	-2.791328	17.266202
C	4.280018	-2.129636	14.804291
H	3.531109	-2.767861	15.313731
H	4.398573	-2.498884	13.777628
C	3.723051	-0.718467	14.697161
H	2.756019	-0.769547	14.170836
H	3.551798	-0.247257	15.678693
C	4.139555	1.061175	13.069915
H	4.040425	2.011691	13.618827
H	3.159074	0.762611	12.664658
C	5.128442	1.203700	11.928520
H	5.172057	0.276583	11.334280
H	4.820037	2.043392	11.284695
C	7.344914	2.228225	11.767618
H	6.817288	2.910482	11.081369
H	7.980970	1.561680	11.162682
C	6.378360	-3.335476	14.939139
H	6.252948	-3.355980	13.855329
H	6.034933	-4.311986	15.335744
N	5.898289	0.147919	16.787803
N	5.590526	-2.221395	15.451617
O	6.301299	2.167239	15.130092
O	4.631457	0.059957	13.940918
O	6.399625	1.464783	12.493210
C	7.553486	-2.029930	12.146617
C	8.855035	-1.420628	12.089048
C	9.901150	-1.980514	11.313159
C	11.104487	-1.231029	11.244044
H	11.944420	-1.614685	10.659688
C	11.188696	-0.014179	11.872187
H	12.086915	0.601072	11.789841
C	10.087322	0.453157	12.631783
C	10.155761	1.799456	13.305864
H	10.647562	2.518681	12.621246
H	10.840537	1.711394	14.164282
C	8.999817	3.024858	15.021569
H	9.768853	3.821520	14.969529
H	8.040861	3.503596	15.226422
C	9.362231	2.093447	16.181660
H	8.937849	2.488908	17.117850
H	10.454813	2.034310	16.306778
C	9.808704	-0.247894	16.288310
H	10.531812	-0.348546	15.458438
H	10.359373	0.000224	17.210049
C	9.083429	-1.546000	16.509083
H	8.467588	-1.490855	17.425239
H	9.834038	-2.343123	16.634050
C	7.864111	-3.184818	15.277026
H	8.470806	-3.657767	14.488838
H	8.099681	-3.686255	16.228864
C	8.137212	3.069135	12.756581
H	7.410049	3.694353	13.290140
H	8.813685	3.738595	12.189179
N	8.987062	-0.250229	12.772412
N	8.868738	2.298595	13.764659
O	8.870917	0.765462	15.980595
O	8.253728	-1.813831	15.395095

O	6.630937	-1.443635	12.844450
C	7.380476	-3.221608	11.441198
H	6.395011	-3.692568	11.442611
C	8.439731	-3.795895	10.707897
H	8.258455	-4.730410	10.171626
C	9.682537	-3.203828	10.632286
H	10.486151	-3.646993	10.041936
C	6.036251	2.475124	16.361701
C	5.945693	3.778138	16.853474
H	6.075902	4.610285	16.158107
C	5.656229	4.027417	18.211235
H	5.596125	5.063901	18.551610
C	5.427712	3.007012	19.109780
H	5.181440	3.214800	20.152317

Yb-anti-KHQ(1+)

SCF (RwB97XD) = -1950.22815543

E(SCF)+ZPE(0 K)= -1949.545301

H(298 K)= -1949.508130

G(298 K)= -1949.610549

Lowest Frequency = 23.2100cm⁻¹

C	5.821005	1.407045	17.300756
C	5.486098	1.666717	18.653693
C	5.187407	0.535342	19.457056
H	4.922389	0.676639	20.507749
C	5.190126	-0.718430	18.899960
H	4.914219	-1.596342	19.487533
C	5.548413	-0.872179	17.537477
C	5.531186	-2.240067	16.904891
H	6.392422	-2.803188	17.298218
H	4.640463	-2.791328	17.266202
C	4.280018	-2.129636	14.804291
H	3.531109	-2.767861	15.313731
H	4.398573	-2.498884	13.777628
C	3.723051	-0.718467	14.697161
H	2.756019	-0.769547	14.170836
H	3.551798	-0.247257	15.678693
C	4.139555	1.061175	13.069915
H	4.040425	2.011691	13.618827
H	3.159074	0.762611	12.664658
C	5.128442	1.203700	11.928520
H	5.172057	0.276583	11.334280
H	4.820037	2.043392	11.284695
C	7.344914	2.228225	11.767618
H	6.817288	2.910482	11.081369
H	7.980970	1.561680	11.162682
C	6.378360	-3.335476	14.939139
H	6.252948	-3.355980	13.855329
H	6.034933	-4.311986	15.335744
N	5.898289	0.147919	16.787803
N	5.590526	-2.221395	15.451617
O	6.301299	2.167239	15.130092
O	4.631457	0.059957	13.940918
O	6.399625	1.464783	12.493210
C	7.553486	-2.029930	12.146617

C	8.855035	-1.420628	12.089048
C	9.901150	-1.980514	11.313159
C	11.104487	-1.231029	11.244044
H	11.944420	-1.614685	10.659688
C	11.188696	-0.014179	11.872187
H	12.086915	0.601072	11.789841
C	10.087322	0.453157	12.631783
C	10.155761	1.799456	13.305864
H	10.647562	2.518681	12.621246
H	10.840537	1.711394	14.164282
C	8.999817	3.024858	15.021569
H	9.768853	3.821520	14.969529
H	8.040861	3.503596	15.226422
C	9.362231	2.093447	16.181660
H	8.937849	2.488908	17.117850
H	10.454813	2.034310	16.306778
C	9.808704	-0.247894	16.288310
H	10.531812	-0.348546	15.458438
H	10.359373	0.000224	17.210049
C	9.083429	-1.546000	16.509083
H	8.467588	-1.490855	17.425239
H	9.834038	-2.343123	16.634050
C	7.864111	-3.184818	15.277026
H	8.470806	-3.657767	14.488838
H	8.099681	-3.686255	16.228864
C	8.137212	3.069135	12.756581
H	7.410049	3.694353	13.290140
H	8.813685	3.738595	12.189179
N	8.987062	-0.250229	12.772412
N	8.868738	2.298595	13.764659
O	8.870917	0.765462	15.980595
O	8.253728	-1.813831	15.395095
O	6.630937	-1.443635	12.844450
C	7.380476	-3.221608	11.441198
H	6.395011	-3.692568	11.442611
C	8.439731	-3.795895	10.707897
H	8.258455	-4.730410	10.171626
C	9.682537	-3.203828	10.632286
H	10.486151	-3.646993	10.041936
C	6.036251	2.475124	16.361701
C	5.945693	3.778138	16.853474
H	6.075902	4.610285	16.158107
C	5.656229	4.027417	18.211235
H	5.596125	5.063901	18.551610
C	5.427712	3.007012	19.109780
H	5.181440	3.214800	20.152317
Yb	6.994421	0.137799	14.416866

Yb3+_Ion

SCF (RwB97XD) = -37.8683700782
 E(SCF)+ZPE(0 K)= -37.868370
 H(298 K)= -37.866010
 G(298 K)= -37.885665

Yb 0.887400 3.945900 9.220400

Yb-syn-KHQ_Ligand(2-)

SCF (RwB97XD) = -1910.49220570

E(SCF)+ZPE(0 K)= -1909.824093

H(298 K)= -1909.789093

G(298 K)= -1909.886224

Lowest Frequency = -38.5923cm⁻¹

N	3.064512	2.642280	9.317809
C	3.133588	1.343235	9.512573
C	4.296972	0.747196	10.048846
H	4.320706	-0.328576	10.229242
C	5.387953	1.537517	10.330474
H	6.292709	1.095024	10.754211
C	5.366307	2.924874	10.030380
C	4.150895	3.426743	9.513239
C	3.980537	4.803398	9.133249
O	2.797089	5.175089	8.727458
C	5.092892	5.628089	9.264744
H	5.020132	6.672651	8.953241
C	6.306371	5.129458	9.793980
H	7.151024	5.815718	9.891092
C	6.458718	3.817310	10.185976
H	7.405324	3.454040	10.589293
N	1.978018	4.421025	11.508006
C	2.630247	5.512064	11.841637
C	3.598393	5.501652	12.871535
H	4.145535	6.415231	13.109347
C	3.834413	4.334037	13.560247
H	4.587682	4.303948	14.351200
C	3.070600	3.170648	13.279652
C	2.136728	3.284427	12.226325
C	1.264761	2.209296	11.845098
O	0.479415	2.413429	10.822215
C	1.358583	1.035185	12.583577
H	0.690602	0.202826	12.350452
C	2.304757	0.913392	13.628674
H	2.353747	-0.030226	14.177300
C	3.157123	1.938165	13.978266
H	3.875677	1.822601	14.791349
C	1.927736	0.544035	9.081333
H	2.259119	-0.443787	8.702397
H	1.285123	0.364309	9.953693
N	1.155293	1.269136	8.074181
C	1.899157	1.385866	6.823079
H	1.927799	0.427074	6.267448
H	2.935994	1.657566	7.056620
C	1.328030	2.453072	5.920859
H	2.011330	2.597494	5.065911
H	0.342914	2.173102	5.505033
O	1.202616	3.663249	6.638828
C	0.846235	4.737747	5.796973
H	-0.186530	4.594025	5.428944
H	1.523000	4.780595	4.925866
C	0.961945	6.020430	6.566479
H	2.004094	6.194132	6.876622
H	0.609234	6.848581	5.930435

O	0.136317	5.908992	7.718936
C	-0.215471	7.153502	8.301535
H	-1.236194	7.047554	8.680731
H	-0.251861	7.928047	7.518579
C	0.768356	7.593396	9.375266
H	1.745356	7.731082	8.892348
H	0.450220	8.584783	9.758999
N	0.950131	6.622182	10.446601
C	2.259847	6.761990	11.083544
H	2.292392	7.630846	11.770599
H	3.010869	6.932894	10.302170
C	-0.097620	6.623722	11.463643
H	-0.252364	7.634078	11.893780
H	0.236824	5.972897	12.280696
C	-1.436057	6.107622	10.972046
H	-2.046220	5.800634	11.838590
H	-2.002326	6.891671	10.440679
O	-1.238097	5.001173	10.110514
C	-2.418862	4.558920	9.463536
H	-2.453022	4.977330	8.441542
H	-3.310279	4.902013	10.011528
C	-2.420629	3.059011	9.435954
H	-2.372178	2.674728	10.469782
H	-3.352619	2.698301	8.964777
O	-1.300104	2.599635	8.710966
C	-1.200735	1.182953	8.819728
H	-2.174825	0.732149	8.561836
H	-0.950417	0.934013	9.862018
C	-0.160420	0.676317	7.855813
H	-0.125193	-0.428869	7.913587
H	-0.496695	0.922075	6.840007

Yb-syn-KHQ(1+)

SCF (RWB97XD) = -1950.23603501
 E(SCF)+ZPE(0 K)= -1949.551688
 H(298 K)= -1949.515159
 G(298 K)= -1949.614564
 Lowest Frequency = 37.9442cm⁻¹

Yb	0.971878	3.958290	9.262481
N	3.064512	2.642280	9.317809
C	3.133588	1.343235	9.512573
C	4.296972	0.747196	10.048846
H	4.320706	-0.328576	10.229242
C	5.387953	1.537517	10.330474
H	6.292709	1.095024	10.754211
C	5.366307	2.924874	10.030380
C	4.150895	3.426743	9.513239
C	3.980537	4.803398	9.133249
O	2.797089	5.175089	8.727458
C	5.092892	5.628089	9.264744
H	5.020132	6.672651	8.953241
C	6.306371	5.129458	9.793980
H	7.151024	5.815718	9.891092
C	6.458718	3.817310	10.185976
H	7.405324	3.454040	10.589293

N	1.978018	4.421025	11.508006
C	2.630247	5.512064	11.841637
C	3.598393	5.501652	12.871535
H	4.145535	6.415231	13.109347
C	3.834413	4.334037	13.560247
H	4.587682	4.303948	14.351200
C	3.070600	3.170648	13.279652
C	2.136728	3.284427	12.226325
C	1.264761	2.209296	11.845098
O	0.479415	2.413429	10.822215
C	1.358583	1.035185	12.583577
H	0.690602	0.202826	12.350452
C	2.304757	0.913392	13.628674
H	2.353747	-0.030226	14.177300
C	3.157123	1.938165	13.978266
H	3.875677	1.822601	14.791349
C	1.927736	0.544035	9.081333
H	2.259119	-0.443787	8.702397
H	1.285123	0.364309	9.953693
N	1.155293	1.269136	8.074181
C	1.899157	1.385866	6.823079
H	1.927799	0.427074	6.267448
H	2.935994	1.657566	7.056620
C	1.328030	2.453072	5.920859
H	2.011330	2.597494	5.065911
H	0.342914	2.173102	5.505033
O	1.202616	3.663249	6.638828
C	0.846235	4.737747	5.796973
H	-0.186530	4.594025	5.428944
H	1.523000	4.780595	4.925866
C	0.961945	6.020430	6.566479
H	2.004094	6.194132	6.876622
H	0.609234	6.848581	5.930435
O	0.136317	5.908992	7.718936
C	-0.215471	7.153502	8.301535
H	-1.236194	7.047554	8.680731
H	-0.251861	7.928047	7.518579
C	0.768356	7.593396	9.375266
H	1.745356	7.731082	8.892348
H	0.450220	8.584783	9.758999
N	0.950131	6.622182	10.446601
C	2.259847	6.761990	11.083544
H	2.292392	7.630846	11.770599
H	3.010869	6.932894	10.302170
C	-0.097620	6.623722	11.463643
H	-0.252364	7.634078	11.893780
H	0.236824	5.972897	12.280696
C	-1.436057	6.107622	10.972046
H	-2.046220	5.800634	11.838590
H	-2.002326	6.891671	10.440679
O	-1.238097	5.001173	10.110514
C	-2.418862	4.558920	9.463536
H	-2.453022	4.977330	8.441542
H	-3.310279	4.902013	10.011528
C	-2.420629	3.059011	9.435954
H	-2.372178	2.674728	10.469782
H	-3.352619	2.698301	8.964777

O	-1.300104	2.599635	8.710966
C	-1.200735	1.182953	8.819728
H	-2.174825	0.732149	8.561836
H	-0.950417	0.934013	9.862018
C	-0.160420	0.676317	7.855813
H	-0.125193	-0.428869	7.913587
H	-0.496695	0.922075	6.840007

Yb-syn-H₂O-KHQ(1+)

SCF (RwB97XD) = -2026.59748734
 E(SCF)+ZPE(0 K)= -2025.887902
 H(298 K)= -2025.849061
 G(298 K)= -2025.953618
 Lowest Frequency = 22.1715cm⁻¹

Yb	1.083592	4.017571	9.114990
N	3.102472	2.629471	9.126157
C	3.123094	1.316062	9.200147
C	4.279612	0.626795	9.630911
H	4.268185	-0.462607	9.692426
C	5.405244	1.342520	9.966206
H	6.304491	0.825908	10.310347
C	5.419911	2.755790	9.841066
C	4.216212	3.353160	9.400269
C	4.093881	4.771865	9.196897
O	2.934783	5.232032	8.808579
C	5.222434	5.542360	9.452837
H	5.176464	6.621334	9.288404
C	6.421335	4.945359	9.906464
H	7.282611	5.589283	10.099350
C	6.538153	3.587529	10.106866
H	7.473625	3.145627	10.453707
N	1.854120	4.488243	11.462743
C	2.365516	5.617277	11.897767
C	3.118006	5.677006	13.093981
H	3.538021	6.629590	13.421131
C	3.308898	4.529715	13.827439
H	3.895626	4.553847	14.748900
C	2.714855	3.310890	13.409380
C	1.980616	3.360727	12.202797
C	1.279623	2.220268	11.685076
O	0.632283	2.376887	10.565777
C	1.355392	1.043496	12.422418
H	0.818801	0.157235	12.075053
C	2.109477	0.987717	13.618084
H	2.149621	0.042569	14.164647
C	2.783413	2.081313	14.115206
H	3.353131	2.019256	15.043799
C	1.866583	0.584631	8.797139
H	2.141566	-0.375767	8.316172
H	1.306558	0.346814	9.708892
N	1.020132	1.387687	7.909997
C	1.685967	1.499372	6.604033
H	1.520362	0.586713	5.998376
H	2.768051	1.580361	6.770290
C	1.266642	2.700160	5.795290

H	1.777659	2.654923	4.817243
H	0.177871	2.711525	5.606965
O	1.634155	3.885347	6.468867
C	1.463295	5.015953	5.642074
H	0.494280	4.942439	5.113340
H	2.263608	5.053732	4.881532
C	1.488419	6.282708	6.452207
H	2.438582	6.369665	7.000951
H	1.365448	7.138580	5.765887
O	0.401050	6.238366	7.367550
C	0.083719	7.467285	7.983068
H	-0.981215	7.423839	8.246981
H	0.197233	8.295481	7.262087
C	0.957724	7.741788	9.189622
H	1.997036	7.796277	8.839193
H	0.699928	8.739399	9.600022
N	0.908028	6.709319	10.226598
C	2.117686	6.833827	11.051191
H	2.072703	7.735108	11.693644
H	2.975776	6.949650	10.376745
C	-0.279899	6.785035	11.083990
H	-0.559826	7.839305	11.280499
H	-0.023765	6.338253	12.054462
C	-1.517145	6.057223	10.596270
H	-2.299388	6.206168	11.361704
H	-1.918147	6.471858	9.654608
O	-1.265499	4.676187	10.438828
C	-2.469037	3.925817	10.475447
H	-3.136685	4.252577	9.653698
H	-2.993891	4.133227	11.424618
C	-2.243321	2.436618	10.389991
H	-1.506829	2.125267	11.145050
H	-3.209789	1.937331	10.586586
O	-1.774282	2.104798	9.103131
C	-1.240292	0.807097	8.939747
H	-2.062177	0.092293	8.755541
H	-0.722963	0.513143	9.863924
C	-0.300802	0.763818	7.745073
H	-0.178245	-0.301026	7.459521
H	-0.808387	1.251354	6.899583
O	-0.829686	3.926488	7.636717
H	-1.512657	3.331702	8.012537
H	-1.184320	4.757382	7.305430

KHQLaΔ_λλλ_λλλ_opt.log

SCF (RwB97XD) = -1942.42343658

E(SCF)+ZPE(0 K)= -1941.740634

H(298 K)= -1941.703805

G(298 K)= -1941.804991

Lowest Frequency = 10.9892cm⁻¹

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C	-3.691406	1.074612	0.378470
N	-2.640801	0.599783	1.296318
O	-2.042382	1.992321	-1.090127
C	-3.251659	1.243277	-1.068524

C	-2.495741	1.466396	2.472611
C	-1.862009	2.809365	2.146508
O	-0.507028	2.691019	1.737213
C	0.456144	2.635049	2.782601
C	1.815536	2.895033	2.173183
O	2.045926	2.002339	1.093430
O	0.506979	2.694746	-1.733366
C	-0.455923	2.634838	-2.778757
C	-1.816642	2.887163	-2.169068
N	2.651158	0.613851	-1.293719
C	2.501561	1.480241	-2.469624
C	1.861339	2.819924	-2.142689
C	3.259056	1.259561	1.071319
C	3.699444	1.093672	-0.375802
C	-2.835688	-0.795757	1.701220
C	2.853241	-0.780474	-1.699297
C	2.494885	-1.774676	-0.621372
C	-2.471942	-1.787668	0.622967
C	1.287579	-2.201337	1.319046
C	1.712432	-3.551115	1.374571
C	2.578880	-3.979508	0.333815
C	2.985254	-3.101837	-0.642736
C	-2.955134	-3.117464	0.643932
C	-2.544036	-3.992630	-0.332890
C	-1.679941	-3.559251	-1.373549
C	-1.262381	-2.207214	-1.317606
La	0.005149	0.676182	0.001338
H	-4.065228	2.046804	0.733731
H	-4.558204	0.391339	0.393755
H	-4.041031	1.784001	-1.615018
H	-3.083217	0.274329	-1.562666
H	3.095783	0.289569	1.565152
H	4.045727	1.804175	1.617849
H	4.068307	2.067871	-0.730753
H	4.569692	0.414812	-0.391432
H	-3.874089	-0.977040	2.040588
H	-2.173545	-0.993716	2.555765
H	3.892496	-0.956178	-2.038978
H	2.191923	-0.981535	-2.553767
C	1.270003	-4.369322	2.444342
H	2.933526	-5.013094	0.327250
H	3.667694	-3.417149	-1.433745
H	-3.635841	-3.436710	1.434857
H	-2.893081	-5.028123	-0.326621
C	-1.233116	-4.374719	-2.443583
N	-1.641641	-1.379130	-0.309818
N	1.662377	-1.370890	0.311526
C	0.439726	-1.623559	2.334011
O	0.081799	-0.374014	2.211409
C	0.047236	-2.467494	3.370586
C	-0.417644	-1.624551	-2.332370
O	-0.066360	-0.373161	-2.209310
C	-0.020657	-2.466018	-3.369243
H	0.431478	1.639560	3.256983
H	0.243959	3.415130	3.533543
H	2.582455	2.768806	2.952744
H	1.872255	3.925573	1.786576

H	-0.426057	1.640010	-3.254193
H	-0.247827	3.416776	-3.528915
H	-1.878695	3.917048	-1.781531
H	-2.582907	2.757681	-2.948736
H	2.378206	3.320427	-1.311810
H	1.921875	3.482965	-3.021565
H	3.474260	1.663931	-2.968144
H	1.857085	0.951422	-3.185354
H	-1.925824	3.471551	3.025799
H	-2.381211	3.307917	1.315922
H	-3.469438	1.645084	2.971002
H	-1.848843	0.940474	3.188284
C	0.457077	-3.818434	3.411078
C	-0.423204	-3.819139	-3.410168
H	-0.082638	-4.439130	-4.242905
H	-1.540759	-5.420400	-2.495167
H	0.602700	-2.056098	-4.167315
H	0.119845	-4.440521	4.243608
H	1.583296	-5.413339	2.495606
H	-0.578341	-2.061200	4.168774

KHQLuΔ_δδδ_δδδ_opt2.log

SCF (RwB97XD) = -1950.78988945

E(SCF)+ZPE(0 K)= -1950.106168

H(298 K)= -1950.069489

G(298 K)= -1950.170115

Lowest Frequency = 23.7976cm⁻¹

81

C	3.634828	-0.774246	-0.455427
N	2.882152	-0.524360	0.769066
O	1.703640	-1.601432	-1.562265
C	3.047442	-1.915926	-1.252194
C	3.141758	-1.536031	1.791089
C	1.869055	-2.074118	2.406647
O	1.007327	-2.495122	1.339426
C	0.067834	-3.487681	1.703715
C	-1.125886	-2.871855	2.392151
O	-1.672626	-1.914340	1.507317
O	-0.945275	-2.509402	-1.449687
C	0.078203	-3.247998	-2.097191
C	1.133990	-2.315958	-2.645178
N	-2.860496	-0.572026	-0.573917
C	-3.180062	-1.662628	-1.491734
C	-1.997870	-2.097357	-2.326205
C	-3.084883	-1.868768	1.523576
C	-3.569110	-0.695900	0.698533
C	3.053769	0.841052	1.251157
C	-3.078477	0.749031	-1.165898
C	-2.428057	1.818540	-0.319673
C	2.417614	1.838269	0.311242
C	-0.924192	2.228466	1.397109
C	-1.282301	3.590708	1.500228
C	-2.255714	4.046542	0.572471
C	-2.847481	3.167413	-0.307455
C	2.854317	3.180557	0.232924

C	2.277066	4.024743	-0.686642
C	1.294015	3.538062	-1.587206
C	0.919090	2.184842	-1.424581
Lu	-0.015206	-0.536460	0.021663
H	0.541281	-4.252150	2.341464
H	-0.262532	-3.966348	0.770565
H	-0.849227	-2.382061	3.340971
H	-1.861053	-3.663837	2.611698
H	-0.350049	-3.878579	-2.893438
H	0.524383	-3.910231	-1.339278
H	1.905014	-2.885458	-3.186698
H	0.689955	-1.576537	-3.327322
H	4.124061	1.098473	1.383799
H	2.569510	0.923719	2.233492
H	-4.159010	0.971031	-1.274587
H	-2.630304	0.760005	-2.168596
C	-0.676405	4.372689	2.518048
H	-2.560268	5.095819	0.587800
H	-3.634281	3.497984	-0.987252
H	3.643350	3.531567	0.899845
H	2.594272	5.068307	-0.751966
C	0.692609	4.293597	-2.626927
N	1.448700	1.392576	-0.459650
N	-1.459552	1.405771	0.467474
C	0.010206	1.597181	2.288921
O	0.295005	0.340763	2.067437
C	0.545793	2.395027	3.293150
C	-0.042420	1.547166	-2.283795
O	-0.361067	0.306959	-2.023686
C	-0.578937	2.318986	-3.307916
H	4.703990	-0.983574	-0.251927
H	3.626326	-2.034142	-2.182834
H	3.091831	-2.872201	-0.699965
H	-4.664062	-0.794145	0.556621
H	-3.398811	0.221184	1.274475
H	-3.451285	-1.747987	2.557367
H	-3.476504	-2.831408	1.146170
H	-1.637239	-1.278794	-2.966399
H	-2.297615	-2.954054	-2.952409
H	-3.514721	-2.531524	-0.909222
H	-4.016397	-1.399068	-2.166579
H	2.104721	-2.943731	3.041621
H	1.357912	-1.301598	2.997904
H	3.792526	-1.148541	2.595452
H	3.687505	-2.375839	1.336646
H	3.592949	0.124565	-1.084377
C	0.204239	3.765580	3.386908
C	-0.212579	3.676116	-3.461734
H	-0.665665	4.248600	-4.274566
H	-1.291483	1.862307	-3.998565
H	0.965219	5.341219	-2.764636
H	0.657200	4.358635	4.184986
H	-0.927837	5.430008	2.615934
H	1.233705	1.952652	4.017185

KHQLuΔ_δδλ_δδλ_opt.log

SCF (RwB97XD) = -1950.78648661
 E(SCF)+ZPE(0 K)= -1950.102776
 H(298 K)= -1950.066105
 G(298 K)= -1950.166356
 Lowest Frequency = 25.2323cm⁻¹

81

C	3.522819	1.060975	-0.221150
N	2.633240	0.855622	0.919906
O	2.517773	-0.884226	-1.198932
C	3.727823	-0.163423	-1.092942
C	3.178928	0.033585	1.993467
C	3.100066	-1.465046	1.742915
O	1.761605	-1.851887	1.471957
C	1.201256	-2.899146	2.247933
C	-0.209277	-2.499045	2.617067
O	-0.935367	-2.179444	1.444383
O	0.489283	-2.714872	-1.199533
C	1.825447	-3.127320	-1.431736
C	2.578675	-1.991166	-2.078593
N	-2.108778	-1.711869	-1.069159
C	-1.654126	-2.414881	-2.261405
C	-0.488521	-3.349003	-2.016211
C	-1.755022	-3.198253	0.913662
C	-2.733980	-2.559614	-0.054980
C	2.175185	2.158983	1.414021
C	-2.996154	-0.610813	-1.447288
C	-3.032697	0.470113	-0.397534
C	1.207875	2.787179	0.439369
C	-1.996320	1.431504	1.437888
C	-3.032848	2.373988	1.630720
C	-4.103727	2.324599	0.700406
C	-4.120922	1.366700	-0.285270
C	0.959417	4.177077	0.380589
C	0.121390	4.668183	-0.595362
C	-0.436526	3.798047	-1.569077
C	-0.133156	2.426706	-1.416548
Lu	0.228610	-0.437138	0.012425
H	2.578223	0.237237	2.889871
H	4.232104	0.294381	2.225148
H	3.460288	-1.980081	2.646833
H	3.738537	-1.793317	0.910655
H	1.790540	-3.058850	3.164466
H	1.216186	-3.835763	1.662244
H	-0.186260	-1.582247	3.220408
H	-0.708638	-3.304886	3.177996
H	1.853739	-4.026257	-2.065812
H	2.280869	-3.375423	-0.461723
H	3.625372	-2.293232	-2.249101
H	2.126326	-1.714591	-3.045546
H	-1.316563	-1.641736	-2.962112
H	-2.467805	-2.998723	-2.738735
H	-0.793598	-4.297099	-1.540882
H	-0.052789	-3.601847	-2.996170
H	3.022780	2.850495	1.588861
H	1.664420	2.007897	2.372528
H	-4.024872	-0.967168	-1.650423

H	-2.623141	-0.167533	-2.379742
C	-2.951336	3.266235	2.730462
H	-4.928639	3.035040	0.794368
H	-4.958123	1.290264	-0.981019
H	1.434320	4.844575	1.101397
H	-0.090241	5.738852	-0.649927
C	-1.230090	4.196160	-2.676241
N	0.625499	1.959498	-0.398988
N	-1.997945	0.545818	0.409777
C	-0.881820	1.323514	2.340820
O	0.029206	0.427694	2.079401
C	-0.860758	2.202680	3.419385
C	-0.565422	1.423210	-2.352013
O	-0.240419	0.184710	-2.097810
C	-1.310353	1.868975	-3.438929
H	3.074550	1.843417	-0.845368
H	4.517741	1.431476	0.098358
H	4.065097	0.165713	-2.090545
H	4.512812	-0.828123	-0.687920
H	-3.361100	-3.350920	-0.511590
H	-3.401645	-1.925736	0.545213
H	-2.331780	-3.672806	1.725549
H	-1.136217	-3.981086	0.446213
C	-1.639085	3.238415	-3.578871
H	-1.488324	5.247596	-2.812245
H	-2.234071	3.542500	-4.443400
H	-1.631656	1.149611	-4.195748
C	-1.883372	3.162472	3.594741
H	-3.737511	4.006179	2.889090
H	-1.823159	3.836918	4.452230
H	-0.044495	2.133732	4.142176

KHQLuΔ_{δλδ}_δλδ_opt.log

SCF (Rwb97XD) = -1950.78598718
 E(SCF)+ZPE(0 K)= -1950.101531
 H(298 K)= -1950.064803
 G(298 K)= -1950.166175
 Lowest Frequency = 12.8609cm⁻¹

81

C	3.500271	-0.702062	-0.790486
N	2.912478	-0.485165	0.526176
O	1.581657	-2.052160	-1.315958
C	2.994292	-1.979816	-1.423279
C	3.342621	-1.487397	1.496762
C	2.243921	-1.880500	2.450822
O	1.133678	-2.370245	1.707636
C	0.205448	-3.001473	2.558364
C	-1.042435	-3.293501	1.778418
O	-1.579891	-2.067899	1.312351
O	-1.131686	-2.370189	-1.710042
C	-0.199577	-2.986047	-2.567790
C	1.051466	-3.276791	-1.792585
N	-2.920711	-0.500212	-0.517352
C	-3.346234	-1.503675	-1.488606
C	-2.247908	-1.885648	-2.447520

C	-2.991990	-1.999272	1.429170
C	-3.505191	-0.722382	0.799966
C	3.131157	0.870920	1.018391
C	-3.147784	0.855318	-1.007540
C	-2.425518	1.875762	-0.165155
C	2.403512	1.888686	0.177383
C	-0.822038	2.225978	1.466939
C	-1.142401	3.593692	1.610425
C	-2.155450	4.086924	0.746815
C	-2.813042	3.233887	-0.109766
C	2.783186	3.249196	0.125800
C	2.120909	4.100780	-0.728557
C	1.110728	3.604151	-1.593558
C	0.798316	2.234153	-1.454114
Lu	-0.004411	-0.542873	0.002490
H	4.210360	1.125126	1.046907
H	2.753028	0.928693	2.048968
H	-4.228465	1.103214	-1.035048
H	-2.770367	0.916923	-2.038178
C	-0.461561	4.347937	2.601474
H	-2.434017	5.142425	0.793572
H	-3.627647	3.590379	-0.742042
H	3.595461	3.608657	0.759392
H	2.393322	5.158016	-0.772290
C	0.425297	4.357609	-2.582031
N	1.406060	1.432753	-0.547283
N	-1.425053	1.423789	0.557778
C	0.152867	1.567421	2.290038
O	0.402157	0.312832	2.027808
C	0.762601	2.336495	3.274407
C	-0.173520	1.572868	-2.278702
O	-0.416318	0.316264	-2.020087
C	-0.788020	2.341553	-3.260410
H	4.608038	-0.745208	-0.758907
H	3.285533	-1.997131	-2.487467
H	3.432662	-2.873280	-0.946317
H	-4.612791	-0.770636	0.770361
H	-3.233472	0.120387	1.447283
H	-3.276409	-2.018087	2.495161
H	-3.431106	-2.893456	0.954313
H	-1.916385	-1.027801	-3.052168
H	-2.616684	-2.683902	-3.115203
H	-3.661563	-2.411490	-0.958614
H	-4.226743	-1.164294	-2.066521
H	2.616185	-2.678562	3.116768
H	1.904240	-1.027107	3.057215
H	4.218217	-1.142163	2.078611
H	3.667408	-2.391370	0.965882
H	0.854506	-3.946533	-0.936744
H	1.773203	-3.776175	-2.457392
H	0.040966	-2.308479	-3.405895
H	-0.614771	-3.924611	-2.978124
H	3.225841	0.140636	-1.436798
H	-1.761975	-3.804398	2.436737
H	-0.839267	-3.953141	0.916266
H	0.627217	-3.940854	2.960041
H	-0.041199	-2.334091	3.402849

C	0.455391	3.711147	3.409454
C	-0.488493	3.718250	-3.391544
H	-1.002525	4.289476	-4.168247
H	0.643128	5.419731	-2.705293
H	-1.507619	1.871435	-3.934578
H	0.965838	4.282844	4.188174
H	-0.685383	5.408430	2.727976
H	1.484262	1.868338	3.947734

KHQLuΔ_{δλ}Δ_{δλ}_opt.log

SCF (RwB97XD) = -1950.79135692

E(SCF)+ZPE(0 K)= -1950.106470

H(298 K)= -1950.070281

G(298 K)= -1950.168483

Lowest Frequency = 36.6030cm⁻¹

81

C	-3.655652	-0.665856	0.306325
N	-2.782428	-0.485324	-0.851058
O	-1.863071	-1.820958	1.395783
C	-3.263395	-1.808216	1.219944
C	-2.925935	-1.503643	-1.883830
C	-2.146697	-2.775755	-1.582425
O	-0.757562	-2.529880	-1.428628
C	-0.001819	-2.628061	-2.629650
C	1.433312	-2.865697	-2.252551
O	1.857733	-1.835074	-1.387001
O	0.751002	-2.520546	1.443018
C	-0.005346	-2.609355	2.644316
C	-1.440873	-2.846499	2.268425
N	2.779736	-0.484459	0.849902
C	2.921236	-1.494918	1.890613
C	2.139649	-2.767868	1.599078
C	3.258015	-1.824227	-1.210900
C	3.652607	-0.675717	-0.306037
C	-2.945723	0.872685	-1.372201
C	2.945700	0.877263	1.360404
C	2.343257	1.876313	0.400878
C	-2.340882	1.878074	-0.420837
C	0.953475	2.177065	-1.429892
C	1.298202	3.540030	-1.572000
C	2.199355	4.057313	-0.604635
C	2.740174	3.231632	0.354447
C	-2.734391	3.234727	-0.385585
C	-2.191364	4.066946	0.566579
C	-1.291431	3.555422	1.538135
C	-0.950220	2.190445	1.407322
Lu	-0.001467	-0.555224	-0.000246
H	-4.011350	1.123840	-1.541400
H	-2.432239	0.942074	-2.338783
H	4.011795	1.127534	1.527958
H	2.432037	0.955278	2.326232
C	0.750518	4.269819	-2.658991
H	2.487519	5.110356	-0.649871
H	3.470424	3.607164	1.072913
H	-3.463730	3.606170	-1.107096

H	-2.476820	5.121066	0.603082
C	-0.741716	4.292813	2.618945
N	-1.438694	1.410621	0.414293
N	1.439915	1.404220	-0.430405
C	0.076174	1.500596	-2.346969
O	-0.227004	0.257383	-2.086839
C	-0.401889	2.247784	-3.418069
C	-0.074501	1.519351	2.329844
O	0.225539	0.273270	2.079951
C	0.405578	2.274180	3.394671
H	-4.711949	-0.808155	0.001388
H	-3.760125	-1.666263	2.195732
H	-3.600519	-2.787435	0.834502
H	4.708605	-0.817818	0.000025
H	3.612545	0.242961	-0.904023
H	3.755336	-1.690906	-2.187608
H	3.592818	-2.801213	-0.817857
H	-1.558350	-3.827051	1.770035
H	-2.055172	-2.846262	3.185410
H	0.095677	-1.671520	3.212180
H	0.348818	-3.461293	3.246978
H	-3.613724	0.257310	0.897192
H	2.047404	-2.872905	-3.169650
H	1.548919	-3.843078	-1.747537
H	-0.358016	-3.483112	-3.226673
H	-0.100944	-1.693508	-3.203316
H	-3.987332	-1.771062	-2.063558
H	-2.533197	-1.084275	-2.820392
H	-2.303877	-3.498509	-2.399177
H	-2.476488	-3.262455	-0.659336
H	2.468781	-3.262572	0.680013
H	2.295252	-3.484401	2.421587
H	2.529210	-1.067499	2.823828
H	3.982111	-1.762932	2.072537
C	-0.067419	3.615714	-3.554235
C	0.074649	3.644056	3.519505
H	0.483785	4.201796	4.365282
H	-0.985725	5.349836	2.736855
H	1.045517	1.795982	4.139801
H	-0.475018	4.167457	-4.404676
H	0.997279	5.325187	-2.785663
H	-1.042996	1.765048	-4.159260

KHQLuΔ_λδδ_λδδ_opt.log

SCF (RwB97XD) = -1950.78961773

E(SCF)+ZPE(0 K)= -1950.105533

H(298 K)= -1950.069153

G(298 K)= -1950.167884

Lowest Frequency = 43.3500cm⁻¹

81

C	3.720161	0.695709	0.506752
N	2.905252	0.590709	-0.711771
O	1.807170	1.796863	1.417817
C	2.898882	0.962411	1.765498
C	3.109447	1.715312	-1.620277

C	1.863120	2.129008	-2.368152
O	0.864947	2.509023	-1.413912
C	-0.155960	3.348667	-1.927559
C	-1.287715	2.529113	-2.494991
O	-1.803971	1.776093	-1.419573
O	-0.868295	2.505308	1.410316
C	0.144876	3.356003	1.921009
C	1.284269	2.548767	2.490803
N	-2.891049	0.566629	0.713921
C	-3.105227	1.691549	1.619787
C	-1.862414	2.118513	2.366087
C	-2.888100	0.930640	-1.764456
C	-3.706998	0.661294	-0.504781
C	3.021621	-0.717998	-1.346656
C	-2.995765	-0.741444	1.352100
C	-2.383403	-1.793819	0.456122
C	2.418832	-1.773469	-0.447812
C	-0.954454	-2.179557	-1.330901
C	-1.294821	-3.547227	-1.418078
C	-2.218120	-4.019258	-0.447411
C	-2.780457	-3.150673	0.460455
C	2.828373	-3.126607	-0.448197
C	2.273930	-3.997723	0.462101
C	1.346274	-3.531411	1.431382
C	0.993344	-2.167191	1.340229
Lu	0.006939	0.596059	0.000834
H	4.459590	1.501509	0.381988
H	4.301301	-0.225655	0.666984
H	3.530493	1.472097	2.511865
H	2.513376	0.036945	2.219018
H	0.255313	4.032849	-2.686106
H	-0.529518	3.947577	-1.083550
H	-0.932480	1.854810	-3.293829
H	-2.066895	3.194410	-2.906629
H	-0.272533	4.038768	2.677485
H	0.512668	3.955660	1.074997
H	2.057418	3.222550	2.899998
H	0.935443	1.873975	3.292048
H	-2.494233	0.006979	-2.214477
H	-3.524167	1.431958	-2.512702
H	-4.452689	1.461657	-0.382406
H	-4.280924	-0.265109	-0.662018
H	4.075191	-0.978633	-1.571247
H	2.472429	-0.701172	-2.298231
H	-4.047015	-1.010928	1.577136
H	-2.447089	-0.717231	2.303786
C	-0.721822	-4.322461	-2.459409
H	-2.505877	-5.073358	-0.449977
H	-3.526824	-3.494354	1.178220
H	3.577993	-3.465456	-1.164868
H	2.571383	-5.049117	0.467719
C	0.780435	-4.308829	2.475003
N	1.492847	-1.348922	0.383894
N	-1.461511	-1.363119	-0.376964
C	-0.067453	-1.539580	-2.264511
O	0.208509	-0.275790	-2.063511
C	0.437248	-2.331072	-3.289003

C	0.100675	-1.532613	2.272119
O	-0.186680	-0.271929	2.067602
C	-0.396719	-2.325713	3.298940
H	-2.110110	2.990602	2.993007
H	-1.461757	1.312279	2.998292
H	-3.905599	1.485052	2.357679
H	-3.433477	2.551533	1.021114
H	2.103130	3.001779	-2.997114
H	1.470289	1.317620	-2.998627
H	3.429516	2.579721	-1.023549
H	3.912005	1.514404	-2.357345
C	-0.059462	-3.697510	3.380613
C	0.112515	-3.706112	-3.366747
H	0.539958	-4.294822	-4.181847
H	-0.962441	-5.383461	-2.544114
H	1.090815	-1.879628	-4.038683
H	-0.481445	-4.287742	4.197455
H	1.030785	-5.367323	2.562791
H	-1.054281	-1.878071	4.047404

KHQLuΔ_λδλ_λδλ_opt.log

SCF (RwB97XD) = -1950.79826200

E(SCF)+ZPE(0 K)= -1950.114154

H(298 K)= -1950.077781

G(298 K)= -1950.176789

Lowest Frequency = 29.8080cm⁻¹

81

C	3.692738	0.876218	-0.161193
N	2.685951	0.529948	-1.171864
O	1.937527	1.821931	1.128374
C	3.123313	1.051624	1.238913
C	2.606614	1.499692	-2.258281
C	1.985895	2.806763	-1.807562
O	0.645528	2.581584	-1.386167
C	-0.374278	3.373791	-1.967369
C	-1.536078	2.483003	-2.326987
O	-1.943543	1.837492	-1.137300
O	-0.645292	2.587735	1.376891
C	0.381169	3.372051	1.957060
C	1.535563	2.471994	2.317453
N	-2.702032	0.552659	1.163736
C	-2.614784	1.522039	2.249886
C	-1.983593	2.823936	1.798781
C	-3.135616	1.076875	-1.247203
C	-3.706156	0.906783	0.153107
C	2.811485	-0.842372	-1.649525
C	-2.838810	-0.818374	1.642122
C	-2.363963	-1.805562	0.604527
C	2.328095	-1.825099	-0.611618
C	-1.131680	-2.121067	-1.333279
C	-1.513462	-3.476221	-1.454361
C	-2.350557	-3.981536	-0.424279
C	-2.796506	-3.151946	0.577856
C	2.749356	-3.175049	-0.584409
C	2.296512	-4.000483	0.418058

C	1.463717	-3.487760	1.447952
C	1.093207	-2.129527	1.326296
Lu	-0.008063	0.609390	-0.004044
H	4.191506	1.813919	-0.452811
H	4.486458	0.111502	-0.119786
H	3.855944	1.589030	1.864346
H	2.893525	0.091332	1.724692
H	1.959659	1.072987	-3.036577
H	3.598324	1.711531	-2.707432
H	1.995149	3.519510	-2.645955
H	2.541302	3.259572	-0.971523
H	-0.004834	3.872493	-2.876450
H	-0.690033	4.147583	-1.246850
H	-1.231860	1.728816	-3.071949
H	-2.361398	3.095721	-2.729238
H	0.016051	3.874847	2.865632
H	0.703250	4.142373	1.235631
H	2.365999	3.078224	2.719005
H	1.225196	1.721110	3.063212
H	-1.971224	1.090254	3.028196
H	-3.604711	1.741966	2.699071
H	-2.535616	3.281216	0.962932
H	-1.986689	3.536801	2.637121
H	-2.913851	0.114488	-1.732571
H	-3.863972	1.619963	-1.872728
H	-4.197102	1.848699	0.444407
H	-4.506169	0.148625	0.112210
H	3.853182	-1.089355	-1.933777
H	2.193507	-0.957890	-2.549414
H	-3.882391	-1.056513	1.926980
H	-2.221271	-0.938530	2.541718
C	-1.070728	-4.209936	-2.584808
H	-2.665628	-5.027406	-0.454742
H	-3.477350	-3.516603	1.348624
H	3.427144	-3.545680	-1.355022
H	2.602840	-5.048934	0.448949
C	1.015007	-4.217297	2.578747
N	1.487454	-1.356832	0.283925
N	-1.519489	-1.344688	-0.291239
C	-0.336532	-1.450722	-2.326779
O	-0.016622	-0.203481	-2.106875
C	0.040095	-2.202231	-3.435420
C	0.303705	-1.452204	2.319572
O	-0.005997	-0.202465	2.099154
C	-0.078991	-2.200073	3.428593
C	0.269711	-3.566113	3.537824
C	-0.319937	-3.565376	-3.544084
H	0.006286	-4.120148	-4.427022
H	-1.345414	-5.260380	-2.693669
H	0.615188	-1.722593	-4.230752
H	-0.061018	-4.117764	4.421041
H	1.280965	-5.269944	2.688024
H	-0.649999	-1.715327	4.223772

KHQLuΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1950.78342069

E(SCF)+ZPE(0 K)= -1950.099461
H(298 K)= -1950.063024
G(298 K)= -1950.161810
Lowest Frequency = 48.7851cm⁻¹

81

C	-3.592630	-0.671526	0.761775
N	-2.924282	-0.531190	-0.536622
O	-1.672708	-2.043461	1.156123
C	-2.647659	-1.245459	1.824042
C	-3.247581	-1.641707	-1.425363
C	-2.163609	-1.964222	-2.423124
O	-0.989857	-2.375499	-1.734931
C	-0.017338	-2.879350	-2.625135
C	1.208504	-3.197128	-1.809888
O	1.669844	-2.033703	-1.154558
O	0.988233	-2.376562	1.735547
C	0.017711	-2.886926	2.624204
C	-1.206850	-3.207053	1.807950
N	2.914770	-0.520762	0.542464
C	3.242771	-1.632393	1.428127
C	2.160184	-1.962288	2.424984
C	2.641520	-1.229840	-1.820207
C	3.583858	-0.654685	-0.756258
C	-3.111371	0.783854	-1.134287
C	3.096578	0.793348	1.143879
C	2.404480	1.835857	0.297518
C	-2.423324	1.826736	-0.285078
C	0.867709	2.196603	-1.399013
C	1.175838	3.570366	-1.504366
C	2.144239	4.059511	-0.587954
C	2.774495	3.200136	0.283468
C	-2.798979	3.189429	-0.267096
C	-2.172254	4.048913	0.606752
C	-1.201808	3.561150	1.521730
C	-0.887960	2.188993	1.412395
Lu	-0.004312	-0.590901	0.002763
H	-4.486364	-1.309810	0.660053
H	-3.951955	0.304476	1.115487
H	-3.202245	-1.867386	2.543483
H	-2.131736	-0.446076	2.377717
H	2.122324	-0.431230	-2.371952
H	3.198888	-1.847550	-2.541132
H	4.480342	-1.289359	-0.656152
H	3.938991	0.323812	-1.107289
H	-4.182239	1.046233	-1.250456
H	-2.661433	0.784570	-2.137268
H	4.166383	1.059609	1.260955
H	2.646425	0.789407	2.146770
C	0.527107	4.333118	-2.510236
H	2.411171	5.118947	-0.604176
H	3.554842	3.556460	0.957618
H	-3.580860	3.544430	-0.940165
H	-2.443594	5.107177	0.626040
C	-0.556311	4.323697	2.529831
N	-1.460332	1.379506	0.490921
N	1.443423	1.386877	-0.479856

C	-0.063959	1.540653	-2.273705
O	-0.304382	0.274091	-2.047742
C	-0.643244	2.319111	-3.267895
C	0.046425	1.534439	2.285237
O	0.292179	0.269556	2.055663
C	0.622411	2.312429	3.281710
H	2.513032	-2.789531	3.065414
H	1.905036	-1.101203	3.062707
H	4.187317	-1.451505	1.979794
H	3.399183	-2.524601	0.807100
H	-2.512963	-2.791126	-3.065899
H	-1.912149	-1.100255	-3.058404
H	-3.400222	-2.536294	-0.806823
H	-4.192878	-1.463309	-1.976563
H	0.212538	-2.120422	-3.394454
H	-0.389147	-3.790540	-3.127282
H	2.001159	-3.629188	-2.440647
H	0.961318	-3.922491	-1.019536
H	-0.215197	-2.131229	3.395793
H	0.393112	-3.798145	3.123619
H	-0.956786	-3.929052	1.015423
H	-1.997828	-3.644127	2.437354
C	0.321386	3.691572	3.383929
C	-0.347985	3.699795	-3.366121
H	-0.833652	4.279239	-4.154845
H	0.741963	5.398378	-2.609641
H	-1.332685	1.854553	-3.976396
H	0.804586	4.270748	4.174363
H	-0.775639	5.387753	2.632311
H	1.313735	1.848695	3.988914

KHQLuΔ_λλ_λλ_opt.log

SCF (RwB97XD) = -1950.79364119
 E(SCF)+ZPE(0 K)= -1950.109845
 H(298 K)= -1950.073407
 G(298 K)= -1950.172468
 Lowest Frequency = 30.7016cm⁻¹

81

C	-3.707962	0.861834	0.343500
N	-2.673620	0.489291	1.312664
O	-1.942443	1.778771	-0.985065
C	-3.168603	1.062789	-1.068221
C	-2.538975	1.443625	2.405604
C	-1.920010	2.746863	1.933883
O	-0.576456	2.575566	1.499633
C	0.397094	2.750817	2.519004
C	1.736132	2.896079	1.842872
O	1.947656	1.787750	0.988857
O	0.577640	2.579527	-1.494938
C	-0.396684	2.750961	-2.514224
C	-1.736488	2.888917	-1.838066
N	2.685111	0.503300	-1.309637
C	2.545694	1.457849	-2.401798
C	1.920399	2.757668	-1.928976
C	3.177284	1.077699	1.071633

C	3.717624	0.880203	-0.340201
C	-2.773254	-0.891864	1.760301
C	2.791653	-0.876970	-1.758425
C	2.343528	-1.842038	-0.687746
C	-2.320537	-1.853845	0.688767
C	1.176653	-2.140253	1.292891
C	1.561498	-3.495407	1.410991
C	2.361812	-4.010760	0.357418
C	2.772974	-3.189718	-0.665405
C	-2.743500	-3.203552	0.665334
C	-2.328398	-4.021787	-0.358149
C	-1.530563	-3.501748	-1.411289
C	-1.152240	-2.144850	-1.292102
Lu	0.005567	0.593265	0.001435
H	-4.195982	1.793501	0.671487
H	-4.505709	0.100525	0.306335
H	-3.896571	1.633808	-1.664380
H	-2.979115	0.107387	-1.576382
H	2.992451	0.121113	1.579272
H	3.902459	1.651929	1.668112
H	4.201155	1.814414	-0.667609
H	4.519008	0.122707	-0.303488
H	-3.802199	-1.155498	2.075396
H	-2.124716	-1.024997	2.636005
H	3.821934	-1.135243	-2.073583
H	2.143915	-1.012567	-2.634347
C	1.159241	-4.223349	2.559978
H	2.676000	-5.056950	0.385552
H	3.425614	-3.561210	-1.457077
H	-3.394350	-3.578811	1.456702
H	-2.637562	-5.069449	-0.387129
C	-1.124801	-4.226846	-2.560844
N	-1.511121	-1.376681	-0.231668
N	1.531818	-1.369523	0.233059
C	0.411096	-1.468692	2.309152
O	0.074742	-0.225369	2.095102
C	0.075106	-2.214010	3.435095
C	-0.389904	-1.468824	-2.307820
O	-0.059573	-0.224051	-2.092816
C	-0.050304	-2.211635	-3.434334
H	0.395096	1.875718	3.188595
H	0.179536	3.666729	3.093458
H	2.525105	2.956824	2.607402
H	1.759445	3.817701	1.236845
H	-0.390306	1.876521	-3.184647
H	-0.183594	3.668488	-3.087772
H	-1.764484	3.809887	-1.231244
H	-2.525697	2.946349	-2.602607
H	2.468360	3.174756	-1.073320
H	1.946565	3.505982	-2.736962
H	3.515129	1.685663	-2.890349
H	1.887255	1.008233	-3.157155
H	-1.949750	3.494327	2.742537
H	-2.470027	3.162102	1.078650
H	-3.509548	1.666281	2.894273
H	-1.878389	0.996666	3.160659
C	0.441404	-3.575118	3.541348

C	-0.410056	-3.574404	-3.541677
H	-0.112911	-4.121941	-4.439235
H	-1.399808	-5.277594	-2.665844
H	0.496830	-1.724257	-4.244596
H	0.146914	-4.124788	4.438477
H	1.439284	-5.272849	2.664143
H	-0.474339	-1.729905	4.245756

KHQTbΔ_δδδ_δδδ_opt.log

SCF (RwB97XD) = -1947.32248925
 E(SCF)+ZPE(0 K)= -1946.639177
 H(298 K)= -1946.602426
 G(298 K)= -1946.703395
 Lowest Frequency = 22.0172cm⁻¹

81

C	3.616356	-0.805667	-0.474650
N	2.862090	-0.552537	0.752328
O	1.700620	-1.697119	-1.563616
C	3.056301	-1.967973	-1.264026
C	3.145161	-1.555303	1.782442
C	1.891077	-2.073927	2.451207
O	1.016836	-2.548978	1.419638
C	0.070769	-3.516892	1.828004
C	-1.137731	-2.869859	2.463625
O	-1.680498	-1.960807	1.524520
O	-0.970428	-2.551476	-1.506354
C	0.045973	-3.300577	-2.150646
C	1.138449	-2.389849	-2.665332
N	-2.853589	-0.591672	-0.586500
C	-3.182178	-1.661041	-1.530407
C	-2.004763	-2.086996	-2.377558
C	-3.094093	-1.931115	1.493148
C	-3.565439	-0.741365	0.683582
C	3.058489	0.814685	1.233839
C	-3.082852	0.739402	-1.157661
C	-2.446347	1.814375	-0.307419
C	2.436987	1.830848	0.304086
C	-0.935648	2.254481	1.399426
C	-1.282404	3.622856	1.464437
C	-2.258539	4.060710	0.530351
C	-2.857977	3.165932	-0.327687
C	2.865907	3.177371	0.262141
C	2.280123	4.040467	-0.634429
C	1.295687	3.573583	-1.544810
C	0.931933	2.212567	-1.422261
Tb	-0.010952	-0.578438	0.025991
H	0.533188	-4.243014	2.517125
H	-0.241324	-4.051133	0.918225
H	-0.876097	-2.327849	3.387983
H	-1.871078	-3.653772	2.715188
H	-0.382038	-3.904545	-2.967802
H	0.459907	-3.988354	-1.397074
H	1.907004	-2.977552	-3.190897
H	0.730356	-1.636074	-3.355525
H	4.134363	1.047756	1.364499

H	2.576462	0.903020	2.217390
H	-4.165924	0.947729	-1.267839
H	-2.631006	0.767615	-2.158995
C	-0.659441	4.433791	2.448221
H	-2.554085	5.112618	0.519749
H	-3.639635	3.487189	-1.017821
H	3.650424	3.518199	0.939591
H	2.588564	5.088059	-0.671311
C	0.679758	4.357903	-2.553798
N	1.475408	1.400267	-0.482494
N	-1.486469	1.412934	0.494811
C	0.011563	1.647144	2.297508
O	0.295973	0.384665	2.116329
C	0.566594	2.477117	3.265912
C	-0.035389	1.593799	-2.291880
O	-0.347067	0.344471	-2.071662
C	-0.587137	2.397612	-3.284197
H	4.689019	-0.991696	-0.268005
H	3.633358	-2.069331	-2.197749
H	3.133497	-2.921968	-0.711801
H	-4.660062	-0.832116	0.534629
H	-3.391688	0.164100	1.277122
H	-3.495751	-1.835167	2.516157
H	-3.461922	-2.889122	1.082308
H	-1.623412	-1.250700	-2.983060
H	-2.317475	-2.913311	-3.037636
H	-3.522366	-2.540979	-0.967898
H	-4.017767	-1.373263	-2.195717
H	2.148933	-2.911208	3.120523
H	1.385750	-1.278445	3.018595
H	3.828746	-1.161562	2.555835
H	3.663649	-2.408408	1.321566
H	3.556044	0.086424	-1.111266
C	0.232109	3.850652	3.322553
C	-0.230564	3.760804	-3.398307
H	-0.696243	4.356031	-4.187425
H	-1.305250	1.959279	-3.980982
H	0.943646	5.411377	-2.660359
H	0.700518	4.466750	4.093879
H	-0.904312	5.495090	2.514835
H	1.266775	2.054779	3.990227

KHQTbΔ_δδλ_δδλ_opt.log

SCF (RwB97XD) = -1947.31813228
 E(SCF)+ZPE(0 K)= -1946.635422
 H(298 K)= -1946.598476
 G(298 K)= -1946.699560
 Lowest Frequency = 20.6508cm⁻¹

81

C	3.535530	1.013174	-0.263190
N	2.647513	0.830102	0.885829
O	2.579141	-0.976034	-1.200553
C	3.777489	-0.235624	-1.089995
C	3.201855	0.026759	1.974021
C	3.118289	-1.480430	1.772935

O	1.777450	-1.870094	1.525634
C	1.213667	-2.898537	2.322431
C	-0.213317	-2.507047	2.642303
O	-0.917075	-2.218617	1.448574
O	0.503234	-2.733179	-1.268124
C	1.828881	-3.203485	-1.436471
C	2.664356	-2.104857	-2.049263
N	-2.094685	-1.730972	-1.075129
C	-1.647374	-2.410118	-2.287945
C	-0.485480	-3.357791	-2.076152
C	-1.708226	-3.245529	0.891848
C	-2.698560	-2.605952	-0.067366
C	2.216120	2.148513	1.373794
C	-3.011927	-0.644329	-1.435460
C	-3.072413	0.434661	-0.383428
C	1.258985	2.807067	0.409104
C	-2.039136	1.444087	1.431809
C	-3.085638	2.380522	1.605792
C	-4.162718	2.293816	0.684860
C	-4.173374	1.317254	-0.282498
C	1.021051	4.199986	0.387483
C	0.159450	4.716561	-0.553974
C	-0.439105	3.871567	-1.525925
C	-0.137125	2.494688	-1.418546
Tb	0.242539	-0.446524	-0.014708
H	2.612763	0.257236	2.871692
H	4.257474	0.292579	2.187200
H	3.484730	-1.963419	2.692399
H	3.750038	-1.838859	0.947726
H	1.778858	-3.015535	3.260880
H	1.259180	-3.856376	1.773174
H	-0.215428	-1.575211	3.223877
H	-0.717710	-3.304782	3.210743
H	1.849528	-4.103791	-2.069364
H	2.226762	-3.468423	-0.445033
H	3.709878	-2.446220	-2.135071
H	2.296151	-1.838622	-3.054459
H	-1.311919	-1.620175	-2.972040
H	-2.468221	-2.976869	-2.773022
H	-0.790074	-4.309414	-1.606796
H	-0.065234	-3.600286	-3.065887
H	3.081241	2.816595	1.553298
H	1.696334	2.005017	2.329444
H	-4.031195	-1.026349	-1.639090
H	-2.650528	-0.185052	-2.365156
C	-3.005611	3.308413	2.675352
H	-4.995933	2.995803	0.768856
H	-5.012037	1.219441	-0.973844
H	1.517006	4.848660	1.111309
H	-0.047029	5.789341	-0.578923
C	-1.278212	4.301497	-2.586166
N	0.655776	2.004312	-0.437795
N	-2.040422	0.535528	0.423678
C	-0.914025	1.377199	2.329054
O	0.005876	0.482140	2.097719
C	-0.893205	2.296715	3.374451
C	-0.620002	1.515326	-2.357752

O	-0.294664	0.267394	-2.156073
C	-1.415828	1.993417	-3.394639
H	3.068845	1.761761	-0.915225
H	4.520196	1.418090	0.046033
H	4.134138	0.067629	-2.089118
H	4.560888	-0.876679	-0.645785
H	-3.314635	-3.399685	-0.534348
H	-3.373768	-1.991478	0.544476
H	-2.278115	-3.753134	1.688619
H	-1.068329	-4.001356	0.408074
C	-1.738852	3.367445	-3.488890
H	-1.534106	5.357635	-2.685171
H	-2.372650	3.695228	-4.316423
H	-1.780833	1.293110	-4.149513
C	-1.925879	3.248481	3.529364
H	-3.799676	4.043236	2.817765
H	-1.864291	3.953067	4.362225
H	-0.067302	2.263738	4.088800

KHQTBΔ_δλδ_δλδ_opt.log

SCF (RWB97XD) = -1947.32139573
 E(SCF)+ZPE(0 K)= -1946.638010
 H(298 K)= -1946.601070
 G(298 K)= -1946.702817
 Lowest Frequency = 20.3935cm⁻¹

81

C	3.511080	-0.757346	-0.795153
N	2.900927	-0.530690	0.512783
O	1.614693	-2.105990	-1.375789
C	3.029028	-2.041249	-1.435482
C	3.327785	-1.527487	1.493557
C	2.248709	-1.870409	2.488205
O	1.116570	-2.376595	1.789417
C	0.186940	-2.941391	2.686488
C	-1.061820	-3.302465	1.935182
O	-1.610262	-2.121277	1.377243
O	-1.109743	-2.380363	-1.789443
C	-0.175919	-2.938661	-2.686235
C	1.075054	-3.290965	-1.934366
N	-2.907599	-0.550718	-0.509431
C	-3.326855	-1.546680	-1.494453
C	-2.244179	-1.879671	-2.488554
C	-3.025252	-2.069607	1.433068
C	-3.517056	-0.787333	0.797100
C	3.143214	0.827697	0.998356
C	-3.160247	0.807749	-0.989509
C	-2.460384	1.844480	-0.147149
C	2.435568	1.862276	0.159839
C	-0.844397	2.243825	1.464882
C	-1.172152	3.613846	1.573437
C	-2.201073	4.076783	0.711388
C	-2.859750	3.200235	-0.119874
C	2.824713	3.221080	0.137289
C	2.159445	4.095519	-0.690965
C	1.134125	3.627805	-1.554740

C	0.816682	2.254985	-1.450916
Tb	-0.003372	-0.592380	0.002207
H	4.227739	1.056920	1.027353
H	2.763734	0.896805	2.027849
H	-4.246507	1.028776	-1.017279
H	-2.781839	0.883906	-2.018860
C	-0.479173	4.404587	2.526333
H	-2.486179	5.131305	0.735369
H	-3.679263	3.537570	-0.756349
H	3.641663	3.562370	0.774949
H	2.436590	5.152237	-0.711276
C	0.435349	4.416515	-2.505093
N	1.435620	1.428863	-0.573794
N	-1.457235	1.416039	0.585019
C	0.155116	1.619082	2.288388
O	0.415779	0.359582	2.066811
C	0.779664	2.427395	3.232646
C	-0.177957	1.625501	-2.276719
O	-0.429138	0.363339	-2.059387
C	-0.808397	2.432263	-3.218380
H	4.618082	-0.790608	-0.740560
H	3.357285	-2.060174	-2.488934
H	3.450987	-2.934557	-0.943078
H	-4.623692	-0.829316	0.741233
H	-3.254108	0.050102	1.455562
H	-3.356271	-2.096002	2.485501
H	-3.437738	-2.964582	0.935678
H	-1.932108	-0.996528	-3.066944
H	-2.618274	-2.656604	-3.177994
H	-3.601477	-2.474368	-0.976624
H	-4.230809	-1.219077	-2.042324
H	2.628875	-2.646776	3.174970
H	1.931714	-0.990997	3.069615
H	4.230651	-1.196394	2.041171
H	3.607041	-2.451713	0.972035
H	0.871976	-4.018965	-1.128862
H	1.792288	-3.747259	-2.634717
H	0.065687	-2.204817	-3.475223
H	-0.594206	-3.845346	-3.159798
H	3.240655	0.080547	-1.450032
H	-1.775406	-3.763871	2.635943
H	-0.854026	-4.028994	1.129533
H	0.611667	-3.845205	3.159808
H	-0.059417	-2.209243	3.475582
C	0.462066	3.801952	3.332779
C	-0.501147	3.809515	-3.313784
H	-1.028040	4.408608	-4.060363
H	0.658554	5.480533	-2.598998
H	-1.547747	1.988795	-3.889321
H	0.984599	4.402477	4.081270
H	-0.710382	5.466567	2.623865
H	1.522492	1.987246	3.901932

KHQTbΔ_{δλλ}Δ_{δλλ}opt.log

SCF (RwB97XD) = -1947.32430041

E(SCF)+ZPE(0 K)= -1946.640476

H(298 K)= -1946.604000
 G(298 K)= -1946.702956
 Lowest Frequency = 36.3519cm⁻¹

81

C	-3.640949	-0.727484	0.302247
N	-2.766724	-0.508933	-0.851164
O	-1.858787	-1.885106	1.406462
C	-3.253983	-1.891099	1.192342
C	-2.915286	-1.492834	-1.920653
C	-2.159605	-2.790233	-1.670110
O	-0.767238	-2.580841	-1.497654
C	0.008291	-2.640418	-2.688345
C	1.437205	-2.900053	-2.295031
O	1.859348	-1.892473	-1.399461
O	0.768382	-2.570491	1.509237
C	-0.007242	-2.623488	2.700139
C	-1.435884	-2.886763	2.308280
N	2.766067	-0.501027	0.849201
C	2.915256	-1.477549	1.925332
C	2.160950	-2.777338	1.683263
C	3.254520	-1.896239	-1.185167
C	3.640724	-0.726694	-0.302514
C	-2.959813	0.859509	-1.344103
C	2.957911	0.870870	1.332922
C	2.368341	1.875881	0.371669
C	-2.370690	1.871529	-0.389936
C	0.958897	2.205856	-1.442247
C	1.294654	3.574562	-1.555538
C	2.207834	4.074134	-0.589522
C	2.761730	3.233222	0.348199
C	-2.764732	3.228816	-0.375958
C	-2.211165	4.076542	0.555802
C	-1.297719	3.584188	1.525282
C	-0.961352	2.214878	1.421588
Tb	-0.000349	-0.591258	-0.000722
H	-4.031905	1.086299	-1.506182
H	-2.451660	0.955050	-2.311671
H	4.029757	1.099600	1.493880
H	2.449263	0.972555	2.299612
C	0.724375	4.331337	-2.611489
H	2.490215	5.129382	-0.616374
H	3.494201	3.599302	1.069288
H	-3.497403	3.589499	-1.099560
H	-2.494021	5.131826	0.575247
C	-0.727742	4.348608	2.575868
N	-1.467579	1.417907	0.450464
N	1.465480	1.415920	-0.465565
C	0.065501	1.549606	-2.361521
O	-0.231358	0.298483	-2.136539
C	-0.437555	2.327202	-3.400435
C	-0.067640	1.565460	2.345407
O	0.229785	0.312920	2.129178
C	0.435083	2.350558	3.378833
H	-4.695612	-0.864109	-0.010353
H	-3.779600	-1.780444	2.157060
H	-3.564627	-2.865140	0.774134

H	4.695346	-0.860842	0.011295
H	3.601369	0.177269	-0.922970
H	3.780174	-1.791475	-2.150524
H	3.565691	-2.867392	-0.760685
H	-1.534295	-3.879321	1.830874
H	-2.063366	-2.871955	3.216161
H	0.075005	-1.664857	3.237022
H	0.343330	-3.449871	3.339865
H	-3.601714	0.180513	0.916808
H	2.064582	-2.890301	-3.203053
H	1.536532	-3.889559	-1.811514
H	-0.341653	-3.470982	-3.322975
H	-0.074814	-1.685070	-3.230950
H	-3.979816	-1.735835	-2.115225
H	-2.510622	-1.043269	-2.837903
H	-2.328542	-3.472896	-2.518832
H	-2.504134	-3.310502	-0.770442
H	2.506163	-3.303222	0.787119
H	2.330447	-3.454186	2.536517
H	2.509862	-1.022227	2.839414
H	3.979969	-1.718185	2.121850
C	-0.110406	3.698833	-3.506946
C	0.107340	3.722765	3.475720
H	0.534371	4.301822	4.298054
H	-0.969055	5.408560	2.670888
H	1.090706	1.891110	4.122191
H	-0.537670	4.271914	-4.333336
H	0.965232	5.390700	-2.713949
H	-1.092970	1.862252	-4.140548

KHQTBΔ_{λδδ}_{λδδ}_opt.log

SCF (RwB97XD) = -1947.32107665
 E(SCF)+ZPE(0 K)= -1946.637127
 H(298 K)= -1946.600750
 G(298 K)= -1946.699164
 Lowest Frequency = 46.2203cm⁻¹

81

C	3.709428	0.738856	0.493944
N	2.877807	0.615225	-0.716517
O	1.830466	1.859853	1.459165
C	2.913829	0.998694	1.768652
C	3.101655	1.721825	-1.649035
C	1.874360	2.120664	-2.435964
O	0.873981	2.557500	-1.511046
C	-0.146996	3.370156	-2.065427
C	-1.290844	2.530144	-2.578998
O	-1.819489	1.845850	-1.462277
O	-0.866445	2.558185	1.505774
C	0.150406	3.377841	2.057408
C	1.298526	2.545321	2.573616
N	-2.860427	0.603170	0.717626
C	-3.089893	1.711817	1.646361
C	-1.864709	2.119466	2.432098
C	-2.898166	0.977807	-1.768869
C	-3.692571	0.718495	-0.493331

C	3.014572	-0.701059	-1.341999
C	-2.990903	-0.711605	1.347595
C	-2.403785	-1.778193	0.451859
C	2.432971	-1.767485	-0.442469
C	-0.976711	-2.197353	-1.332150
C	-1.314221	-3.568124	-1.387108
C	-2.240238	-4.019208	-0.408398
C	-2.802674	-3.134358	0.483564
C	2.838856	-3.121672	-0.469462
C	2.281018	-4.006305	0.425595
C	1.352731	-3.556601	1.402785
C	1.008090	-2.187801	1.343039
Tb	0.008535	0.642841	0.000655
H	4.434477	1.554455	0.352336
H	4.306119	-0.173373	0.649523
H	3.570363	1.481753	2.511786
H	2.519148	0.071278	2.210730
H	0.261328	4.006058	-2.866831
H	-0.507513	4.021678	-1.255247
H	-0.944731	1.804247	-3.335707
H	-2.061958	3.179205	-3.030080
H	-0.261087	4.014245	2.856787
H	0.507528	4.028576	1.245098
H	2.066438	3.199778	3.022355
H	0.956156	1.820293	3.332856
H	-2.498384	0.050871	-2.207387
H	-3.557119	1.454613	-2.513899
H	-4.421633	1.531010	-0.354607
H	-4.284747	-0.197200	-0.645756
H	4.072729	-0.938744	-1.569115
H	2.460905	-0.699427	-2.291684
H	-4.047954	-0.953711	1.575193
H	-2.437618	-0.703968	2.297456
C	-0.733098	-4.369288	-2.403577
H	-2.526568	-5.073537	-0.389530
H	-3.545406	-3.465854	1.210778
H	3.583286	-3.451851	-1.195538
H	2.572802	-5.059197	0.410395
C	0.775884	-4.357205	2.422126
N	1.516100	-1.355351	0.403831
N	-1.489063	-1.364266	-0.395880
C	-0.083231	-1.578635	-2.276374
O	0.191385	-0.309605	-2.112190
C	0.432086	-2.399057	-3.273759
C	0.111471	-1.570441	2.285181
O	-0.169742	-0.303433	2.116637
C	-0.399493	-2.390036	3.285480
H	-2.133670	2.960381	3.092399
H	-1.463372	1.290972	3.035669
H	-3.909379	1.489079	2.357539
H	-3.399571	2.587044	1.060086
H	2.139002	2.960644	-3.099196
H	1.477208	1.288068	-3.036617
H	3.407074	2.600564	-1.065787
H	3.922137	1.500736	-2.359582
C	-0.069574	-3.764633	3.335322
C	0.109346	-3.775525	-3.318784

H	0.545152	-4.384803	-4.114173
H	-0.971842	-5.432455	-2.462621
H	1.093016	-1.966773	-4.028334
H	-0.502121	-4.373371	4.132899
H	1.020193	-5.418893	2.484893
H	-1.062609	-1.958545	4.038589

KHQTbΔ_λδλ_λδλ_opt.log

SCF (RwB97XD) = -1947.32864350
 E(SCF)+ZPE(0 K)= -1946.645614
 H(298 K)= -1946.608924
 G(298 K)= -1946.708946
 Lowest Frequency = 26.8304cm⁻¹

81

C	3.681570	0.930091	-0.187812
N	2.663364	0.558819	-1.182783
O	1.967958	1.899729	1.146876
C	3.142962	1.107710	1.223114
C	2.588799	1.505637	-2.294787
C	1.977649	2.831191	-1.884822
O	0.633302	2.627543	-1.467897
C	-0.385327	3.393690	-2.085629
C	-1.561256	2.495860	-2.380703
O	-1.969947	1.919130	-1.154750
O	-0.628307	2.633579	1.460077
C	0.397775	3.389653	2.077887
C	1.564946	2.480412	2.372844
N	-2.678504	0.584874	1.174831
C	-2.594734	1.530859	2.286885
C	-1.970603	2.850365	1.876966
C	-3.152625	1.138606	-1.231041
C	-3.692993	0.966152	0.179851
C	2.811007	-0.818281	-1.653160
C	-2.839644	-0.790743	1.645144
C	-2.390606	-1.791917	0.609416
C	2.352402	-1.814981	-0.617306
C	-1.159737	-2.146289	-1.326063
C	-1.531222	-3.507890	-1.408860
C	-2.369044	-3.990004	-0.367711
C	-2.818458	-3.140259	0.615823
C	2.767304	-3.167365	-0.623541
C	2.309690	-4.012664	0.360046
C	1.476462	-3.522431	1.401073
C	1.118141	-2.157317	1.318168
Tb	-0.007222	0.643893	-0.003965
H	4.159683	1.873175	-0.495196
H	4.487798	0.178163	-0.155201
H	3.900266	1.626858	1.835124
H	2.906719	0.146964	1.705845
H	1.939098	1.062224	-3.061680
H	3.582839	1.694264	-2.748277
H	2.000776	3.519566	-2.743409
H	2.530297	3.303666	-1.057750
H	-0.021596	3.829488	-3.029184
H	-0.684070	4.215422	-1.412696

H	-1.271384	1.697216	-3.084488
H	-2.382734	3.094098	-2.811845
H	0.038336	3.828849	3.021512
H	0.704484	4.208530	1.405056
H	2.392215	3.070662	2.803927
H	1.267430	1.684621	3.076666
H	-1.949482	1.081011	3.053789
H	-3.586911	1.729202	2.740311
H	-2.518541	3.328165	1.049817
H	-1.987051	3.538963	2.735529
H	-2.925726	0.175630	-1.713791
H	-3.904819	1.665125	-1.843057
H	-4.161847	1.913851	0.487307
H	-4.506534	0.222145	0.147151
H	3.854884	-1.041788	-1.947895
H	2.185439	-0.946612	-2.546672
H	-3.885722	-1.004052	1.939639
H	-2.215630	-0.925269	2.538814
C	-1.073885	-4.273915	-2.511344
H	-2.677488	-5.038294	-0.372137
H	-3.492916	-3.491998	1.398118
H	3.438417	-3.525626	-1.405753
H	2.608071	-5.063862	0.364594
C	1.011695	-4.283954	2.503569
N	1.523384	-1.363324	0.296135
N	-1.557299	-1.348363	-0.304072
C	-0.357893	-1.500945	-2.333318
O	-0.045265	-0.245321	-2.155445
C	0.036914	-2.288231	-3.411446
C	0.322550	-1.504212	2.325383
O	0.022156	-0.245616	2.147475
C	-0.079885	-2.287585	3.403534
C	0.258530	-3.658305	3.473662
C	-0.314752	-3.655616	-3.481502
H	0.025307	-4.236185	-4.342413
H	-1.341385	-5.328930	-2.589718
H	0.620164	-1.831101	-4.214111
H	-0.087159	-4.235522	4.334585
H	1.269001	-5.341500	2.582003
H	-0.658702	-1.824793	4.206164

KHQTBΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1947.31682136

E(SCF)+ZPE(0 K)= -1946.632858

H(298 K)= -1946.596477

G(298 K)= -1946.694855

Lowest Frequency = 46.9865cm⁻¹

81

C	-3.580914	-0.720875	0.750610
N	-2.880761	-0.568829	-0.534946
O	-1.728052	-2.161444	1.205420
C	-2.671585	-1.298866	1.836332
C	-3.210661	-1.672110	-1.437055
C	-2.153908	-1.957654	-2.474788
O	-0.961637	-2.381363	-1.827985

C	0.012531	-2.816269	-2.753780
C	1.229580	-3.231447	-1.967066
O	1.726342	-2.149560	-1.204939
O	0.960854	-2.382693	1.827970
C	-0.011290	-2.825455	2.752151
C	-1.226339	-3.243584	1.963917
N	2.871983	-0.557481	0.540829
C	3.206646	-1.661859	1.439819
C	2.150908	-1.955226	2.476409
C	2.666239	-1.280811	-1.832816
C	3.572979	-0.702606	-0.745059
C	-3.097551	0.748606	-1.129853
C	3.082678	0.759154	1.139637
C	2.416395	1.819245	0.294516
C	-2.435856	1.809227	-0.281792
C	0.883842	2.214279	-1.401041
C	1.191783	3.590725	-1.473997
C	2.162149	4.058604	-0.547881
C	2.790140	3.182633	0.308703
C	-2.815684	3.170969	-0.291915
C	-2.191511	4.047197	0.567195
C	-1.218973	3.580924	1.491845
C	-0.904920	2.206089	1.414803
Tb	-0.004313	-0.641198	0.002645
H	-4.471059	-1.358488	0.618851
H	-3.948608	0.252663	1.102225
H	-3.263432	-1.869351	2.569611
H	-2.129493	-0.500894	2.368977
H	2.120788	-0.483391	-2.362842
H	3.260606	-1.846287	-2.567934
H	4.465650	-1.337056	-0.615156
H	3.936851	0.273508	-1.093514
H	-4.175273	0.979052	-1.246316
H	-2.645821	0.762705	-2.131915
H	4.159318	0.994131	1.257066
H	2.630611	0.768242	2.141625
C	0.538097	4.378890	-2.456394
H	2.429307	5.118096	-0.541986
H	3.566503	3.526387	0.993897
H	-3.593677	3.513275	-0.975986
H	-2.463413	5.105495	0.564464
C	-0.568756	4.369055	2.476568
N	-1.479679	1.379689	0.510661
N	1.462240	1.387755	-0.499324
C	-0.053220	1.578725	-2.287414
O	-0.294368	0.307005	-2.097309
C	-0.639960	2.385439	-3.255721
C	0.034874	1.572027	2.299343
O	0.281556	0.301934	2.105499
C	0.618029	2.378441	3.270062
H	2.517102	-2.765792	3.130542
H	1.916636	-1.074988	3.095916
H	4.170778	-1.484173	1.956844
H	3.327229	-2.566726	0.829500
H	-2.516533	-2.768068	-3.131096
H	-1.924053	-1.074591	-3.091905
H	-3.326976	-2.579269	-0.829323

H	-4.175734	-1.497297	-1.953301
H	0.253203	-1.994422	-3.451848
H	-0.368156	-3.674153	-3.336525
H	2.010730	-3.625803	-2.636645
H	0.960713	-4.019645	-1.247755
H	-0.255868	-2.007271	3.453158
H	0.373409	-3.683590	3.331885
H	-0.953767	-4.028075	1.241953
H	-2.005705	-3.643851	2.632070
C	0.316278	3.759068	3.339536
C	-0.344276	3.767572	-3.321141
H	-0.835722	4.367160	-4.091079
H	0.752918	5.446230	-2.530335
H	-1.335959	1.939878	-3.970066
H	0.805059	4.358533	4.111265
H	-0.788288	5.435211	2.553679
H	1.315921	1.933830	3.983150

KHQTbΔ_λλ_λλ_opt.log

SCF (RwB97XD) = -1947.32407866
 E(SCF)+ZPE(0 K)= -1946.640620
 H(298 K)= -1946.604105
 G(298 K)= -1946.703450
 Lowest Frequency = 27.4277cm⁻¹

81

C	-3.686580	0.908828	0.359022
N	-2.634950	0.518428	1.309526
O	-1.978497	1.872545	-1.004394
C	-3.185809	1.123181	-1.063482
C	-2.510281	1.452027	2.427698
C	-1.899946	2.774300	1.998116
O	-0.551252	2.628000	1.573577
C	0.419245	2.734270	2.606406
C	1.762739	2.924014	1.945883
O	1.979579	1.884728	1.007728
O	0.547482	2.632554	-1.570093
C	-0.423775	2.732941	-2.602779
C	-1.768394	2.913691	-1.942047
N	2.644743	0.536436	-1.307007
C	2.514010	1.469620	-2.424815
C	1.895149	2.787748	-1.994687
C	3.191630	1.142996	1.066314
C	3.693828	0.933275	-0.356350
C	-2.762521	-0.865527	1.758188
C	2.781321	-0.846478	-1.756226
C	2.360625	-1.829098	-0.691011
C	-2.335108	-1.844952	0.692693
C	1.198673	-2.163448	1.289533
C	1.569381	-3.525792	1.369778
C	2.367026	-4.019859	0.303315
C	2.782111	-3.179589	-0.702402
C	-2.747244	-3.198332	0.703750
C	-2.326344	-4.035463	-0.302170
C	-1.532153	-3.535627	-1.368514
C	-1.170894	-2.170772	-1.287940

Tb	0.004528	0.632790	0.001302
H	-4.160649	1.840396	0.706229
H	-4.489213	0.152583	0.331894
H	-3.945515	1.676995	-1.636686
H	-2.985961	0.171971	-1.577271
H	2.997705	0.189924	1.578951
H	3.947701	1.701022	1.640234
H	4.161358	1.868407	-0.702834
H	4.501665	0.182557	-0.329955
H	-3.795293	-1.100242	2.082337
H	-2.110365	-1.009813	2.629726
H	3.815535	-1.074257	-2.080720
H	2.129876	-0.994690	-2.627645
C	1.152144	-4.283737	2.493485
H	2.671849	-5.069206	0.305358
H	3.425864	-3.539559	-1.506554
H	-3.388476	-3.562954	1.507821
H	-2.623875	-5.086900	-0.304451
C	-1.109658	-4.290404	-2.492390
N	-1.540745	-1.382800	-0.246615
N	1.563081	-1.372676	0.248403
C	0.431573	-1.512986	2.320334
O	0.108200	-0.259955	2.145788
C	0.076714	-2.291763	3.418391
C	-0.408240	-1.514785	-2.318546
O	-0.093428	-0.259622	-2.143613
C	-0.048024	-2.290812	-3.416800
H	0.414810	1.816208	3.216171
H	0.200216	3.609979	3.240314
H	2.548306	2.925047	2.716523
H	1.792062	3.887386	1.410153
H	-0.413469	1.815174	-3.212915
H	-0.210508	3.610304	-3.236368
H	-1.803890	3.876585	-1.405829
H	-2.554010	2.910040	-2.712625
H	2.434507	3.223057	-1.142393
H	1.938045	3.512450	-2.823709
H	3.488131	1.673890	-2.913335
H	1.857331	1.003095	-3.171560
H	-1.947601	3.498402	2.827401
H	-2.442061	3.206392	1.145937
H	-3.485728	1.649816	2.916237
H	-1.850644	0.989500	3.174313
C	0.430086	-3.658469	3.486850
C	-0.391938	-3.659916	-3.485595
H	-0.079504	-4.231347	-4.362897
H	-1.371693	-5.347012	-2.567695
H	0.502839	-1.822975	-4.236059
H	0.121631	-4.232256	4.364023
H	1.421506	-5.338517	2.568547
H	-0.477336	-1.827931	4.237777

KHQLaΔ_δδδ_δδδ_opt.log

SCF (Rwb97XD) = -1942.42487633
E(SCF)+ZPE(0 K)= -1941.742882
H(298 K)= -1941.705709

G(298 K)= -1941.807554
Lowest Frequency = 24.3228cm⁻¹

81

C	3.615262	-0.868898	-0.581880
N	2.872669	-0.649267	0.663077
O	1.724271	-1.946735	-1.585609
C	3.121764	-2.058031	-1.383840
C	3.194407	-1.662990	1.674037
C	2.017845	-2.042519	2.547281
O	1.014075	-2.615544	1.706190
C	0.021148	-3.379956	2.367233
C	-1.171126	-2.533789	2.760729
O	-1.719902	-1.960899	1.582641
O	-1.006483	-2.613781	-1.711341
C	-0.010040	-3.371588	-2.374644
C	1.178419	-2.518837	-2.765434
N	-2.874801	-0.660776	-0.661176
C	-3.191417	-1.671962	-1.676275
C	-2.012768	-2.042444	-2.550593
C	-3.116681	-2.079044	1.379914
C	-3.616335	-0.889212	0.582832
C	3.099272	0.708101	1.176515
C	-3.108053	0.697563	-1.168993
C	-2.504255	1.762052	-0.280721
C	2.489936	1.773376	0.292973
C	-0.978731	2.239369	1.408729
C	-1.327838	3.610484	1.439451
C	-2.323031	4.022928	0.513580
C	-2.925375	3.111092	-0.321970
C	2.904161	3.124355	0.340103
C	2.297018	4.036775	-0.491335
C	1.303737	3.623345	-1.418817
C	0.961731	2.250325	-1.394157
La	-0.000875	-0.686095	0.000945
H	0.446720	-3.876639	3.254994
H	-0.299561	-4.158965	1.658879
H	-0.875024	-1.714996	3.436547
H	-1.915296	-3.168129	3.267739
H	-0.433249	-3.867486	-3.263973
H	0.314167	-4.151284	-1.668645
H	1.925596	-3.148421	-3.273955
H	0.878828	-1.699630	-3.439204
H	4.181869	0.908034	1.305729
H	2.624597	0.779477	2.166193
H	-4.191598	0.892658	-1.297657
H	-2.633453	0.775484	-2.158220
C	-0.684188	4.460643	2.374265
H	-2.621111	5.073761	0.484991
H	-3.708969	3.417608	-1.016702
H	3.686305	3.431814	1.036053
H	2.589727	5.088982	-0.458154
C	0.655468	4.474311	-2.349700
N	1.535645	1.385881	-0.521945
N	-1.548080	1.375852	0.532601
C	0.005442	1.673510	2.300387
O	0.307003	0.409303	2.172467

C	0.585819	2.547498	3.216118
C	-0.019565	1.683292	-2.288233
O	-0.314386	0.416950	-2.165937
C	-0.604638	2.558323	-3.199969
H	4.699142	-1.000175	-0.390454
H	3.646997	-2.055454	-2.352605
H	3.340615	-3.020417	-0.888468
H	-4.699517	-1.025255	0.390799
H	-3.505156	0.003281	1.211207
H	-3.642247	-2.083534	2.348487
H	-3.330084	-3.040446	0.880268
H	-1.601297	-1.161726	-3.069024
H	-2.337835	-2.793612	-3.289918
H	-3.528401	-2.588441	-1.172373
H	-4.027903	-1.343178	-2.321223
H	2.346827	-2.794917	3.283618
H	1.602210	-1.165814	3.069217
H	4.029567	-1.332820	2.319997
H	3.535533	-2.575866	1.166401
H	3.499546	0.025531	-1.206649
C	0.242195	3.917786	3.238348
C	-0.268210	3.930484	-3.216067
H	-0.761258	4.578266	-3.944988
H	-1.335307	2.165574	-3.910814
H	0.902390	5.536833	-2.379346
H	0.731735	4.564858	3.970256
H	-0.936671	5.521716	2.408621
H	1.318479	2.155386	3.925264

KHQLaΔ_{δδλ}Δ_{δδλ}_opt.log

SCF (RwB97XD) = -1942.41778323
 E(SCF)+ZPE(0 K)= -1941.736471
 H(298 K)= -1941.699058
 G(298 K)= -1941.802644
 Lowest Frequency = 7.7884cm⁻¹

81

C	3.612149	0.928243	-0.329588
N	2.712329	0.820530	0.821759
O	2.685571	-1.111891	-1.192764
C	3.882588	-0.370125	-1.068845
C	3.242803	0.052164	1.951778
C	3.136455	-1.465602	1.844161
O	1.790910	-1.848112	1.624101
C	1.224360	-2.869556	2.424448
C	-0.225689	-2.506490	2.680590
O	-0.908124	-2.266817	1.464858
O	0.517517	-2.738762	-1.411323
C	1.814761	-3.299649	-1.482108
C	2.779716	-2.261679	-2.010548
N	-2.109485	-1.775434	-1.074085
C	-1.669960	-2.408010	-2.319038
C	-0.507334	-3.367738	-2.164761
C	-1.643998	-3.314964	0.874516
C	-2.662260	-2.697710	-0.075545
C	2.325274	2.171331	1.266546

C	-3.072225	-0.710122	-1.393175
C	-3.202453	0.323651	-0.299599
C	1.433630	2.881239	0.273923
C	-2.188042	1.418331	1.483981
C	-3.308717	2.260043	1.697705
C	-4.414617	2.066406	0.828936
C	-4.376762	1.097194	-0.145542
C	1.303955	4.288461	0.244071
C	0.447647	4.859198	-0.669964
C	-0.267333	4.053766	-1.595178
C	-0.059496	2.656017	-1.496671
La	0.247523	-0.411175	-0.066953
H	2.655334	0.342871	2.833363
H	4.301681	0.310825	2.157314
H	3.496694	-1.888295	2.796089
H	3.764716	-1.887146	1.045896
H	1.751310	-2.944100	3.389981
H	1.316732	-3.843400	1.909236
H	-0.267036	-1.556818	3.233355
H	-0.726530	-3.297342	3.262633
H	1.825692	-4.188029	-2.132806
H	2.115613	-3.609655	-0.467890
H	3.802795	-2.675047	-1.980006
H	2.541002	-1.994966	-3.054552
H	-1.347243	-1.590256	-2.979036
H	-2.497454	-2.954459	-2.816002
H	-0.799538	-4.313904	-1.676159
H	-0.136820	-3.617174	-3.173064
H	3.215964	2.792875	1.483543
H	1.748877	2.056466	2.195423
H	-4.067479	-1.129099	-1.637948
H	-2.702644	-0.191010	-2.289083
C	-3.267979	3.210989	2.748189
H	-5.305616	2.686583	0.954405
H	-5.231740	0.926661	-0.802041
H	1.872905	4.904947	0.942021
H	0.322977	5.944414	-0.701727
C	-1.145343	4.547241	-2.593242
N	0.754344	2.120082	-0.554497
N	-2.158019	0.508645	0.476775
C	-1.021896	1.469585	2.335594
O	-0.038486	0.643298	2.107125
C	-1.037041	2.420953	3.353270
C	-0.688635	1.716622	-2.395253
O	-0.441943	0.444445	-2.238072
C	-1.534150	2.257219	-3.360749
H	3.146787	1.628067	-1.035653
H	4.589938	1.361714	-0.036848
H	4.286678	-0.123929	-2.065787
H	4.641630	-0.986769	-0.553925
H	-3.243801	-3.509692	-0.555103
H	-3.363241	-2.126516	0.549250
H	-2.194118	-3.874506	1.650654
H	-0.964987	-4.024491	0.372928
C	-1.754081	3.650532	-3.444603
H	-1.323664	5.620332	-2.679331
H	-2.427750	4.024562	-4.219347

H	-2.018205	1.583159	-4.071052
C	-2.144570	3.275652	3.543616
H	-4.120587	3.870787	2.917065
H	-2.107042	4.004346	4.356979
H	-0.175374	2.483945	4.021705

KHQLaΔ_{δλδ}_δλδ_opt.log

SCF (RwB97XD) = -1942.42984924
 E(SCF)+ZPE(0 K)= -1941.747045
 H(298 K)= -1941.710126
 G(298 K)= -1941.810850
 Lowest Frequency = 35.9667cm⁻¹

81

C	3.572031	-0.920584	-0.782997
N	2.919751	-0.654813	0.500345
O	1.675162	-2.158917	-1.555141
C	3.086156	-2.189928	-1.449872
C	3.316118	-1.637502	1.511560
C	2.278767	-1.850609	2.585190
O	1.095797	-2.378410	1.996568
C	0.146004	-2.713721	2.987315
C	-1.113221	-3.214865	2.336386
O	-1.672724	-2.173708	1.555940
O	-1.092019	-2.379935	-1.996113
C	-0.140221	-2.706315	-2.987934
C	1.122244	-3.201320	-2.338604
N	-2.926713	-0.671814	-0.495291
C	-3.317012	-1.654455	-1.508888
C	-2.278533	-1.858441	-2.583195
C	-3.083523	-2.212936	1.450967
C	-3.577181	-0.944825	0.787454
C	3.201695	0.709411	0.960096
C	-3.217066	0.691788	-0.951643
C	-2.563529	1.752308	-0.098760
C	2.541382	1.768075	0.110124
C	-0.911863	2.256113	1.453551
C	-1.278616	3.621504	1.514273
C	-2.358313	4.016747	0.681270
C	-3.012091	3.093129	-0.100099
C	2.981368	3.111727	0.115238
C	2.321738	4.033332	-0.663577
C	1.244637	3.633531	-1.497766
C	0.886585	2.265669	-1.440857
La	-0.003328	-0.687069	0.002337
H	4.293900	0.894540	1.002495
H	2.806150	0.812583	1.980990
H	-4.310390	0.870229	-0.993862
H	-2.821822	0.800063	-1.972143
C	-0.567536	4.484106	2.386813
H	-2.677054	5.061868	0.680432
H	-3.858085	3.383830	-0.724987
H	3.825452	3.406077	0.741001
H	2.633788	5.080463	-0.659778
C	0.528108	4.494020	-2.367931
N	1.517613	1.388923	-0.620442

N	-1.537332	1.377655	0.630719
C	0.153528	1.709707	2.256936
O	0.453068	0.448776	2.107788
C	0.801969	2.594058	3.114936
C	-0.175316	1.714745	-2.245774
O	-0.466933	0.451555	-2.100038
C	-0.829326	2.597329	-3.101365
H	4.673634	-0.985426	-0.674991
H	3.532537	-2.244340	-2.457794
H	3.394855	-3.100418	-0.906464
H	-4.678389	-1.016041	0.679448
H	-3.367537	-0.104031	1.461544
H	-3.529305	-2.272611	2.458857
H	-3.386902	-3.123863	0.905296
H	-2.027806	-0.917104	-3.097166
H	-2.667442	-2.582414	-3.320796
H	-3.483563	-2.624033	-1.021780
H	-4.275887	-1.375449	-1.987272
H	2.672148	-2.573734	3.321246
H	2.021836	-0.912002	3.101132
H	4.273160	-1.353628	1.990742
H	3.488835	-2.604811	1.022086
H	0.929959	-4.087183	-1.706779
H	1.828859	-3.494056	-3.132620
H	0.081529	-1.808315	-3.591377
H	-0.539514	-3.494552	-3.651298
H	3.357451	-0.079332	-1.454944
H	-1.818020	-3.514480	3.129446
H	-0.915211	-4.097606	1.701962
H	0.550244	-3.501316	3.648447
H	-0.081553	-1.818922	3.593344
C	0.441631	3.959212	3.164810
C	-0.477675	3.964879	-3.147433
H	-1.025161	4.620446	-3.828960
H	0.786580	5.552937	-2.419516
H	-1.624893	2.214973	-3.745099
H	0.984952	4.616347	3.848157
H	-0.832762	5.541202	2.441378
H	1.599956	2.214980	3.757612

KHQLaΔ_δλλ_δλλ_opt.log

SCF (RwB97XD) = -1942.42664428
 E(SCF)+ZPE(0 K)= -1941.744085
 H(298 K)= -1941.707200
 G(298 K)= -1941.807923
 Lowest Frequency = 21.5255cm⁻¹

81

C	-3.646701	-0.860755	0.291893
N	-2.776755	-0.560024	-0.850464
O	-1.866138	-1.976698	1.450495
C	-3.243886	-2.047157	1.149504
C	-2.911901	-1.476763	-1.986101
C	-2.190335	-2.809206	-1.829015
O	-0.794023	-2.664548	-1.624522
C	0.013730	-2.631384	-2.795499

C	1.434470	-2.939086	-2.393227
O	1.866378	-1.985134	-1.442475
O	0.794697	-2.653279	1.636834
C	-0.013155	-2.613491	2.807508
C	-1.433672	-2.924525	2.407087
N	2.775965	-0.552276	0.848856
C	2.911130	-1.460884	1.990999
C	2.191146	-2.795143	1.842512
C	3.244129	-2.052879	-1.140921
C	3.646297	-0.860559	-0.291200
C	-3.019980	0.825260	-1.284664
C	3.018523	0.836086	1.273435
C	2.461620	1.850543	0.301541
C	-2.463460	1.846763	-0.319916
C	1.001591	2.255731	-1.462748
C	1.350792	3.625823	-1.533276
C	2.311237	4.077100	-0.588930
C	2.879874	3.201399	0.305837
C	-2.882043	3.197444	-0.333854
C	-2.313696	4.079611	0.554722
C	-1.353239	3.635317	1.502374
C	-1.003660	2.264847	1.441617
La	-0.000342	-0.636905	-0.000530
H	-4.100388	1.011906	-1.442464
H	-2.514176	0.970974	-2.248368
H	4.098832	1.024310	1.430034
H	2.512607	0.988312	2.236070
C	0.742419	4.440326	-2.521692
H	2.608205	5.128680	-0.592564
H	3.634640	3.536633	1.018991
H	-3.636803	3.527432	-1.049455
H	-2.610906	5.131122	0.550833
C	-0.745165	4.456989	2.485025
N	-1.542350	1.429468	0.518396
N	1.540554	1.427033	-0.533695
C	0.049834	1.656507	-2.368278
O	-0.259533	0.398948	-2.207100
C	-0.497602	2.496994	-3.335434
C	-0.051752	1.672315	2.351387
O	0.258123	0.413760	2.199102
C	0.495337	2.519816	3.312614
H	-4.695064	-1.014226	-0.033938
H	-3.832298	-2.003790	2.082977
H	-3.474753	-3.016865	0.675478
H	4.694632	-1.011443	0.035927
H	3.635724	0.019331	-0.947461
H	3.832595	-2.015402	-2.074613
H	3.475466	-3.019300	-0.660468
H	-1.504267	-3.941661	1.980191
H	-2.074115	-2.875516	3.304811
H	0.045666	-1.611603	3.266020
H	0.327059	-3.377661	3.526042
H	-3.636277	0.023563	0.942164
H	2.074863	-2.895178	-3.291251
H	1.505709	-3.953537	-1.960098
H	-0.326037	-3.400159	-3.509315
H	-0.045759	-1.632325	-3.260104

H	-3.976604	-1.684343	-2.217378
H	-2.480966	-0.968498	-2.859933
H	-2.372883	-3.414787	-2.732364
H	-2.562672	-3.389911	-0.977722
H	2.564258	-3.380948	0.995051
H	2.374145	-3.394610	2.749831
H	2.478612	-0.946884	2.860719
H	3.975851	-1.665609	2.224722
C	-0.153196	3.865580	-3.397227
C	0.150539	3.888709	3.364683
H	0.612932	4.512931	4.133147
H	-0.999987	5.516529	2.541721
H	1.199635	2.105299	4.037718
H	-0.615814	4.484204	-4.170071
H	0.996968	5.499500	-2.585948
H	-1.201819	2.077138	-4.057538

KHQLaΔ_λδδ_λδδ_opt.log

SCF (RwB97XD) = -1942.42366214
 E(SCF)+ZPE(0 K)= -1941.741211
 H(298 K)= -1941.704401
 G(298 K)= -1941.804195
 Lowest Frequency = 36.7292cm⁻¹

81

C	3.726944	0.921830	0.471050
N	2.880562	0.727684	-0.725070
O	1.873937	1.939067	1.602085
C	2.971416	1.057592	1.785454
C	3.102543	1.788871	-1.717445
C	1.907726	2.089563	-2.595752
O	0.870760	2.623056	-1.769986
C	-0.165406	3.310704	-2.453313
C	-1.308118	2.391157	-2.816027
O	-1.870205	1.918769	-1.604443
O	-0.873131	2.620753	1.765724
C	0.157326	3.319111	2.446822
C	1.307773	2.410323	2.812232
N	-2.867051	0.705907	0.726555
C	-3.097821	1.767833	1.716116
C	-1.905335	2.080834	2.593290
C	-2.960216	1.027444	-1.784955
C	-3.714789	0.889827	-0.470204
C	3.057068	-0.607192	-1.311575
C	-3.032577	-0.628757	1.316710
C	-2.479011	-1.710556	0.419025
C	2.512651	-1.690996	-0.410678
C	-1.018175	-2.207664	-1.320862
C	-1.368705	-3.578095	-1.326197
C	-2.331672	-3.979687	-0.361644
C	-2.903184	-3.058137	0.485210
C	2.948045	-3.035180	-0.472965
C	2.384257	-3.958993	0.376609
C	1.418097	-3.562613	1.340126
C	1.056085	-2.195195	1.330751
La	0.006726	0.755290	0.000612

H	4.335695	1.826644	0.330263
H	4.439836	0.088332	0.582321
H	3.658642	1.474367	2.542048
H	2.597393	0.090459	2.154313
H	0.232048	3.798733	-3.357639
H	-0.527361	4.094541	-1.770972
H	-0.954001	1.535235	-3.417357
H	-2.065781	2.951440	-3.391779
H	-0.244105	3.806535	3.349717
H	0.512625	4.103890	1.762068
H	2.060644	2.978693	3.386339
H	0.960879	1.553224	3.416101
H	-2.578034	0.062166	-2.150305
H	-3.650792	1.435837	-2.543062
H	-4.330540	1.790326	-0.332231
H	-4.421165	0.050464	-0.578995
H	4.122886	-0.806365	-1.539092
H	2.498783	-0.646587	-2.258791
H	-4.096764	-0.836132	1.544558
H	-2.474250	-0.660929	2.264161
C	-0.761093	-4.434620	-2.278981
H	-2.632046	-5.029143	-0.313597
H	-3.664754	-3.355615	1.207744
H	3.712008	-3.328413	-1.194709
H	2.693335	-5.006053	0.331572
C	0.817817	-4.421335	2.295583
N	1.579509	-1.321670	0.436335
N	-1.548974	-1.335907	-0.429044
C	-0.084582	-1.644417	-2.265583
O	0.198665	-0.371610	-2.172020
C	0.462333	-2.524206	-3.195338
C	0.117823	-1.636975	2.273820
O	-0.176087	-0.366870	2.176419
C	-0.421581	-2.518516	3.206296
H	-2.207336	2.840762	3.333263
H	-1.525413	1.188823	3.116558
H	-3.961941	1.530908	2.367109
H	-3.344064	2.690687	1.173982
H	2.203635	2.850006	-3.337655
H	1.535500	1.193040	-3.116801
H	3.340872	2.715198	-1.177702
H	3.968785	1.557499	-2.367621
C	-0.074264	-3.888360	3.201261
C	0.126589	-3.896904	-3.186175
H	0.587707	-4.549665	-3.931281
H	-1.011620	-5.496591	-2.294310
H	1.158917	-2.135693	-3.941696
H	-0.529789	-4.542722	3.948399
H	1.077261	-5.481113	2.314084
H	-1.121359	-2.133632	3.951545

KHQLaΔ_λδλ_λδλ_opt.log

SCF (RwB97XD) = -1942.42721527
E(SCF)+ZPE(0 K)= -1941.745936
H(298 K)= -1941.708571
G(298 K)= -1941.811282

Lowest Frequency = 27.6234cm⁻¹

81

C	3.692726	1.073979	-0.197752
N	2.680608	0.632886	-1.174781
O	2.024461	2.030511	1.217284
C	3.190859	1.220201	1.229138
C	2.599049	1.528667	-2.334743
C	1.967260	2.870877	-2.012172
O	0.611699	2.680938	-1.629148
C	-0.403160	3.379415	-2.328750
C	-1.596008	2.469961	-2.508423
O	-2.028085	2.047546	-1.225870
O	-0.609855	2.686486	1.620092
C	0.410780	3.375644	2.320581
C	1.595761	2.455903	2.499987
N	-2.696086	0.656075	1.166241
C	-2.607160	1.551677	2.325820
C	-1.963839	2.888242	2.002683
C	-3.201345	1.247219	-1.237852
C	-3.704496	1.105229	0.189019
C	2.880784	-0.754565	-1.609375
C	-2.908070	-0.729458	1.601466
C	-2.505730	-1.747274	0.561191
C	2.470055	-1.768443	-0.568541
C	-1.234435	-2.191809	-1.335508
C	-1.630887	-3.550360	-1.373519
C	-2.518899	-3.972587	-0.347965
C	-2.972110	-3.082575	0.597048
C	2.925557	-3.107502	-0.603591
C	2.465056	-3.993251	0.341897
C	1.580412	-3.563220	1.367124
C	1.195031	-2.201499	1.328287
La	-0.007654	0.684397	-0.004311
H	4.098091	2.046758	-0.515066
H	4.548583	0.377576	-0.185246
H	3.975527	1.707991	1.833494
H	2.955004	0.245866	1.685985
H	1.963778	1.035667	-3.083962
H	3.595614	1.701898	-2.788074
H	2.018603	3.513629	-2.904718
H	2.489640	3.390299	-1.192965
H	-0.043467	3.685510	-3.324145
H	-0.684117	4.284725	-1.764095
H	-1.315130	1.586392	-3.108525
H	-2.403650	3.023661	-3.018427
H	0.053397	3.684041	3.316097
H	0.699667	4.278945	1.756711
H	2.407978	3.002453	3.010438
H	1.307291	1.574400	3.099543
H	-1.976302	1.053726	3.075477
H	-3.602323	1.733607	2.778820
H	-2.481558	3.411602	1.183040
H	-2.009917	3.531966	2.894813
H	-2.973788	0.270990	-1.694840
H	-3.981806	1.741732	-1.842193
H	-4.102013	2.081294	0.506183

H	-4.565959	0.415782	0.176511
H	3.929586	-0.934938	-1.915698
H	2.246674	-0.923533	-2.491428
H	-3.958423	-0.900802	1.907657
H	-2.275603	-0.903377	2.483720
C	-1.139409	-4.380226	-2.412345
H	-2.852907	-5.012847	-0.327883
H	-3.671144	-3.395197	1.374454
H	3.622111	-3.426236	-1.380741
H	2.790627	-5.036194	0.322469
C	1.082147	-4.388457	2.406400
N	1.620470	-1.364487	0.347901
N	-1.652942	-1.350809	-0.355553
C	-0.368537	-1.613693	-2.335799
O	-0.038522	-0.355297	-2.223999
C	0.070415	-2.470272	-3.343279
C	0.333860	-1.615788	2.328218
O	0.014132	-0.354808	2.215720
C	-0.112100	-2.468180	3.336178
C	0.257409	-3.831264	3.359956
C	-0.310205	-3.830312	-3.366250
H	0.064152	-4.461794	-4.175581
H	-1.428724	-5.431647	-2.451858
H	0.710798	-2.067728	-4.131518
H	-0.122106	-4.459208	4.169636
H	1.362905	-5.442171	2.446534
H	-0.749208	-2.059964	4.124154

KHQLaΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1942.42259001
 E(SCF)+ZPE(0 K)= -1941.739863
 H(298 K)= -1941.703148
 G(298 K)= -1941.802317
 Lowest Frequency = 43.0274cm⁻¹

81

C	-3.599088	-0.840345	0.744138
N	-2.874740	-0.654167	-0.528845
O	-1.803742	-2.312371	1.331865
C	-2.710610	-1.355051	1.872362
C	-3.185538	-1.746188	-1.458932
C	-2.163134	-1.957051	-2.551647
O	-0.943393	-2.405155	-1.975192
C	0.040352	-2.700822	-2.948951
C	1.257365	-3.241904	-2.235505
O	1.803295	-2.300429	-1.330053
O	0.943493	-2.405509	1.976728
C	-0.038860	-2.707605	2.949924
C	-1.253305	-3.253044	2.235423
N	2.866369	-0.641921	0.534442
C	3.182423	-1.734867	1.461666
C	2.161258	-1.953221	2.554050
C	2.705821	-1.337834	-1.868430
C	3.591697	-0.821347	-0.738948
C	-3.123970	0.670129	-1.107959
C	3.109240	0.682032	1.117059

C	2.482401	1.764746	0.268735
C	-2.502041	1.753623	-0.257016
C	0.931713	2.236712	-1.396566
C	1.250686	3.614165	-1.412759
C	2.246076	4.033679	-0.489614
C	2.875722	3.121638	0.326430
C	-2.901690	3.108808	-0.311334
C	-2.276295	4.021752	0.506963
C	-1.278945	3.604597	1.429062
C	-0.953575	2.228686	1.409463
La	-0.003942	-0.725713	0.002718
H	-4.446709	-1.528404	0.590540
H	-4.031167	0.113923	1.076867
H	-3.331840	-1.826350	2.651692
H	-2.141330	-0.529597	2.333253
H	2.132843	-0.514086	-2.327778
H	3.329363	-1.804672	-2.648599
H	4.442775	-1.505486	-0.586963
H	4.018974	0.135883	-1.069342
H	-4.207687	0.862302	-1.235086
H	-2.658874	0.711005	-2.103734
H	4.192000	0.878969	1.245009
H	2.643585	0.718125	2.112784
C	0.578314	4.457705	-2.333540
H	2.523720	5.089651	-0.448023
H	3.660475	3.433700	1.017307
H	-3.687917	3.418913	-1.001417
H	-2.558863	5.076517	0.467986
C	-0.610469	4.448977	2.351908
N	-1.541972	1.363336	0.549939
N	1.524179	1.371985	-0.539212
C	-0.041075	1.655094	-2.287287
O	-0.297429	0.378878	-2.167328
C	-0.650700	2.521563	-3.189827
C	0.021915	1.649399	2.298741
O	0.284213	0.374689	2.175623
C	0.627525	2.516458	3.203417
H	2.545361	-2.727586	3.240969
H	1.958976	-1.035716	3.129575
H	4.173066	-1.581891	1.934131
H	3.239602	-2.662078	0.875091
H	-2.543507	-2.731473	-3.240571
H	-1.964900	-1.037197	-3.124832
H	-3.238543	-2.675154	-0.874746
H	-4.176779	-1.596611	-1.931228
H	0.279295	-1.783650	-3.516904
H	-0.338401	-3.463532	-3.652516
H	2.018084	-3.556112	-2.969068
H	0.976396	-4.119072	-1.634156
H	-0.282063	-1.792578	3.519535
H	0.343456	-3.469850	3.652063
H	-0.968191	-4.127673	1.632330
H	-2.012505	-3.572316	2.968373
C	0.311311	3.894274	3.213955
C	-0.340878	3.900852	-3.196964
H	-0.851170	4.543916	-3.918092
H	0.804076	5.525015	-2.359750

H	-1.377771	2.119736	-3.899210
H	0.818625	4.537923	3.936661
H	-0.841183	5.515161	2.380747
H	1.356458	2.116256	3.911808

MacropaLaΔ_δδδ_δδδ_opt.log

SCF (RwB97XD) = -1861.92003121
 E(SCF)+ZPE(0 K)= -1861.310793
 H(298 K)= -1861.275493
 G(298 K)= -1861.373699
 Lowest Frequency = 33.0679cm⁻¹

73

C	3.618769	-0.846323	-0.543780
N	2.860157	-0.613383	0.690140
O	1.737551	-1.910699	-1.576467
C	3.129970	-2.038432	-1.343370
C	3.175705	-1.618601	1.713826
C	1.994774	-1.991933	2.582269
O	0.993735	-2.564668	1.735184
C	-0.001735	-3.333153	2.388807
C	-1.201250	-2.489642	2.764362
O	-1.732042	-1.915214	1.576842
O	-0.986297	-2.568057	-1.734618
C	0.011360	-3.333886	-2.388028
C	1.208451	-2.487045	-2.763815
N	-2.858346	-0.621849	-0.690113
C	-3.171039	-1.628322	-1.713435
C	-1.989100	-1.998598	-2.581815
C	-3.124109	-2.046950	1.343891
C	-3.616301	-0.856517	0.543888
C	3.092463	0.747542	1.196203
C	-3.094523	0.738258	-1.196613
C	-2.543278	1.800297	-0.272811
C	2.538027	1.807750	0.272206
C	-1.013800	2.284761	1.409209
C	-1.443544	3.602113	1.499112
C	-2.467535	4.014340	0.646791
C	-3.040627	3.102961	-0.237101
C	3.031520	3.111874	0.236233
C	2.455705	4.021390	-0.647806
C	1.432911	3.605976	-1.500018
C	1.007069	2.287376	-1.409861
La	0.000993	-0.673180	-0.000013
H	0.416520	-3.823129	3.283405
H	-0.310261	-4.117314	1.680648
H	-0.917474	-1.671626	3.446052
H	-1.953594	-3.124205	3.258345
H	-0.405492	-3.825298	-3.282492
H	0.322125	-4.116966	-1.679652
H	1.962639	-3.119588	-3.257577
H	0.922334	-1.670077	-3.445779
H	4.172917	0.930101	1.357351
H	2.588135	0.852825	2.169527
H	-4.175476	0.917647	-1.357963
H	-2.590331	0.844753	-2.169882

H	-0.974690	4.263715	2.227866
H	-2.832708	5.042765	0.681433
H	-3.858989	3.396885	-0.895903
H	3.849033	3.408336	0.894954
H	2.817830	5.050885	-0.682642
H	0.962081	4.266058	-2.228876
N	1.532943	1.437850	-0.521141
N	-1.537135	1.433517	0.520643
C	0.085867	1.710853	2.302196
O	0.270843	0.444747	2.139959
O	0.708308	2.449606	3.038842
C	-0.090919	1.710065	-2.302715
O	-0.272140	0.443447	-2.140272
O	-0.715584	2.446864	-3.039441
H	4.699212	-0.979565	-0.336689
H	3.674998	-2.053239	-2.300808
H	3.325335	-2.997477	-0.832603
H	-4.696360	-0.992902	0.336838
H	-3.518315	0.033508	1.178774
H	-3.669034	-2.062927	2.301369
H	-3.316813	-3.006735	0.833504
H	-1.578248	-1.119020	-3.101835
H	-2.309993	-2.752143	-3.320027
H	-3.514955	-2.545661	-1.215855
H	-4.001018	-1.291821	-2.361982
H	2.317772	-2.744233	3.320830
H	1.581283	-1.113314	3.101850
H	4.004695	-1.279500	2.362280
H	3.522257	-2.535130	1.216582
H	3.518253	0.043198	-1.178971

MacropaLaΔ_δδλ_δδλ_opt.log

SCF (RwB97XD) = -1861.91456304
 E(SCF)+ZPE(0 K)= -1861.306347
 H(298 K)= -1861.270664
 G(298 K)= -1861.370448
 Lowest Frequency = 25.5337cm⁻¹

73

C	3.605428	0.943567	-0.263370
N	2.669277	0.853712	0.861132
O	2.688360	-1.093138	-1.149536
C	3.887661	-0.359452	-0.990451
C	3.157732	0.101769	2.022735
C	3.084055	-1.417957	1.924493
O	1.755715	-1.830643	1.648568
C	1.176420	-2.863442	2.426808
C	-0.277535	-2.504645	2.665325
O	-0.940369	-2.246139	1.440273
O	0.514131	-2.697017	-1.442659
C	1.807855	-3.269434	-1.505768
C	2.790699	-2.227258	-1.991079
N	-2.111263	-1.723434	-1.108188
C	-1.670488	-2.347354	-2.359090
C	-0.511922	-3.312953	-2.209138
C	-1.672067	-3.286932	0.826936

C	-2.678340	-2.655584	-0.125791
C	2.286450	2.216098	1.279540
C	-3.070814	-0.652123	-1.425919
C	-3.224409	0.353871	-0.310588
C	1.440497	2.925566	0.248537
C	-2.189678	1.476681	1.440019
C	-3.325176	2.234040	1.700186
C	-4.455556	2.009748	0.917159
C	-4.414674	1.047727	-0.089543
C	1.376950	4.314943	0.146088
C	0.532132	4.877521	-0.808820
C	-0.202030	4.050411	-1.657822
C	-0.061821	2.676587	-1.508754
La	0.257128	-0.414211	-0.067020
H	2.521672	0.392482	2.869959
H	4.200954	0.380501	2.274851
H	3.407988	-1.824182	2.896085
H	3.754672	-1.836652	1.160126
H	1.688651	-2.951575	3.398690
H	1.277490	-3.829144	1.898864
H	-0.329603	-1.565547	3.234312
H	-0.788374	-3.304639	3.225273
H	1.821267	-4.139410	-2.180554
H	2.088630	-3.610572	-0.495581
H	3.809865	-2.648218	-1.948408
H	2.574603	-1.934588	-3.032785
H	-1.348465	-1.526040	-3.014350
H	-2.499464	-2.887710	-2.859073
H	-0.808914	-4.263100	-1.731537
H	-0.136170	-3.552207	-3.217621
H	3.179637	2.826538	1.513091
H	1.681590	2.137190	2.195651
H	-4.060183	-1.068767	-1.693771
H	-2.698666	-0.105992	-2.307212
H	-3.298356	2.965526	2.508208
H	-5.372717	2.574479	1.096482
H	-5.291703	0.841551	-0.705115
H	1.973111	4.943478	0.809317
H	0.456277	5.963229	-0.896741
H	-0.869264	4.435029	-2.429540
N	0.720238	2.149161	-0.560911
N	-2.147421	0.586309	0.441996
C	-0.918463	1.600353	2.280772
O	-0.079119	0.641797	2.089338
O	-0.777481	2.556464	3.017338
C	-0.787668	1.664251	-2.395642
O	-0.368267	0.455452	-2.239481
O	-1.692365	2.037717	-3.115830
H	3.169084	1.644180	-0.987994
H	4.577034	1.372010	0.055088
H	4.321544	-0.118040	-1.975780
H	4.626249	-0.981035	-0.453523
H	-3.257808	-3.459472	-0.620566
H	-3.385437	-2.090929	0.498513
H	-2.230138	-3.855652	1.590159
H	-0.987353	-3.989493	0.323785

MacropaLaΔ_δλδ_δλδ_opt.log

SCF (RwB97XD) = -1861.92551980

E(SCF)+ZPE(0 K)= -1861.316008

H(298 K)= -1861.280755

G(298 K)= -1861.378754

Lowest Frequency = 35.2014cm⁻¹

73

C	3.577759	-0.893184	-0.734368
N	2.904186	-0.614130	0.536160
O	1.690853	-2.127951	-1.535330
C	3.100289	-2.166628	-1.399206
C	3.291331	-1.587274	1.562652
C	2.242776	-1.794306	2.625541
O	1.067818	-2.328971	2.022140
C	0.106779	-2.669098	3.000925
C	-1.142616	-3.170435	2.331481
O	-1.687195	-2.129426	1.537159
O	-1.063785	-2.332663	-2.020120
C	-0.102176	-2.672118	-2.998577
C	1.148069	-3.170667	-2.328640
N	-2.903115	-0.619603	-0.535727
C	-3.288571	-1.594316	-1.561364
C	-2.239631	-1.800530	-2.624034
C	-3.096553	-2.170699	1.401031
C	-3.576233	-0.898694	0.735033
C	3.188230	0.754336	0.988546
C	-3.189492	0.747976	-0.989312
C	-2.586463	1.800029	-0.090806
C	2.583390	1.804580	0.089141
C	-0.936691	2.298122	1.463924
C	-1.374346	3.608867	1.595286
C	-2.471480	4.010671	0.834322
C	-3.099287	3.094627	-0.005461
C	3.094006	3.099980	0.002675
C	2.464631	4.014228	-0.837891
C	1.368175	3.609896	-1.598493
C	0.932758	2.298522	-1.465996
La	0.000624	-0.677211	0.000246
H	4.279946	0.923273	1.069310
H	2.755422	0.893275	1.991404
H	-4.281494	0.914978	-1.070248
H	-2.756889	0.886776	-1.992277
H	-0.854070	4.273295	2.285551
H	-2.847916	5.033114	0.905279
H	-3.971937	3.378590	-0.595366
H	3.966177	3.385936	0.592325
H	2.839325	5.037249	-0.909735
H	0.846755	4.272840	-2.289324
N	1.514744	1.440990	-0.619486
N	-1.517205	1.438873	0.618144
C	0.237797	1.737546	2.260304
O	0.410737	0.472509	2.087859
O	0.920958	2.480587	2.936957
C	-0.240780	1.735248	-2.261872
O	-0.411516	0.470059	-2.088366

O	-0.925247	2.476542	-2.939122
H	4.677012	-0.958061	-0.607275
H	3.567024	-2.233497	-2.396835
H	3.391029	-3.073147	-0.840161
H	-4.675367	-0.965607	0.607968
H	-3.378601	-0.062431	1.419069
H	-3.563201	-2.237485	2.398706
H	-3.385688	-3.078234	0.842802
H	-1.978923	-0.859530	-3.133458
H	-2.623025	-2.521726	-3.366644
H	-3.469615	-2.564969	-1.081584
H	-4.238320	-1.302622	-2.049051
H	2.627410	-2.514182	3.368792
H	1.980485	-0.853287	3.134117
H	4.240604	-1.293536	2.050040
H	3.473997	-2.558047	1.083732
H	0.943401	-4.054839	-1.698615
H	1.868081	-3.465386	-3.109453
H	0.131767	-1.780544	-3.606792
H	-0.498104	-3.462225	-3.661302
H	3.378646	-0.057883	-1.419150
H	-1.862114	-3.465623	3.112590
H	-0.936439	-4.054872	1.702320
H	0.504046	-3.457878	3.664426
H	-0.128680	-1.777326	3.608260

MacropaLaΔ_δλλ_δλλ_opt.log

SCF (RwB97XD) = -1861.92280131
 E(SCF)+ZPE(0 K)= -1861.313203
 H(298 K)= -1861.278087
 G(298 K)= -1861.375577
 Lowest Frequency = 27.3478cm⁻¹

73

C	-3.652466	-0.849688	0.245176
N	-2.766776	-0.501591	-0.872135
O	-1.872535	-1.943781	1.429093
C	-3.240487	-2.043827	1.086911
C	-2.882485	-1.373299	-2.046536
C	-2.188269	-2.721581	-1.919574
O	-0.794581	-2.605866	-1.668712
C	0.043256	-2.586866	-2.818829
C	1.450984	-2.901969	-2.381585
O	1.873326	-1.943213	-1.428872
O	0.795633	-2.605338	1.669021
C	-0.042208	-2.586513	2.819138
C	-1.449810	-2.902239	2.381937
N	2.766996	-0.500388	0.872177
C	2.883063	-1.371915	2.046677
C	2.189367	-2.720481	1.919888
C	3.241324	-2.042656	-1.086695
C	3.652822	-0.848254	-0.245098
C	-3.028319	0.893486	-1.267404
C	3.027969	0.894842	1.267284
C	2.536186	1.887354	0.240843
C	-2.536926	1.886322	-0.241089

C	1.052245	2.291803	-1.499617
C	1.512609	3.591222	-1.666196
C	2.535246	4.035325	-0.828882
C	3.068335	3.172139	0.124964
C	-3.069585	3.170910	-0.125369
C	-2.536835	4.034425	0.828369
C	-1.514021	3.590830	1.665737
C	-1.053143	2.291574	1.499319
La	0.000131	-0.616170	0.000026
H	-4.106832	1.058368	-1.454023
H	-2.498695	1.099899	-2.209660
H	4.106412	1.060185	1.453896
H	2.498246	1.101149	2.209508
H	1.067994	4.214202	-2.442632
H	2.928142	5.049267	-0.927829
H	3.882764	3.489100	0.778149
H	-3.884140	3.487468	-0.778591
H	-2.930131	5.048224	0.927192
H	-1.069653	4.214082	2.442096
N	-1.540890	1.485315	0.549324
N	1.540310	1.485855	-0.549523
C	-0.046176	1.693745	-2.376542
O	-0.242941	0.436814	-2.174047
O	-0.663213	2.413768	-3.137478
C	0.045511	1.694055	2.376318
O	0.242776	0.437180	2.173969
O	0.662263	2.414413	3.137169
H	-4.690366	-1.018241	-0.104830
H	-3.854142	-2.036953	2.004797
H	-3.429843	-3.008923	0.587537
H	4.690793	-1.016345	0.104922
H	3.679715	0.020799	-0.916256
H	3.854965	-2.035633	-2.004589
H	3.431084	-3.007618	-0.587215
H	-1.501323	-3.912760	1.937598
H	-2.111023	-2.872953	3.265080
H	0.002824	-1.593413	3.297103
H	0.284196	-3.358847	3.535047
H	-3.679714	0.019432	0.916234
H	2.112184	-2.872538	-3.264733
H	1.502902	-3.912409	-1.937108
H	-0.282838	-3.359428	-3.534632
H	-0.002172	-1.593851	-3.296932
H	-3.943652	-1.553741	-2.312665
H	-2.419835	-0.835951	-2.886044
H	-2.351243	-3.287218	-2.851487
H	-2.596099	-3.331083	-1.105369
H	2.597425	-3.329924	1.105755
H	2.352567	-3.285942	2.851868
H	2.420221	-0.834650	2.886132
H	3.944304	-1.551913	2.312811

MacropaLaΔ_δλλ_λδλ.log

SCF (RwB97XD) = -1861.92467977
E(SCF)+ZPE(0 K)= -1861.315000
H(298 K)= -1861.279854

G(298 K)= -1861.377327
 Lowest Frequency = 32.4894cm⁻¹

73

La	0.878267	3.986601	9.179094
N	3.144985	2.608587	9.218658
C	3.171543	1.278445	9.302768
C	4.313858	0.615239	9.750403
H	4.324290	-0.473204	9.823255
C	5.429325	1.369733	10.106781
H	6.329740	0.871585	10.471879
C	5.397100	2.757798	9.976169
C	4.225213	3.340284	9.511735
C	4.073894	4.848366	9.313961
O	2.949866	5.189571	8.784216
H	6.246457	3.397042	10.218132
N	1.899722	4.421922	11.620405
C	2.453822	5.577230	11.987797
C	3.302583	5.647245	13.093277
H	3.751156	6.599659	13.379612
C	3.570473	4.483442	13.808468
H	4.242899	4.512961	14.668195
C	2.961363	3.287614	13.429996
C	2.114901	3.307604	12.330009
C	1.376588	2.065313	11.841028
O	0.537286	2.311059	10.894868
H	3.116481	2.347616	13.960046
C	1.908911	0.553293	8.896248
H	2.172446	-0.431329	8.463191
H	1.321521	0.368547	9.808635
N	1.096329	1.337991	7.954572
C	1.792036	1.468143	6.669669
H	1.788148	0.511259	6.110998
H	2.840994	1.721766	6.871055
C	1.219723	2.548245	5.777845
H	1.864841	2.640917	4.887239
H	0.201448	2.312024	5.419645
O	1.196851	3.774537	6.482247
C	0.969764	4.899380	5.655491
H	-0.039794	4.836164	5.210357
H	1.711832	4.925560	4.838865
C	1.108151	6.149911	6.482029
H	2.130617	6.235776	6.886384
H	0.882158	7.022709	5.847547
O	0.172260	6.071660	7.552019
C	-0.134851	7.303404	8.185146
H	-1.175941	7.224000	8.515178
H	-0.097954	8.120066	7.445305
C	0.820096	7.637547	9.322249
H	1.832597	7.705550	8.900076
H	0.560904	8.642935	9.711673
N	0.874098	6.643632	10.398406
C	2.142383	6.781223	11.133212
H	2.140493	7.691212	11.763696
H	2.961248	6.885538	10.405735
C	-0.238260	6.713944	11.351119
H	-0.371677	7.744295	11.737577

H	0.031665	6.082827	12.208501
C	-1.581723	6.227810	10.839866
H	-2.248559	6.092138	11.708917
H	-2.071821	6.956858	10.173203
O	-1.418475	4.992138	10.169396
C	-2.627486	4.371765	9.759751
H	-2.911745	4.736305	8.756431
H	-3.438241	4.624823	10.462332
C	-2.444352	2.877360	9.768236
H	-2.139721	2.544670	10.776173
H	-3.403420	2.396243	9.506655
O	-1.447328	2.507280	8.834508
C	-1.223327	1.098730	8.849001
H	-2.175186	0.580155	8.640779
H	-0.864600	0.810065	9.849364
C	-0.230723	0.740005	7.770166
H	-0.163132	-0.363011	7.705361
H	-0.641580	1.085282	6.811708
O	1.638449	0.978674	12.317789
O	4.958060	5.593062	9.690072

MacropaLaΔ_λδδ_λδδ_opt.log

SCF (RwB97XD) = -1861.91734482

E(SCF)+ZPE(0 K)= -1861.308114

H(298 K)= -1861.272975

G(298 K)= -1861.370481

Lowest Frequency = 30.0201cm⁻¹

73

C	3.730162	0.922840	0.416774
N	2.866524	0.699215	-0.762196
O	1.880228	1.875812	1.602149
C	2.998016	1.012594	1.747009
C	3.080221	1.737302	-1.783106
C	1.876858	2.019225	-2.653840
O	0.848120	2.562902	-1.821877
C	-0.190384	3.252426	-2.499929
C	-1.345471	2.337421	-2.831394
O	-1.880928	1.875051	-1.602165
O	-0.849109	2.562550	1.821866
C	0.189115	3.252496	2.499918
C	1.344580	2.337965	2.831379
N	-2.866766	0.698058	0.762187
C	-3.080888	1.736084	1.783069
C	-1.877649	2.018480	2.653821
C	-2.998328	1.011327	-1.747024
C	-3.730470	0.921310	-0.416806
C	3.048727	-0.645631	-1.328123
C	-3.048444	-0.646845	1.328143
C	-2.557686	-1.724079	0.391412
C	2.558425	-1.723044	-0.391357
C	-1.080148	-2.244852	-1.325175
C	-1.540045	-3.552203	-1.403503
C	-2.556343	-3.939447	-0.529804
C	-3.088920	-3.013941	0.364439
C	3.090212	-3.012678	-0.364347

C	2.558025	-3.938389	0.529917
C	1.541553	-3.551558	1.403597
C	1.081098	-2.244406	1.325233
La	-0.000124	0.746483	0.000006
H	4.285339	1.860486	0.274141
H	4.489541	0.127618	0.503444
H	3.691414	1.426908	2.498825
H	2.649973	0.032308	2.106001
H	0.197887	3.723052	-3.417088
H	-0.534855	4.049955	-1.824333
H	-1.011311	1.476902	-3.437091
H	-2.114334	2.898404	-3.390740
H	-0.199344	3.722956	3.417082
H	0.533257	4.050170	1.824327
H	2.113213	2.899266	3.390722
H	1.010775	1.477310	3.437077
H	-2.649829	0.031177	-2.105950
H	-3.691887	1.425296	-2.498881
H	-4.286027	1.858737	-0.274208
H	-4.489527	0.125782	-0.503475
H	4.110535	-0.828622	-1.582215
H	2.467345	-0.726363	-2.259658
H	-4.110186	-0.830255	1.582212
H	-2.467054	-0.727315	2.259696
H	-1.104290	-4.224823	-2.142702
H	-2.947920	-4.958295	-0.557246
H	-3.901787	-3.287051	1.038763
H	3.903200	-3.285458	-1.038658
H	2.950037	-4.957069	0.557388
H	1.106079	-4.224347	2.142808
N	1.560944	-1.381209	0.423374
N	-1.560356	-1.381837	-0.423333
C	-0.012840	-1.680961	-2.261268
O	0.150449	-0.406325	-2.136922
O	0.598803	-2.425882	-2.999529
C	0.013544	-1.680947	2.261307
O	-0.150278	-0.406382	2.136934
O	-0.597789	-2.426111	2.999579
H	-2.163313	2.769293	3.408947
H	-1.503688	1.113884	3.158890
H	-3.938594	1.485117	2.436322
H	-3.328114	2.674320	1.268595
H	2.162223	2.770143	-3.408975
H	1.503241	1.114483	-3.158902
H	3.327096	2.675644	-1.268656
H	3.938010	1.486652	-2.436371

MacropaLaΔ_λδλ_λδλ_opt.log

SCF (RwB97XD) = -1861.92270640
E(SCF)+ZPE(0 K)= -1861.314567
H(298 K)= -1861.278952
G(298 K)= -1861.378549
Lowest Frequency = 27.5355cm⁻¹

73

C	3.691777	1.092107	-0.298546
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N	2.661753	0.595763	-1.228713
O	2.047652	1.967097	1.189706
C	3.243704	1.201945	1.148384
C	2.537390	1.443664	-2.421858
C	1.904346	2.792832	-2.136950
O	0.567386	2.611586	-1.686089
C	-0.474256	3.312800	-2.343612
C	-1.669070	2.400302	-2.486341
O	-2.048039	1.966597	-1.189842
O	-0.567896	2.611628	1.685831
C	0.473588	3.313027	2.343413
C	1.668572	2.400758	2.486189
N	-2.661838	0.595281	1.228654
C	-2.537651	1.443333	2.421709
C	-1.904910	2.792612	2.136646
C	-3.243912	1.201166	-1.148490
C	-3.691979	1.091294	0.298440
C	2.893083	-0.800081	-1.625874
C	-2.892843	-0.800578	1.625949
C	-2.589017	-1.783832	0.523140
C	2.589473	-1.783305	-0.522980
C	-1.296836	-2.239941	-1.353111
C	-1.856242	-3.502020	-1.503123
C	-2.837084	-3.894410	-0.593163
C	-3.223498	-3.022610	0.421871
C	3.224243	-3.021924	-0.421592
C	2.838022	-3.893723	0.593517
C	1.857081	-3.501478	1.503431
C	1.297381	-2.239544	1.353299
La	-0.000045	0.651522	-0.000036
H	4.018494	2.091025	-0.622726
H	4.590222	0.451547	-0.332379
H	4.031751	1.713680	1.727320
H	3.064781	0.216270	1.607367
H	1.889690	0.911416	-3.132233
H	3.519651	1.607227	-2.907983
H	1.908927	3.387646	-3.063345
H	2.455931	3.362541	-1.371759
H	-0.151048	3.628029	-3.348275
H	-0.737837	4.212445	-1.762101
H	-1.409511	1.523942	-3.105675
H	-2.498466	2.954647	-2.958548
H	0.150276	3.628182	3.348066
H	0.737023	4.212728	1.761924
H	2.497850	2.955275	2.958401
H	1.409168	1.524362	3.105536
H	-1.889826	0.911303	3.132134
H	-3.519943	1.606730	2.907828
H	-2.456607	3.362088	1.371366
H	-1.909652	3.387552	3.062959
H	-3.064750	0.215510	-1.607418
H	-4.032072	1.712685	-1.727463
H	-4.018987	2.090137	0.622560
H	-4.590246	0.450486	0.332288
H	3.929905	-0.948292	-1.982843
H	2.221342	-1.040921	-2.465344
H	-3.929628	-0.948995	1.982942

H	-2.221036	-1.041186	2.465433
H	-1.522899	-4.135258	-2.325666
H	-3.310870	-4.874209	-0.681275
H	-4.001400	-3.299787	1.134919
H	4.002218	-3.298984	-1.134606
H	3.312035	-4.873403	0.681723
H	1.523878	-4.134717	2.326031
N	1.642152	-1.428253	0.346023
N	-1.641790	-1.428640	-0.345907
C	-0.261600	-1.676640	-2.325301
O	-0.067363	-0.409878	-2.188858
O	0.306106	-2.424284	-3.097400
C	0.262015	-1.676394	2.325437
O	0.067482	-0.409690	2.188876
O	-0.305513	-2.424096	3.097611

MacropaLaΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1861.91647434
 E(SCF)+ZPE(0 K)= -1861.306363
 H(298 K)= -1861.271504
 G(298 K)= -1861.367597
 Lowest Frequency = 37.6005cm-1

73

C	-3.603668	-0.823026	0.713637
N	-2.863605	-0.622783	-0.549524
O	-1.798665	-2.267153	1.335435
C	-2.720114	-1.312199	1.856019
C	-3.169788	-1.704101	-1.496152
C	-2.142351	-1.898828	-2.585953
O	-0.927774	-2.358807	-2.003494
C	0.059350	-2.659599	-2.972638
C	1.268936	-3.204340	-2.250283
O	1.803683	-2.263196	-1.335020
O	0.932969	-2.356369	2.003917
C	-0.053444	-2.659225	2.973139
C	-1.261783	-3.206880	2.250902
N	2.864755	-0.616133	0.549661
C	3.173468	-1.696680	1.496353
C	2.146579	-1.893721	2.586256
C	2.722984	-1.306280	-1.855786
C	3.605326	-0.814770	-0.713463
C	-3.115921	0.705587	-1.122054
C	3.114034	0.712866	1.122080
C	2.538163	1.793155	0.237337
C	-2.542416	1.787288	-0.237503
C	0.972653	2.274070	-1.411044
C	1.376847	3.599501	-1.491065
C	2.408211	4.017728	-0.649306
C	3.012326	3.104917	0.212206
C	-3.019556	3.097975	-0.212570
C	-2.417498	4.012295	0.648778
C	-1.385176	3.596534	1.490587
C	-0.977976	2.272012	1.410764
La	0.000765	-0.721427	0.000075
H	-4.429656	-1.533850	0.550217

H	-4.068677	0.119487	1.036732
H	-3.342806	-1.778850	2.636546
H	-2.162067	-0.476561	2.311877
H	2.163075	-0.472039	-2.311917
H	3.346807	-1.771714	-2.636137
H	4.433055	-1.523535	-0.549911
H	4.068020	0.128830	-1.036701
H	-4.197736	0.881347	-1.278012
H	-2.623997	0.778982	-2.104190
H	4.195434	0.891076	1.278124
H	2.621813	0.785264	2.104144
H	0.886458	4.262974	-2.203808
H	2.755465	5.052572	-0.676384
H	3.836920	3.403674	0.860910
H	-3.844846	3.394750	-0.861298
H	-2.767098	5.046352	0.675699
H	-0.896286	4.261223	2.203226
N	-1.527624	1.417054	0.542382
N	1.524239	1.420506	-0.542525
C	-0.122700	1.678221	-2.291625
O	-0.258476	0.403134	-2.140251
O	-0.783350	2.400557	-3.010182
C	0.118720	1.678794	2.291443
O	0.257409	0.404003	2.140236
O	0.777704	2.402729	3.009921
H	2.524082	-2.657899	3.287468
H	1.941598	-0.966793	3.145705
H	4.161716	-1.536673	1.970378
H	3.231904	-2.633612	0.925404
H	-2.518068	-2.663809	-3.287248
H	-1.939335	-0.971402	-3.145299
H	-3.226116	-2.641134	-0.925157
H	-4.158363	-1.546390	-1.970263
H	0.304755	-1.744962	-3.541931
H	-0.318967	-3.421066	-3.677394
H	2.038556	-3.515031	-2.975456
H	0.982918	-4.083337	-1.654141
H	-0.300926	-1.745033	3.542249
H	0.326627	-3.419683	3.678041
H	-0.973760	-4.085353	1.654953
H	-2.030696	-3.519166	2.976139

MacropaLaΔ_λλλ_λλλ_opt.log

SCF (RwB97XD) = -1861.91950610
 E(SCF)+ZPE(0 K)= -1861.310570
 H(298 K)= -1861.275173
 G(298 K)= -1861.374090
 Lowest Frequency = 23.0001cm⁻¹

73

C	-3.691993	1.140098	0.469405
N	-2.632338	0.600349	1.337075
O	-2.075063	1.863640	-1.138178
C	-3.330868	1.208132	-1.005055
C	-2.446610	1.415644	2.545758
C	-1.787460	2.755092	2.258551

O	-0.441987	2.623123	1.817634
C	0.530268	2.522296	2.851589
C	1.894067	2.742503	2.239859
O	2.074675	1.863937	1.138395
O	0.441438	2.623449	-1.817346
C	-0.530806	2.522543	-2.851304
C	-1.894644	2.742387	-2.239530
N	2.632230	0.601101	-1.337035
C	2.446322	1.416497	-2.545623
C	1.786878	2.755766	-2.258258
C	3.330632	1.208740	1.005172
C	3.691760	1.140989	-0.469300
C	-2.868772	-0.802791	1.699089
C	2.868985	-0.801942	-1.699213
C	2.601783	-1.765330	-0.569437
C	-2.601351	-1.765984	0.569198
C	1.345025	-2.231464	1.326357
C	1.934422	-3.479364	1.481452
C	2.913691	-3.858895	0.565207
C	3.265369	-2.988613	-0.463157
C	-3.264640	-2.989416	0.462788
C	-2.912759	-3.859496	-0.565676
C	-1.933590	-3.479625	-1.481888
C	-1.344495	-2.231601	-1.326657
La	-0.000060	0.661214	0.000024
H	-3.937663	2.160456	0.796728
H	-4.622555	0.553621	0.573650
H	-4.112453	1.778727	-1.531229
H	-3.262757	0.210303	-1.464732
H	3.262758	0.210834	1.464717
H	4.112089	1.779447	1.531415
H	3.937181	2.161449	-0.796489
H	4.622464	0.554750	-0.573632
H	-3.898520	-0.950281	2.076194
H	-2.181073	-1.073537	2.515702
H	3.898767	-0.949152	-2.076333
H	2.181352	-1.072748	-2.515862
H	1.622732	-4.111539	2.313241
H	3.411032	-4.826569	0.657148
H	4.039123	-3.255484	-1.184665
H	-4.038322	-3.256557	1.184274
H	-3.409866	-4.827282	-0.657721
H	-1.621752	-4.111633	-2.313749
N	-1.659445	-1.418738	-0.310079
N	1.659785	-1.418411	0.309872
C	0.307219	-1.694224	2.308980
O	0.071130	-0.435704	2.167579
O	-0.223705	-2.451005	3.097952
C	-0.306818	-1.694003	-2.309222
O	-0.071018	-0.435444	-2.167673
O	0.224279	-2.450568	-3.098284
H	0.474015	1.524502	3.316983
H	0.351207	3.299773	3.613403
H	2.655668	2.557145	3.012876
H	1.998508	3.780327	1.882727
H	-0.474345	1.524819	-3.316823
H	-0.351919	3.300153	-3.613023

H	-1.999294	3.780142	-1.882259
H	-2.656216	2.556975	-3.012562
H	2.308981	3.302899	-1.460407
H	1.817740	3.384488	-3.163100
H	3.408138	1.598632	-3.064531
H	1.805062	0.844831	-3.230482
H	-1.818467	3.383705	3.163463
H	-2.309677	3.302200	1.460756
H	-3.408465	1.597507	3.064689
H	-1.805225	0.844038	3.230549

MacropaLuΔ_δδδ_δδδ_opt.log

SCF (RwB97XD) = -1870.28497173
 E(SCF)+ZPE(0 K)= -1869.674292
 H(298 K)= -1869.639441
 G(298 K)= -1869.736259
 Lowest Frequency = 36.4536cm-1

73

C	3.627013	-0.782489	-0.401162
N	2.854984	-0.504974	0.806623
O	1.711033	-1.615643	-1.530065
C	3.047441	-1.935852	-1.185747
C	3.107820	-1.496244	1.853620
C	1.832360	-2.045088	2.452083
O	0.990626	-2.478435	1.371433
C	0.054351	-3.478900	1.724014
C	-1.154123	-2.866694	2.388602
O	-1.680886	-1.904882	1.493283
O	-0.933297	-2.506155	-1.464281
C	0.091328	-3.256691	-2.097034
C	1.163341	-2.332691	-2.625401
N	-2.835003	-0.556057	-0.607922
C	-3.158934	-1.644339	-1.530556
C	-1.975147	-2.090251	-2.354884
C	-3.094413	-1.856564	1.484268
C	-3.559716	-0.678590	0.656984
C	3.038759	0.868477	1.266325
C	-3.057653	0.763986	-1.204041
C	-2.441208	1.840092	-0.341803
C	2.446757	1.853794	0.286177
C	-0.933287	2.262081	1.371043
C	-1.317737	3.591897	1.467133
C	-2.294208	4.049579	0.582262
C	-2.884404	3.161724	-0.315368
C	2.923882	3.158768	0.156933
C	2.360027	3.993536	-0.803785
C	1.367442	3.495371	-1.646436
C	0.949478	2.186629	-1.452798
Lu	-0.015566	-0.559379	0.017692
H	0.523143	-4.235905	2.373509
H	-0.255361	-3.965252	0.787684
H	-0.899275	-2.379574	3.344661
H	-1.895107	-3.658022	2.588586
H	-0.331010	-3.880169	-2.901524
H	0.518154	-3.925870	-1.334087

H	1.945243	-2.906455	-3.145736
H	0.739193	-1.595330	-3.322252
H	4.110003	1.109168	1.415334
H	2.536461	0.995139	2.237311
H	-4.138445	0.971291	-1.330268
H	-2.593356	0.796235	-2.200580
H	-0.857713	4.226296	2.225096
H	-2.620140	5.091266	0.611815
H	-3.684638	3.484683	-0.982794
H	3.731757	3.508433	0.801458
H	2.713873	5.020785	-0.911961
H	0.915408	4.081707	-2.446701
N	1.449183	1.411465	-0.483081
N	-1.451240	1.439525	0.455730
C	0.087002	1.605906	2.289551
O	0.261006	0.353611	2.026644
O	0.661584	2.257773	3.136574
C	-0.103830	1.524312	-2.328767
O	-0.330177	0.295754	-2.004465
O	-0.656793	2.153373	-3.206803
H	4.691336	-0.991650	-0.175412
H	3.642522	-2.078042	-2.102239
H	3.070736	-2.880116	-0.612989
H	-4.653269	-0.767070	0.501372
H	-3.390801	0.235657	1.238495
H	-3.478013	-1.740206	2.512078
H	-3.480407	-2.816219	1.095043
H	-1.605364	-1.277873	-2.997510
H	-2.275481	-2.948809	-2.977574
H	-3.508247	-2.509760	-0.951718
H	-3.985604	-1.368730	-2.211310
H	2.067220	-2.911342	3.091347
H	1.307199	-1.276760	3.035707
H	3.731579	-1.081177	2.664393
H	3.679081	-2.333710	1.426853
H	3.603013	0.103589	-1.049219

MacropaLuΔ_δδλ_δδλ_opt.log

SCF (RwB97XD) = -1870.28291903
 E(SCF)+ZPE(0 K)= -1869.672440
 H(298 K)= -1869.637477
 G(298 K)= -1869.734813
 Lowest Frequency = 30.6315cm⁻¹

73

C	3.541809	1.028165	-0.216662
N	2.624816	0.855470	0.909629
O	2.531224	-0.915063	-1.190393
C	3.751141	-0.212642	-1.062361
C	3.144615	0.058207	2.016859
C	3.081519	-1.444786	1.795859
O	1.751794	-1.846456	1.495926
C	1.175797	-2.879744	2.281033
C	-0.233099	-2.460656	2.633192
O	-0.945134	-2.146962	1.448346
O	0.494116	-2.722217	-1.185194

C	1.828364	-3.156238	-1.394747
C	2.599204	-2.038454	-2.051597
N	-2.090716	-1.700722	-1.082325
C	-1.635596	-2.404110	-2.276421
C	-0.476664	-3.344036	-2.023594
C	-1.745422	-3.179126	0.907740
C	-2.719565	-2.553450	-0.072946
C	2.187406	2.179219	1.372285
C	-2.987137	-0.607934	-1.468447
C	-3.059407	0.455187	-0.402711
C	1.266134	2.814577	0.359428
C	-2.005652	1.461059	1.397133
C	-3.068606	2.325212	1.616848
C	-4.170364	2.235207	0.767965
C	-4.177819	1.274468	-0.238733
C	1.083039	4.192194	0.241040
C	0.252515	4.675096	-0.767935
C	-0.333295	3.782638	-1.665782
C	-0.093694	2.428711	-1.479312
Lu	0.252705	-0.453512	0.001550
H	2.518305	0.281265	2.890810
H	4.189330	0.331057	2.269664
H	3.418300	-1.938019	2.720355
H	3.743796	-1.789182	0.989227
H	1.756872	-3.034165	3.203236
H	1.186521	-3.822601	1.705986
H	-0.206651	-1.539140	3.228844
H	-0.747874	-3.253546	3.198233
H	1.851898	-4.066851	-2.011760
H	2.268944	-3.391475	-0.414922
H	3.646388	-2.348217	-2.201462
H	2.163130	-1.774864	-3.029346
H	-1.300961	-1.633117	-2.980787
H	-2.451449	-2.985564	-2.751572
H	-0.791295	-4.294232	-1.558712
H	-0.026819	-3.590218	-2.998506
H	3.049073	2.849670	1.555357
H	1.644408	2.072024	2.321795
H	-4.005941	-0.977978	-1.692006
H	-2.609395	-0.143594	-2.391991
H	-3.012028	3.029621	2.447065
H	-5.030511	2.893791	0.904206
H	-5.040808	1.154327	-0.895588
H	1.590293	4.872391	0.926862
H	0.087449	5.749494	-0.871191
H	-0.953889	4.102817	-2.503046
N	0.643966	1.971313	-0.463929
N	-1.991716	0.582372	0.387004
C	-0.786241	1.422640	2.305070
O	0.022982	0.460500	2.023709
O	-0.643210	2.259890	3.173501
C	-0.614870	1.343102	-2.409498
O	-0.190971	0.167463	-2.091505
O	-1.373866	1.624231	-3.315440
H	3.117697	1.804808	-0.865267
H	4.532900	1.394821	0.117403
H	4.119551	0.094986	-2.055649

H	4.513639	-0.883256	-0.626981
H	-3.333385	-3.351108	-0.535480
H	-3.402487	-1.927178	0.518421
H	-2.324463	-3.660001	1.713834
H	-1.109136	-3.952322	0.448530

MacropaLuΔ_{δλδ}_δλδ_opt.log

SCF (RwB97XD) = -1870.28136799
 E(SCF)+ZPE(0 K)= -1869.670420
 H(298 K)= -1869.635350
 G(298 K)= -1869.733738
 Lowest Frequency = 15.8167cm⁻¹

73

C	3.516896	-0.736272	-0.691439
N	2.889332	-0.476694	0.599706
O	1.599352	-2.048881	-1.306442
C	3.018969	-2.022945	-1.307490
C	3.302227	-1.447888	1.613150
C	2.174918	-1.845108	2.530222
O	1.102114	-2.356713	1.743074
C	0.165840	-3.034400	2.548542
C	-1.052381	-3.319340	1.720358
O	-1.582553	-2.083381	1.266141
O	-1.105046	-2.349679	-1.753199
C	-0.161732	-2.933299	-2.621623
C	1.077225	-3.255135	-1.840870
N	-2.891619	-0.486054	-0.545427
C	-3.316849	-1.488050	-1.521693
C	-2.221563	-1.855671	-2.487529
C	-2.994086	-1.995239	1.393809
C	-3.490317	-0.710414	0.766456
C	3.118589	0.891503	1.056666
C	-3.133033	0.868121	-1.038407
C	-2.449861	1.896657	-0.174570
C	2.444693	1.896725	0.158656
C	-0.838273	2.258116	1.448765
C	-1.196345	3.589148	1.600630
C	-2.219964	4.082281	0.791138
C	-2.874332	3.222978	-0.087359
C	2.872627	3.220641	0.050853
C	2.225975	4.067079	-0.845148
C	1.203262	3.563426	-1.648866
C	0.841103	2.235910	-1.477442
Lu	-0.003389	-0.570104	0.000897
H	4.201184	1.123142	1.109872
H	2.710963	1.004595	2.073361
H	-4.216938	1.094769	-1.084207
H	-2.737105	0.954347	-2.062308
H	-0.680105	4.196844	2.344129
H	-2.529699	5.126570	0.866390
H	-3.710122	3.569666	-0.696846
H	3.705028	3.575426	0.660345
H	2.538907	5.109146	-0.936256
H	0.688518	4.160450	-2.401977
N	1.418745	1.447427	-0.564054

N	-1.419588	1.459204	0.548037
C	0.224324	1.571796	2.289367
O	0.356018	0.323008	1.994125
O	0.865074	2.196010	3.110063
C	-0.231171	1.549565	-2.306082
O	-0.374950	0.306106	-1.995764
O	-0.869388	2.170750	-3.130918
H	4.622206	-0.788432	-0.621261
H	3.385203	-2.090852	-2.345942
H	3.390517	-2.909553	-0.765989
H	-4.597651	-0.747498	0.726454
H	-3.218465	0.126946	1.421338
H	-3.270846	-2.010429	2.461538
H	-3.447974	-2.882326	0.920837
H	-1.894382	-0.990420	-3.084127
H	-2.588972	-2.647528	-3.162964
H	-3.623340	-2.400983	-0.995635
H	-4.201418	-1.148001	-2.091794
H	2.530933	-2.634575	3.214178
H	1.803957	-0.991088	3.116546
H	4.142772	-1.065111	2.220703
H	3.672151	-2.354814	1.117845
H	0.870760	-3.962218	-1.017798
H	1.811114	-3.722279	-2.515816
H	0.088607	-2.224906	-3.430772
H	-0.570942	-3.855618	-3.071980
H	3.275253	0.090490	-1.371672
H	-1.791801	-3.853174	2.336208
H	-0.813434	-3.951192	0.847179
H	0.594867	-3.978341	2.930515
H	-0.116317	-2.401569	3.408351

MacropaLuΔ_δλλ_δλλ_opt.log

SCF (RwB97XD) = -1870.28676273
 E(SCF)+ZPE(0 K)= -1869.675879
 H(298 K)= -1869.641074
 G(298 K)= -1869.737583
 Lowest Frequency = 37.4453cm⁻¹

73

C	-3.647318	-0.672637	0.278217
N	-2.761806	-0.468459	-0.867040
O	-1.857133	-1.829573	1.374330
C	-3.257306	-1.821763	1.183629
C	-2.900079	-1.463455	-1.925173
C	-2.146847	-2.752232	-1.635026
O	-0.755635	-2.528975	-1.451547
C	0.016618	-2.631155	-2.642199
C	1.446000	-2.864038	-2.244110
O	1.857755	-1.828598	-1.374674
O	0.756500	-2.529080	1.451020
C	-0.015732	-2.631880	2.641629
C	-1.445036	-2.865124	2.243470
N	2.761981	-0.467740	0.867026
C	2.900564	-1.462932	1.924933
C	2.147789	-2.751901	1.634463

C	3.257923	-1.820397	-1.183956
C	3.647571	-0.671365	-0.278266
C	-2.938827	0.896182	-1.369715
C	2.938528	0.896848	1.370011
C	2.368500	1.892881	0.388109
C	-2.369083	1.892192	-0.387627
C	0.965444	2.189850	-1.433407
C	1.338532	3.517933	-1.583867
C	2.254217	4.043470	-0.672814
C	2.796188	3.218190	0.309585
C	-2.797161	3.217360	-0.308841
C	-2.255431	4.042604	0.673720
C	-1.339600	3.517152	1.584676
C	-0.966116	2.189212	1.433950
Lu	0.000109	-0.584643	-0.000030
H	-4.005988	1.131340	-1.547739
H	-2.416762	1.003439	-2.331123
H	4.005603	1.132321	1.548136
H	2.416376	1.003718	2.331417
H	0.914225	4.098007	-2.403659
H	2.568955	5.086514	-0.745029
H	3.548630	3.590700	1.006344
H	-3.549712	3.589786	-1.005527
H	-2.570475	5.085541	0.746140
H	-0.915474	4.097186	2.404590
N	-1.437512	1.424199	0.444717
N	1.437073	1.424777	-0.444333
C	-0.003062	1.487657	-2.372932
O	-0.214461	0.256617	-2.052044
O	-0.517565	2.097898	-3.288089
C	0.002581	1.487107	2.373348
O	0.214389	0.256213	2.052171
O	0.516851	2.097294	3.288671
H	-4.698440	-0.818571	-0.041083
H	-3.763092	-1.692135	2.156227
H	-3.584072	-2.799039	0.786551
H	4.698736	-0.817046	0.041009
H	3.623353	0.244709	-0.881605
H	3.763677	-1.690376	-2.156518
H	3.584994	-2.797667	-0.787115
H	-1.555312	-3.839318	1.732101
H	-2.072623	-2.873971	3.150928
H	0.080847	-1.703768	3.226154
H	0.330086	-3.491282	3.238058
H	-3.623384	0.243300	0.881773
H	2.073590	-2.872417	-3.151571
H	1.556600	-3.838340	-1.733020
H	-0.328916	-3.490496	-3.238881
H	-0.080274	-1.702892	-3.226436
H	-3.961875	-1.709900	-2.128410
H	-2.484487	-1.027169	-2.843883
H	-2.298317	-3.455395	-2.469216
H	-2.500056	-3.254142	-0.728892
H	2.501186	-3.253475	0.728216
H	2.299489	-3.455207	2.468490
H	2.484791	-1.027002	2.843730
H	3.962438	-1.709060	2.128145

MacropaLuΔ_δλλ_λδλ_opt.log

SCF (RwB97XD) = -1870.28346304
E(SCF)+ZPE(0 K)= -1869.672200
H(298 K)= -1869.637390
G(298 K)= -1869.733918
Lowest Frequency = 39.2156cm⁻¹

73

Lu	0.921946	3.984196	9.233439
N	3.057879	2.678749	9.289645
C	3.137795	1.356545	9.449031
C	4.307069	0.763843	9.925505
H	4.352316	-0.317126	10.065746
C	5.405791	1.572044	10.206392
H	6.327009	1.128134	10.589140
C	5.332440	2.942503	9.959047
C	4.130541	3.451545	9.488924
C	3.923738	4.921314	9.157196
O	2.731495	5.179875	8.740037
H	6.171719	3.621243	10.112156
N	1.952537	4.393440	11.523286
C	2.581549	5.507395	11.895755
C	3.483200	5.501085	12.960739
H	3.999361	6.419659	13.243906
C	3.701694	4.311403	13.650139
H	4.410995	4.282312	14.479734
C	2.980424	3.170869	13.297005
C	2.103115	3.267059	12.227041
C	1.226355	2.119930	11.757448
O	0.466322	2.450603	10.769345
H	3.070115	2.222010	13.826370
C	1.919139	0.564068	9.043792
H	2.241239	-0.420534	8.650628
H	1.305238	0.373633	9.937069
N	1.129199	1.297443	8.055718
C	1.855290	1.424270	6.794876
H	1.877145	0.470030	6.231782
H	2.896506	1.693770	7.012612
C	1.269885	2.497863	5.911336
H	1.932842	2.643676	5.041233
H	0.273058	2.226501	5.519812
O	1.168814	3.707963	6.637503
C	0.813693	4.787096	5.797472
H	-0.219528	4.644550	5.431231
H	1.489628	4.828953	4.926174
C	0.931040	6.067339	6.569177
H	1.973856	6.250485	6.871174
H	0.569607	6.895347	5.938341
O	0.113204	5.947036	7.726690
C	-0.221050	7.190773	8.325302
H	-1.244401	7.096253	8.700522
H	-0.242943	7.974919	7.552083
C	0.769179	7.598425	9.403933
H	1.750875	7.723683	8.927175
H	0.468657	8.588890	9.802615

N	0.931091	6.608896	10.463730
C	2.233423	6.751282	11.118264
H	2.255595	7.625068	11.798287
H	3.007348	6.912820	10.353758
C	-0.126781	6.606576	11.471247
H	-0.281534	7.613587	11.908172
H	0.197284	5.950494	12.288720
C	-1.462269	6.097692	10.964590
H	-2.077508	5.775521	11.821653
H	-2.025476	6.889042	10.442167
O	-1.259813	5.004202	10.084939
C	-2.439111	4.580883	9.417557
H	-2.449085	5.004320	8.397454
H	-3.332737	4.936261	9.953157
C	-2.458410	3.081638	9.385163
H	-2.441059	2.692152	10.418024
H	-3.381170	2.731316	8.889296
O	-1.322798	2.616871	8.687147
C	-1.221787	1.198774	8.812523
H	-2.195829	0.746039	8.560083
H	-0.966872	0.957989	9.855659
C	-0.183822	0.689870	7.848844
H	-0.136409	-0.413286	7.920144
H	-0.526414	0.920500	6.831550
O	1.306152	1.025270	12.276476
O	4.822357	5.719953	9.328484

MacropaLuΔ_λδδ_λδδ_opt.log

SCF (RwB97XD) = -1870.28214670
 E(SCF)+ZPE(0 K)= -1869.671664
 H(298 K)= -1869.636835
 G(298 K)= -1869.733106
 Lowest Frequency = 38.1730cm⁻¹

73

C	3.718138	0.695911	0.443107
N	2.876414	0.574705	-0.757266
O	1.814861	1.774448	1.401363
C	2.921674	0.947890	1.719611
C	3.075603	1.686038	-1.686852
C	1.820362	2.097131	-2.418269
O	0.843674	2.492586	-1.444958
C	-0.176150	3.344772	-1.940458
C	-1.324271	2.534037	-2.485893
O	-1.815396	1.774074	-1.401150
O	-0.844424	2.492151	1.445248
C	0.175140	3.344584	1.940860
C	1.323505	2.534129	2.486199
N	-2.876549	0.573695	0.757314
C	-3.076102	1.684875	1.687006
C	-1.821009	2.096288	2.418497
C	-2.921932	0.947192	-1.719516
C	-3.718310	0.694752	-0.443049
C	2.996070	-0.739733	-1.383958
C	-2.995804	-0.740847	1.383868
C	-2.435991	-1.797128	0.460088

C	2.436600	-1.796291	-0.460287
C	-1.004784	-2.200414	-1.322757
C	-1.403424	-3.524743	-1.426360
C	-2.348509	-3.991273	-0.511902
C	-2.890767	-3.115838	0.425769
C	2.891818	-3.114853	-0.426104
C	2.349845	-3.990569	0.511469
C	1.404596	-3.524452	1.425967
C	1.005514	-2.200245	1.322503
Lu	-0.000088	0.614141	0.000037
H	4.436557	1.517135	0.302364
H	4.323680	-0.212093	0.590180
H	3.564552	1.457385	2.455832
H	2.553684	0.017608	2.177314
H	0.228649	4.023480	-2.707019
H	-0.527471	3.948693	-1.090494
H	-0.992520	1.864435	-3.298601
H	-2.112233	3.203613	-2.871968
H	-0.229869	4.023075	2.707502
H	0.526282	3.948713	1.090970
H	2.111263	3.203899	2.872354
H	0.991957	1.864330	3.298827
H	-2.553629	0.017103	-2.177359
H	-3.564983	1.456581	-2.455660
H	-4.437042	1.515685	-0.302200
H	-4.323508	-0.213461	-0.590247
H	4.047708	-0.985172	-1.629841
H	2.426774	-0.754993	-2.325294
H	-4.047371	-0.986640	1.629704
H	-2.426524	-0.756034	2.325213
H	-0.978462	-4.148540	-2.213060
H	-2.685413	-5.029251	-0.547953
H	-3.663243	-3.444881	1.122259
H	3.664411	-3.443563	-1.122621
H	2.687097	-5.028438	0.547413
H	0.979837	-4.148475	2.212598
N	1.479745	-1.386293	0.373474
N	-1.479280	-1.386723	-0.373638
C	-0.019963	-1.543510	-2.280629
O	0.159347	-0.287426	-2.030669
O	0.520699	-2.194510	-3.149135
C	0.020474	-1.543775	2.280447
O	-0.159244	-0.287720	2.030636
O	-0.519979	-2.195054	3.148873
H	-2.052877	2.961953	3.059522
H	-1.413414	1.280355	3.033311
H	-3.864079	1.463531	2.432766
H	-3.413152	2.555381	1.108942
H	2.051942	2.962935	-3.059211
H	1.413011	1.281131	-3.033157
H	3.412402	2.556591	-1.108713
H	3.863626	1.465008	-2.432656

MacropaLuΔ_λδλ_λδλ_opt.log

SCF (RwB97XD) = -1870.29245718
E(SCF)+ZPE(0 K)= -1869.681866

H(298 K)= -1869.647122
 G(298 K)= -1869.743498
 Lowest Frequency = 35.3387cm⁻¹

73

C	3.690800	0.914394	-0.247602
N	2.660432	0.532893	-1.222311
O	1.952936	1.808312	1.098980
C	3.161426	1.068259	1.169590
C	2.543663	1.479541	-2.327949
C	1.936823	2.794637	-1.884546
O	0.613689	2.578448	-1.403260
C	-0.426184	3.373727	-1.945597
C	-1.588143	2.477949	-2.290054
O	-1.953549	1.807842	-1.098555
O	-0.614598	2.577804	1.403912
C	0.424958	3.373383	1.946415
C	1.587286	2.477995	2.290642
N	-2.660555	0.531520	1.222400
C	-2.544151	1.477913	2.328293
C	-1.937818	2.793362	1.885243
C	-3.161748	1.067335	-1.169360
C	-3.691064	0.912890	0.247789
C	2.811219	-0.842780	-1.687983
C	-2.810809	-0.844340	1.687688
C	-2.397525	-1.824763	0.618467
C	2.398326	-1.823664	-0.619036
C	-1.155874	-2.152022	-1.311373
C	-1.600243	-3.458240	-1.452374
C	-2.477344	-3.955358	-0.488384
C	-2.901321	-3.124691	0.544720
C	2.902640	-3.123412	-0.545656
C	2.478989	-3.954540	0.487211
C	1.601689	-3.458042	1.451340
C	1.156803	-2.151960	1.310709
Lu	-0.000069	0.620203	0.000058
H	4.143615	1.870378	-0.552212
H	4.513969	0.180247	-0.236058
H	3.898196	1.620579	1.776063
H	2.971518	0.101060	1.658672
H	1.877334	1.031504	-3.077294
H	3.520992	1.683047	-2.810053
H	1.909550	3.485259	-2.740507
H	2.522669	3.272428	-1.083673
H	-0.082830	3.892034	-2.853477
H	-0.729916	4.130636	-1.202786
H	-1.299393	1.741287	-3.058349
H	-2.431489	3.087637	-2.656729
H	0.081408	3.891337	2.854423
H	0.728369	4.130589	1.203776
H	2.430394	3.087937	2.657440
H	1.298852	1.741041	3.058775
H	-1.877646	1.029937	3.077517
H	-3.521557	1.680913	2.810454
H	-2.523842	3.271137	1.084491
H	-1.910815	3.483766	2.741389
H	-2.971464	0.100339	-1.658696

H	-3.898735	1.619527	-1.775687
H	-4.144242	1.868620	0.552654
H	-4.513955	0.178434	0.236047
H	3.849943	-1.059683	-2.003025
H	2.169127	-1.001769	-2.567388
H	-3.849451	-1.061738	2.002657
H	-2.168668	-1.003324	2.567056
H	-1.263744	-4.042441	-2.309184
H	-2.851578	-4.978840	-0.556530
H	-3.618263	-3.473611	1.289504
H	3.619721	-3.471837	-1.290537
H	2.853628	-4.977893	0.555069
H	1.265421	-4.042620	2.307984
N	1.514230	-1.381563	0.276180
N	-1.513607	-1.382059	-0.276627
C	-0.254069	-1.471326	-2.330851
O	-0.045372	-0.225827	-2.068289
O	0.206998	-2.107366	-3.257082
C	0.254734	-1.471899	2.330376
O	0.045569	-0.226407	2.068161
O	-0.206093	-2.108375	3.256426

MacropaLuΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1870.27650515
 E(SCF)+ZPE(0 K)= -1869.666676
 H(298 K)= -1869.631563
 G(298 K)= -1869.728969
 Lowest Frequency = 39.4027cm⁻¹

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C	-3.585944	-0.671509	0.718957
N	-2.890821	-0.519569	-0.566123
O	-1.674718	-2.047398	1.141688
C	-2.661563	-1.251323	1.794640
C	-3.213243	-1.622345	-1.469203
C	-2.124145	-1.936975	-2.461950
O	-0.961414	-2.364214	-1.760023
C	0.015583	-2.880732	-2.638654
C	1.227334	-3.205638	-1.805992
O	1.680649	-2.041031	-1.142907
O	0.968431	-2.362287	1.758758
C	-0.006915	-2.882826	2.636830
C	-1.217508	-3.211056	1.803782
N	2.892359	-0.510957	0.566281
C	3.218000	-1.613120	1.468915
C	2.129618	-1.931677	2.461204
C	2.664910	-1.241096	-1.795086
C	3.587903	-0.660141	-0.718881
C	-3.090810	0.797887	-1.159910
C	3.088076	0.806840	1.160644
C	2.438371	1.853249	0.287184
C	-2.444363	1.845942	-0.286002
C	0.893932	2.219612	-1.403679
C	1.245698	3.555669	-1.524438
C	2.227350	4.047693	-0.663193
C	2.849724	3.185541	0.236169

C	-2.859862	3.176910	-0.234200
C	-2.240107	4.040476	0.665625
C	-1.256890	3.551030	1.526552
C	-0.900990	2.216136	1.405019
Lu	0.000601	-0.615619	-0.000107
H	-4.475851	-1.310293	0.594082
H	-3.956459	0.300058	1.073623
H	-3.229312	-1.874736	2.501954
H	-2.154780	-0.455601	2.361548
H	2.155537	-0.446014	-2.360565
H	3.234239	-1.861775	-2.503532
H	4.479236	-1.297030	-0.594544
H	3.956252	0.312577	-1.072689
H	-4.163964	1.038329	-1.293047
H	-2.622923	0.829959	-2.155766
H	4.160445	1.050674	1.293975
H	2.620039	0.837030	2.156487
H	0.756999	4.169174	-2.281658
H	2.529597	5.095761	-0.712435
H	3.651224	3.534729	0.888693
H	-3.662497	3.523983	-0.886458
H	-2.545618	5.087568	0.715480
H	-0.770090	4.165632	2.284105
N	-1.451361	1.411722	0.490461
N	1.446772	1.416350	-0.489578
C	-0.132289	1.534305	-2.292358
O	-0.264643	0.277263	-2.020147
O	-0.745100	2.163157	-3.129065
C	0.127281	1.533392	2.293298
O	0.263290	0.276879	2.020444
O	0.738292	2.163615	3.130293
H	2.477744	-2.749895	3.114824
H	1.864351	-1.063135	3.084463
H	4.158241	-1.420061	2.022318
H	3.380148	-2.512372	0.859641
H	-2.469845	-2.755978	-3.115875
H	-1.861821	-1.067295	-3.084869
H	-3.372360	-2.522383	-0.860290
H	-4.154258	-1.431975	-2.022214
H	0.260435	-2.127542	-3.409047
H	-0.359283	-3.789753	-3.141695
H	2.029666	-3.638742	-2.423080
H	0.966400	-3.929780	-1.019142
H	-0.254358	-2.131165	3.407892
H	0.370917	-3.791043	3.139109
H	-0.954075	-3.933604	1.016301
H	-2.018424	-3.647412	2.420418

MacropaLuΔ_λλλ_λλλ_opt.log

SCF (RwB97XD) = -1870.28844292
E(SCF)+ZPE(0 K)= -1869.677825
H(298 K)= -1869.643119
G(298 K)= -1869.739329
Lowest Frequency = 34.4722cm⁻¹

C	-3.707552	0.893215	0.403331
N	-2.655667	0.495298	1.344155
O	-1.957738	1.770502	-0.974696
C	-3.198906	1.075923	-1.020897
C	-2.496040	1.432609	2.450707
C	-1.887789	2.741167	1.981510
O	-0.551416	2.575170	1.517960
C	0.439139	2.751425	2.521734
C	1.767146	2.888579	1.824448
O	1.957387	1.770886	0.974759
O	0.550892	2.575356	-1.517868
C	-0.439704	2.751430	-2.521634
C	-1.767739	2.888270	-1.824340
N	2.655590	0.495932	-1.344141
C	2.495762	1.433249	-2.450658
C	1.887227	2.741659	-1.981418
C	3.198701	1.076566	1.020934
C	3.707389	0.894037	-0.403301
C	-2.775569	-0.888806	1.782990
C	2.775794	-0.888129	-1.783032
C	2.381875	-1.847123	-0.685903
C	-2.381437	-1.847670	0.685822
C	1.195316	-2.154571	1.280936
C	1.634985	-3.462948	1.417112
C	2.479866	-3.972721	0.431790
C	2.877662	-3.150739	-0.617981
C	-2.876928	-3.151396	0.617853
C	-2.478950	-3.973248	-0.431950
C	-1.634189	-3.463247	-1.417257
C	-1.194813	-2.154776	-1.281032
Lu	-0.000048	0.617363	0.000004
H	-4.161439	1.838348	0.739784
H	-4.527105	0.154494	0.390200
H	-3.930355	1.653820	-1.605414
H	-3.037804	0.114529	-1.527494
H	3.037798	0.115110	1.527478
H	3.930025	1.654588	1.605485
H	4.161069	1.839285	-0.739710
H	4.527104	0.155495	-0.390204
H	-3.801414	-1.129058	2.123229
H	-2.106894	-1.057539	2.640764
H	3.801692	-1.128142	-2.123284
H	2.107155	-1.056971	-2.640813
H	1.318424	-4.038748	2.287080
H	2.848735	-4.998449	0.495064
H	3.569228	-3.509043	-1.382131
H	-3.568410	-3.509886	1.381993
H	-2.847586	-4.999057	-0.495261
H	-1.317503	-4.038941	-2.287249
N	-1.527762	-1.390505	-0.232644
N	1.528096	-1.390185	0.232578
C	0.322002	-1.473427	2.324645
O	0.088368	-0.233791	2.058933
O	-0.098539	-2.105157	3.273004
C	-0.321655	-1.473398	-2.324719
O	-0.088283	-0.233723	-2.058959
O	0.099016	-2.104999	-3.273107

H	0.442792	1.880875	3.197552
H	0.233302	3.670154	3.095367
H	2.568462	2.948218	2.575797
H	1.786329	3.805799	1.212037
H	-0.443171	1.880902	-3.197482
H	-0.234069	3.670223	-3.095235
H	-1.787121	3.805462	-1.211894
H	-2.569068	2.947764	-2.575688
H	2.452584	3.167984	-1.141520
H	1.899646	3.480352	-2.797992
H	3.456398	1.649040	-2.960396
H	1.823480	0.971131	-3.186158
H	-1.900375	3.479835	2.798103
H	-2.453236	3.167389	1.141621
H	-3.456723	1.648175	2.960452
H	-1.823660	0.970611	3.186191

Macropa2-_ligand_opt.log

SCF (RwB97XD) = -1830.14717483
 E(SCF)+ZPE(0 K)= -1829.546180
 H(298 K)= -1829.510704
 G(298 K)= -1829.612072
 Lowest Frequency = 19.9838cm⁻¹

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N	3.841451	3.130788	8.905548
C	3.798678	1.905070	8.379525
C	4.819492	1.401542	7.573866
H	4.754430	0.384789	7.177028
C	5.896167	2.234142	7.263685
H	6.709847	1.874582	6.625622
C	5.891303	3.532702	7.745648
C	4.841371	3.947075	8.582607
C	4.800235	5.426253	9.053586
O	4.201347	5.663645	10.114790
H	6.657167	4.265813	7.489989
N	-0.040372	4.917020	12.921994
C	1.048258	5.001695	12.150792
C	2.020104	3.996570	12.092458
H	2.856938	4.101191	11.393447
C	1.877334	2.912886	12.958173
H	2.627833	2.115508	12.965158
C	0.778017	2.860528	13.809243
C	-0.201503	3.860859	13.724223
C	-1.527077	3.689709	14.514668
O	-2.552419	4.102262	13.937193
H	0.619062	2.055780	14.528921
C	2.555514	1.086547	8.667854
H	2.742662	0.022669	8.379363
H	2.406954	1.107201	9.756132
N	1.377598	1.638200	8.041081
C	1.386236	1.743520	6.597230
H	0.521832	1.194008	6.174731
H	2.289791	1.270981	6.172625
C	1.354636	3.181767	6.094809
H	0.938820	3.221124	5.061767

H	0.690962	3.776380	6.745699
O	2.664660	3.669594	6.102415
C	2.829313	5.059808	6.078896
H	2.403701	5.497002	5.148672
H	3.916899	5.222440	6.083737
C	2.276399	5.824844	7.267351
H	2.400096	5.236281	8.191840
H	2.900318	6.731053	7.373204
O	0.915964	6.175552	7.087664
C	0.532600	7.320964	7.791770
H	-0.563768	7.390521	7.694560
H	0.956773	8.229364	7.306474
C	0.946258	7.386212	9.260873
H	2.045166	7.402775	9.320891
H	0.597172	8.387095	9.630093
N	0.481721	6.312119	10.098768
C	1.232638	6.268071	11.347261
H	0.961329	7.122261	12.010004
H	2.297518	6.348997	11.083614
C	-0.962508	6.235469	10.229080
H	-1.431567	7.220418	10.003653
H	-1.222434	5.996404	11.273395
C	-1.579751	5.171284	9.324101
H	-2.665554	5.374389	9.196168
H	-1.102014	5.212684	8.333122
O	-1.387715	3.871768	9.803164
C	-2.344229	3.426311	10.732239
H	-3.314720	3.278482	10.208491
H	-2.494459	4.126748	11.576654
C	-1.875387	2.121307	11.349369
H	-1.092414	2.331351	12.090785
H	-2.718002	1.672984	11.897197
O	-1.408880	1.185004	10.404396
C	-0.049131	1.342549	10.071501
H	0.540883	0.562186	10.592788
H	0.340310	2.325308	10.379409
C	0.091406	1.235356	8.563078
H	-0.190465	0.201512	8.239404
H	-0.670966	1.918351	8.158441
O	-1.414688	3.105325	15.608813
O	5.356531	6.215239	8.260487

MacropaTbΔ_δδδ_δδδ_opt.log

SCF (RwB97XD) = -1866.81747521
 E(SCF)+ZPE(0 K)= -1866.207698
 H(298 K)= -1866.172621
 G(298 K)= -1866.270326
 Lowest Frequency = 29.1368cm⁻¹

73

C	3.564862	-0.712824	-0.639981
N	2.834997	-0.558373	0.620351
O	1.692855	-1.926114	-1.516274
C	3.106771	-1.906418	-1.450076
C	3.167472	-1.621592	1.573249
C	1.987754	-2.061222	2.408174

O	0.965770	-2.530469	1.521997
C	-0.049470	-3.295405	2.150492
C	-1.157618	-2.396800	2.651444
O	-1.703653	-1.699407	1.541966
O	-0.996840	-2.522393	-1.449205
C	-0.046902	-3.489251	-1.853368
C	1.167543	-2.834765	-2.468863
N	-2.841987	-0.532677	-0.779802
C	-3.118025	-1.519547	-1.830144
C	-1.860775	-2.040887	-2.488839
C	-3.051779	-1.982197	1.211480
C	-3.610198	-0.811739	0.434107
C	3.064489	0.774578	1.190390
C	-3.054142	0.840428	-1.242339
C	-2.479690	1.847938	-0.274176
C	2.462776	1.850400	0.317115
C	-0.971275	2.225595	1.449005
C	-1.394673	3.536966	1.613883
C	-2.398881	4.009001	0.769508
C	-2.965133	3.151953	-0.170403
C	2.911397	3.170599	0.301609
C	2.318576	4.069129	-0.583224
C	1.330557	3.625698	-1.462532
C	0.943342	2.295313	-1.381991
Tb	0.011507	-0.586622	-0.021145
H	0.374619	-3.895496	2.972114
H	-0.444610	-3.986677	1.390076
H	-0.768626	-1.645968	3.355547
H	-1.932991	-2.992089	3.157474
H	-0.501367	-4.209245	-2.553698
H	0.253653	-4.031249	-0.944153
H	1.909018	-3.612675	-2.713450
H	0.917153	-2.288633	-3.393566
H	4.146575	0.971660	1.321183
H	2.593324	0.826965	2.183398
H	-4.131085	1.053742	-1.390172
H	-2.555480	0.971920	-2.214803
H	-0.937231	4.146293	2.393662
H	-2.757654	5.036445	0.858042
H	-3.776599	3.485413	-0.818933
H	3.713619	3.485465	0.970495
H	2.647423	5.110127	-0.603754
H	0.861530	4.272218	-2.204579
N	1.471696	1.459894	-0.483472
N	-1.479163	1.428363	0.502165
C	0.099050	1.591058	2.329665
O	0.313475	0.348796	2.054596
O	0.674239	2.258203	3.165006
C	-0.099826	1.665844	-2.297814
O	-0.268969	0.405165	-2.077700
O	-0.696448	2.350712	-3.103283
H	4.657090	-0.800251	-0.474674
H	3.533012	-1.822151	-2.463850
H	3.456967	-2.862804	-1.021652
H	-4.678618	-1.000550	0.210533
H	-3.567218	0.069416	1.087647
H	-3.643338	-2.108590	2.132593

H	-3.105017	-2.925762	0.639717
H	-1.349977	-1.246468	-3.051841
H	-2.115868	-2.876379	-3.160921
H	-3.653013	-2.373358	-1.389787
H	-3.783881	-1.105869	-2.607540
H	2.301364	-2.889402	3.064870
H	1.595797	-1.232230	3.016401
H	3.990063	-1.317583	2.246402
H	3.527311	-2.498054	1.017753
H	3.401860	0.188826	-1.242667

MacropaTbΔ_δδλ_δδλ_opt.log

SCF (RwB97XD) = -1866.81465787
 E(SCF)+ZPE(0 K)= -1866.204456
 H(298 K)= -1866.169495
 G(298 K)= -1866.266498
 Lowest Frequency = 31.4766cm⁻¹

73

C	3.551405	0.997552	-0.233346
N	2.627935	0.844066	0.893191
O	2.589395	-0.984271	-1.179386
C	3.797231	-0.262510	-1.040813
C	3.143934	0.059868	2.015932
C	3.081757	-1.449736	1.833535
O	1.752591	-1.857668	1.544879
C	1.172020	-2.881410	2.337598
C	-0.253931	-2.476658	2.643105
O	-0.942789	-2.183004	1.440021
O	0.503482	-2.720425	-1.269304
C	1.826446	-3.206555	-1.420675
C	2.678867	-2.117150	-2.025397
N	-2.084204	-1.699226	-1.099834
C	-1.634261	-2.374172	-2.315983
C	-0.480106	-3.329867	-2.098696
C	-1.718960	-3.216483	0.868838
C	-2.698342	-2.582118	-0.103770
C	2.214351	2.180914	1.350365
C	-3.004252	-0.614337	-1.464401
C	-3.106729	0.431740	-0.383349
C	1.312749	2.848712	0.340741
C	-2.061118	1.473293	1.404505
C	-3.145691	2.309734	1.629542
C	-4.255565	2.180328	0.796452
C	-4.247427	1.217066	-0.208402
C	1.158236	4.231490	0.244615
C	0.317419	4.744808	-0.740581
C	-0.312165	3.877512	-1.633395
C	-0.094086	2.515953	-1.475396
Tb	0.258385	-0.448419	-0.022560
H	2.515510	0.301927	2.883506
H	4.187670	0.338622	2.265730
H	3.418871	-1.915414	2.772547
H	3.744482	-1.816128	1.036821
H	1.727811	-3.003562	3.280533
H	1.214343	-3.838811	1.788096

H	-0.254605	-1.546367	3.226683
H	-0.772842	-3.268542	3.206253
H	1.844111	-4.108612	-2.050830
H	2.209298	-3.472922	-0.423750
H	3.722977	-2.465061	-2.095684
H	2.326470	-1.849537	-3.035632
H	-1.298599	-1.583941	-2.999331
H	-2.456643	-2.935494	-2.803510
H	-0.795676	-4.283640	-1.641122
H	-0.047001	-3.565115	-3.084276
H	3.091317	2.827033	1.547048
H	1.656615	2.080616	2.292522
H	-4.012272	-1.003986	-1.702338
H	-2.629537	-0.121959	-2.375032
H	-3.098402	3.024938	2.451082
H	-5.133038	2.813882	0.940855
H	-5.113356	1.073023	-0.856495
H	1.689998	4.891829	0.931246
H	0.172813	5.823736	-0.825799
H	-0.952422	4.222840	-2.445483
N	0.663454	2.031337	-0.487166
N	-2.038581	0.588550	0.400092
C	-0.826822	1.481866	2.297971
O	-0.014641	0.512274	2.052985
O	-0.679966	2.361894	3.122714
C	-0.675473	1.456871	-2.404388
O	-0.237645	0.270728	-2.151778
O	-1.492732	1.769405	-3.247572
H	3.116778	1.746124	-0.907893
H	4.532111	1.393071	0.098412
H	4.185838	0.025858	-2.032240
H	4.557120	-0.911893	-0.570171
H	-3.301341	-3.378073	-0.582873
H	-3.389743	-1.976445	0.499098
H	-2.295900	-3.728798	1.657100
H	-1.065421	-3.965895	0.394185

MacropaTbΔ_{δλδ}_δλδ_opt.log

SCF (RwB97XD) = -1866.81684073
 E(SCF)+ZPE(0 K)= -1866.206203
 H(298 K)= -1866.171150
 G(298 K)= -1866.269147
 Lowest Frequency = 22.4195cm⁻¹

73

C	3.521393	-0.765689	-0.732297
N	2.883710	-0.515232	0.558916
O	1.629068	-2.102359	-1.351129
C	3.046541	-2.055419	-1.364636
C	3.296484	-1.497469	1.563530
C	2.201814	-1.829285	2.543275
O	1.083515	-2.345423	1.825150
C	0.141805	-2.915126	2.707029
C	-1.090310	-3.282279	1.932180
O	-1.625957	-2.102541	1.354194
O	-1.079721	-2.349691	-1.822093

C	-0.137263	-2.920631	-2.702361
C	1.095145	-3.284264	-1.926300
N	-2.882788	-0.520317	-0.559174
C	-3.293854	-1.504128	-1.562969
C	-2.198191	-1.835864	-2.541640
C	-3.043539	-2.058610	1.366073
C	-3.520489	-0.770492	0.732078
C	3.136433	0.848187	1.029880
C	-3.137414	0.842258	-1.031553
C	-2.486091	1.874986	-0.147389
C	2.483247	1.879049	0.144912
C	-0.867407	2.275721	1.462155
C	-1.249247	3.601474	1.606013
C	-2.293551	4.068216	0.807735
C	-2.937111	3.192652	-0.062494
C	2.932150	3.197350	0.058651
C	2.287089	4.070998	-0.812396
C	1.243488	3.601760	-1.610138
C	0.863786	2.275550	-1.464890
Tb	0.000527	-0.604018	0.000273
H	4.223347	1.054918	1.089844
H	2.724272	0.958740	2.045093
H	-4.224619	1.047278	-1.092107
H	-2.725032	0.952416	-2.046733
H	-0.731876	4.226164	2.334509
H	-2.623146	5.106590	0.880568
H	-3.780649	3.521826	-0.670978
H	3.775234	3.528494	0.666696
H	2.615001	5.109827	-0.886315
H	0.725097	4.224865	-2.339267
N	1.445709	1.460331	-0.578499
N	-1.447982	1.458637	0.576587
C	0.231882	1.629535	2.291711
O	0.375555	0.373823	2.037471
O	0.889231	2.294643	3.066669
C	-0.234367	1.626575	-2.293748
O	-0.375888	0.370903	-2.038081
O	-0.892826	2.289671	-3.069490
H	4.626400	-0.803214	-0.652096
H	3.407746	-2.097068	-2.406335
H	3.440270	-2.944358	-0.842706
H	-4.625394	-0.810117	0.651497
H	-3.274397	0.059523	1.406950
H	-3.405766	-2.100033	2.407428
H	-3.434800	-2.948901	0.844586
H	-1.873165	-0.951539	-3.110765
H	-2.564434	-2.607771	-3.240217
H	-3.585931	-2.434257	-1.059329
H	-4.184340	-1.160536	-2.121646
H	2.569424	-2.599813	3.242661
H	1.876084	-0.944623	3.111473
H	4.186959	-1.152295	2.121259
H	3.589222	-2.427846	1.060744
H	0.872076	-4.013876	-1.127736
H	1.825953	-3.740468	-2.612195
H	0.125149	-2.191932	-3.489383
H	-0.557027	-3.823605	-3.180987

H	3.273534	0.063137	-1.407981
H	-1.820346	-3.737641	2.619468
H	-0.866522	-4.013686	1.135454
H	0.562671	-3.816366	3.187948
H	-0.121297	-2.184643	3.492165

MacropaTbΔ_{δλλ}Δ_{δλλ}_opt.log

SCF (RwB97XD) = -1866.81983104
 E(SCF)+ZPE(0 K)= -1866.209387
 H(298 K)= -1866.174486
 G(298 K)= -1866.271211
 Lowest Frequency = 32.2474cm⁻¹

73

C	-3.639276	-0.724642	0.263311
N	-2.748715	-0.476546	-0.872520
O	-1.862031	-1.880211	1.382063
C	-3.254965	-1.895728	1.144145
C	-2.885432	-1.431503	-1.971588
C	-2.159321	-2.746647	-1.734652
O	-0.766162	-2.564004	-1.526036
C	0.031046	-2.630766	-2.702328
C	1.451107	-2.891906	-2.282142
O	1.861628	-1.880917	-1.381840
O	0.765569	-2.564035	1.526373
C	-0.031680	-2.630418	2.702659
C	-1.451810	-2.891209	2.282487
N	2.748727	-0.477240	0.872582
C	2.885143	-1.432063	1.971803
C	2.158671	-2.747041	1.735051
C	3.254552	-1.896853	-1.143892
C	3.639231	-0.725780	-0.263198
C	-2.955363	0.899411	-1.342104
C	2.955789	0.898727	1.341959
C	2.406873	1.897284	0.351057
C	-2.406138	1.897949	-0.351355
C	0.982094	2.225573	-1.450160
C	1.368323	3.551102	-1.591823
C	2.308222	4.055770	-0.693481
C	2.852853	3.217053	0.275707
C	-2.851693	3.217874	-0.276217
C	-2.306801	4.056567	0.692845
C	-1.367072	3.551738	1.591275
C	-0.981266	2.226064	1.449821
Tb	-0.000002	-0.605690	0.000031
H	-4.028197	1.109729	-1.516399
H	-2.436910	1.038072	-2.301745
H	4.028685	1.108745	1.516227
H	2.437377	1.037689	2.301579
H	0.934206	4.145996	-2.395718
H	2.635636	5.095116	-0.762781
H	3.616725	3.576221	0.966995
H	-3.615442	3.577180	-0.967570
H	-2.633881	5.096030	0.761978
H	-0.932771	4.146620	2.395079
N	-1.463572	1.446468	0.476637

N	1.464156	1.445974	-0.476856
C	-0.017105	1.551523	-2.381950
O	-0.215395	0.308627	-2.103673
O	-0.565283	2.198033	-3.252454
C	0.017721	1.551840	2.381713
O	0.215629	0.308843	2.103614
O	0.566096	2.198306	3.252124
H	-4.686863	-0.867069	-0.068647
H	-3.795883	-1.802045	2.101950
H	-3.548281	-2.867487	0.710335
H	4.686763	-0.868513	0.068803
H	3.624655	0.172924	-0.892829
H	3.795518	-1.803465	-2.101700
H	3.547545	-2.868653	-0.709957
H	-1.540023	-3.878022	1.792246
H	-2.096124	-2.886230	3.178222
H	0.043416	-1.680416	3.255614
H	0.307485	-3.463858	3.338965
H	-3.624383	0.174139	0.892828
H	2.095414	-2.887216	-3.177883
H	1.539047	-3.878685	-1.791782
H	-0.308365	-3.464193	-3.338520
H	-0.043789	-1.680815	-3.255405
H	-3.948770	-1.650171	-2.196908
H	-2.450580	-0.962328	-2.864860
H	-2.318701	-3.404924	-2.603692
H	-2.532774	-3.284421	-0.857023
H	2.531997	-3.285059	0.857517
H	2.317845	-3.405226	2.604197
H	2.450385	-0.962626	2.864984
H	3.948411	-1.650990	2.197195

MacropaTbΔ_{δλλ}_{λδλ}_opt.log

SCF (RwB97XD) = -1866.81840133
 E(SCF)+ZPE(0 K)= -1866.207715
 H(298 K)= -1866.172799
 G(298 K)= -1866.269598
 Lowest Frequency = 36.7686cm⁻¹

73

Tb	0.902576	3.981891	9.212035
N	3.089828	2.658969	9.274685
C	3.150013	1.334654	9.418356
C	4.306441	0.720749	9.899234
H	4.338520	-0.362303	10.026190
C	5.408989	1.513946	10.207536
H	6.320411	1.054292	10.595159
C	5.352142	2.890085	9.987819
C	4.163557	3.421006	9.506904
C	3.977707	4.903281	9.206807
O	2.808081	5.185307	8.744333
H	6.194548	3.557300	10.171478
N	1.937313	4.401641	11.552171
C	2.547005	5.529576	11.914774
C	3.444068	5.549559	12.983521
H	3.943468	6.479280	13.260183

C	3.684251	4.368999	13.681153
H	4.391181	4.359898	14.513237
C	2.992934	3.209776	13.329215
C	2.114075	3.279702	12.258050
C	1.275151	2.099780	11.792339
O	0.481742	2.402687	10.822449
H	3.107595	2.264169	13.859586
C	1.917901	0.564850	9.007111
H	2.221950	-0.418325	8.597131
H	1.310345	0.372177	9.904173
N	1.122214	1.318077	8.033183
C	1.842963	1.440425	6.765364
H	1.860404	0.481345	6.210748
H	2.885115	1.708822	6.980321
C	1.262672	2.508901	5.869958
H	1.925593	2.636243	4.996910
H	0.262271	2.243080	5.483595
O	1.177584	3.726455	6.584516
C	0.867010	4.819961	5.744694
H	-0.157149	4.700993	5.346370
H	1.570136	4.858241	4.894934
C	0.985291	6.090703	6.535734
H	2.022198	6.245917	6.873556
H	0.664252	6.934230	5.903346
O	0.126579	5.976518	7.664796
C	-0.207831	7.213517	8.275091
H	-1.234937	7.112797	8.638868
H	-0.220075	8.008892	7.512615
C	0.772428	7.603835	9.370318
H	1.762690	7.717730	8.908266
H	0.479962	8.596973	9.767852
N	0.908749	6.611559	10.434931
C	2.202410	6.758832	11.111997
H	2.212632	7.645049	11.775782
H	2.989175	6.905659	10.357506
C	-0.162788	6.633410	11.431055
H	-0.301241	7.646612	11.858798
H	0.142632	5.976908	12.255812
C	-1.505797	6.145675	10.924431
H	-2.138304	5.880752	11.788810
H	-2.042311	6.927565	10.360893
O	-1.321210	5.006851	10.102171
C	-2.515307	4.519710	9.509921
H	-2.607951	4.925735	8.486791
H	-3.391714	4.842891	10.093279
C	-2.471485	3.018514	9.500847
H	-2.371695	2.646347	10.535453
H	-3.409269	2.624820	9.070140
O	-1.365635	2.584086	8.736422
C	-1.222742	1.167253	8.828158
H	-2.189144	0.692157	8.587215
H	-0.937161	0.910368	9.859642
C	-0.193553	0.709680	7.828325
H	-0.134585	-0.394993	7.854235
H	-0.556088	0.979187	6.827571
O	1.416778	1.005839	12.300733
O	4.874382	5.687724	9.444790

MacropaTbΔ_λδδ_λδδ_opt.log

SCF (RwB97XD) = -1866.81379310

E(SCF)+ZPE(0 K)= -1866.203916

H(298 K)= -1866.168891

G(298 K)= -1866.266077

Lowest Frequency = 34.8662cm⁻¹

73

C	3.707509	0.743274	0.444431
N	2.856078	0.599468	-0.751331
O	1.829797	1.828176	1.451450
C	2.929377	0.977729	1.733539
C	3.073556	1.691961	-1.705147
C	1.838297	2.081799	-2.481401
O	0.852066	2.529556	-1.543504
C	-0.168781	3.351122	-2.085601
C	-1.325063	2.516729	-2.578443
O	-1.830162	1.827889	-1.451317
O	-0.852580	2.529251	1.543700
C	0.168089	3.351001	2.085855
C	1.324554	2.516823	2.578629
N	-2.856184	0.598802	0.751374
C	-3.073894	1.691178	1.705273
C	-1.838720	2.081216	2.481561
C	-2.929561	0.977231	-1.733470
C	-3.707644	0.742516	-0.444380
C	2.999498	-0.722814	-1.366274
C	-2.999335	-0.723557	1.366216
C	-2.462509	-1.790528	0.441697
C	2.462910	-1.789968	-0.441827
C	-1.024859	-2.226460	-1.330297
C	-1.432682	-3.549693	-1.416320
C	-2.389915	-3.995341	-0.503859
C	-2.930020	-3.105029	0.421153
C	2.930715	-3.104366	-0.421374
C	2.390809	-3.994863	0.503578
C	1.433477	-3.549491	1.416069
C	1.025360	-2.226342	1.330139
Tb	-0.000060	0.650890	0.000031
H	4.402938	1.581808	0.293312
H	4.336996	-0.149411	0.585753
H	3.591599	1.459953	2.471583
H	2.553095	0.042022	2.173577
H	0.233119	3.980106	-2.895324
H	-0.511365	4.009201	-1.272901
H	-0.998208	1.793741	-3.346289
H	-2.105412	3.168484	-3.008294
H	-0.233946	3.979835	2.895627
H	0.510526	4.009216	1.273203
H	2.104764	3.168716	3.008524
H	0.997861	1.793708	3.346425
H	-2.553082	0.041636	-2.173578
H	-3.591886	1.459369	-2.471478
H	-4.403249	1.580893	-0.293200
H	-4.336942	-0.150291	-0.585768

H	4.055951	-0.943917	-1.613385
H	2.427962	-0.755917	-2.306112
H	-4.055745	-0.944900	1.613293
H	-2.427810	-0.756613	2.306061
H	-1.004360	-4.189495	-2.188239
H	-2.735092	-5.030927	-0.529174
H	-3.706229	-3.420865	1.119575
H	3.706995	-3.419980	-1.119817
H	2.736219	-5.030373	0.528822
H	1.005297	-4.189442	2.187943
N	1.503480	-1.397614	0.396165
N	-1.503164	-1.397903	-0.396265
C	-0.021271	-1.594245	-2.288654
O	0.147093	-0.329642	-2.080015
O	0.543378	-2.275410	-3.118643
C	0.021633	-1.594418	2.288542
O	-0.146994	-0.329833	2.080002
O	-0.542877	-2.275767	3.118473
H	-2.094050	2.914614	3.156007
H	-1.434098	1.242659	3.068324
H	-3.883883	1.452975	2.421263
H	-3.390203	2.577826	1.140253
H	2.093451	2.915302	-3.155785
H	1.433850	1.243203	-3.068227
H	3.389681	2.578633	-1.140061
H	3.883592	1.453981	-2.421159

MacropaTbΔ_{λδλ}λ_{δλ}_opt.log

SCF (RwB97XD) = -1866.82308018
 E(SCF)+ZPE(0 K)= -1866.213004
 H(298 K)= -1866.178092
 G(298 K)= -1866.275144
 Lowest Frequency = 29.1414cm⁻¹

73

C	3.682240	0.960109	-0.268601
N	2.643764	0.551030	-1.228042
O	1.983097	1.870554	1.121172
C	3.182176	1.111955	1.158352
C	2.532122	1.472120	-2.360265
C	1.927201	2.803173	-1.961853
O	0.598502	2.604783	-1.491137
C	-0.440525	3.370652	-2.076307
C	-1.614737	2.465481	-2.352681
O	-1.983136	1.870429	-1.121285
O	-0.598565	2.604843	1.491002
C	0.440444	3.370801	2.076087
C	1.614689	2.465692	2.352523
N	-2.643765	0.551027	1.228015
C	-2.532149	1.472175	2.360193
C	-1.927263	2.803226	1.961722
C	-3.182200	1.111804	-1.158411
C	-3.682251	0.960034	0.268555
C	2.818608	-0.830074	-1.681960
C	-2.818577	-0.830058	1.682004
C	-2.445383	-1.818521	0.605841

C	2.445441	-1.818489	-0.605742
C	-1.200733	-2.187406	-1.317039
C	-1.674093	-3.484953	-1.448679
C	-2.573397	-3.951401	-0.489832
C	-2.982809	-3.105013	0.536763
C	2.982900	-3.104963	-0.536594
C	2.573512	-3.951304	0.490049
C	1.674197	-3.484826	1.448872
C	1.200804	-2.187299	1.317161
Tb	-0.000003	0.635377	-0.000015
H	4.109431	1.923484	-0.585526
H	4.520391	0.242917	-0.268063
H	3.941384	1.647771	1.752594
H	2.987894	0.142654	1.642756
H	1.868613	1.004471	-3.100306
H	3.513022	1.655454	-2.842560
H	1.914960	3.468536	-2.838284
H	2.504967	3.302289	-1.168050
H	-0.102179	3.820802	-3.022153
H	-0.729950	4.181054	-1.386200
H	-1.338175	1.679409	-3.075657
H	-2.453869	3.060003	-2.752845
H	0.102097	3.821024	3.021897
H	0.729832	4.181151	1.385902
H	2.453805	3.060272	2.752635
H	1.338158	1.679668	3.075565
H	-1.868628	1.004580	3.100258
H	-3.513055	1.655504	2.842478
H	-2.505049	3.302302	1.167908
H	-1.915026	3.468620	2.838130
H	-2.987904	0.142479	-1.642761
H	-3.941423	1.647571	-1.752678
H	-4.109451	1.923423	0.585425
H	-4.520393	0.242832	0.268065
H	3.856323	-1.020994	-2.015816
H	2.162659	-1.010094	-2.547517
H	-3.856288	-1.020984	2.015867
H	-2.162626	-1.010016	2.547573
H	-1.341423	-4.086940	-2.294620
H	-2.972902	-4.965528	-0.554489
H	-3.710217	-3.433415	1.280689
H	3.710315	-3.433388	-1.280503
H	2.973043	-4.965418	0.554762
H	1.341543	-4.086776	2.294846
N	1.552075	-1.401892	0.292006
N	-1.552025	-1.401951	-0.291928
C	-0.268827	-1.540420	-2.334631
O	-0.071903	-0.284698	-2.116224
O	0.224494	-2.213168	-3.217767
C	0.268881	-1.540281	2.334718
O	0.071927	-0.284576	2.116244
O	-0.224426	-2.212995	3.217888

MacropaTbΔ_λλδ_λλδ_opt.log

SCF (RwB97XD) = -1866.81005689

E(SCF)+ZPE(0 K)= -1866.199750

H(298 K)= -1866.164921
 G(298 K)= -1866.261019
 Lowest Frequency = 39.6774cm⁻¹

73

C	-3.578725	-0.723292	0.714373
N	-2.859248	-0.554053	-0.559913
O	-1.722645	-2.153236	1.189690
C	-2.679833	-1.297299	1.809732
C	-3.183505	-1.647963	-1.478753
C	-2.120772	-1.918092	-2.512894
O	-0.936049	-2.355019	-1.856163
C	0.043042	-2.796560	-2.774280
C	1.249426	-3.216597	-1.974525
O	1.735757	-2.133578	-1.203700
O	0.950434	-2.361886	1.840775
C	-0.025728	-2.816593	2.755563
C	-1.229311	-3.238648	1.952659
N	2.861966	-0.539415	0.557370
C	3.193240	-1.637521	1.468678
C	2.132158	-1.921709	2.500750
C	2.687332	-1.266961	-1.817524
C	3.582558	-0.695197	-0.718029
C	-3.086279	0.767382	-1.146287
C	3.080642	0.779346	1.152839
C	2.455271	1.843389	0.282968
C	-2.467763	1.829379	-0.269035
C	0.910262	2.249335	-1.400776
C	1.270892	3.585489	-1.495801
C	2.260608	4.053659	-0.630221
C	2.878214	3.172652	0.254362
C	-2.899691	3.155501	-0.230755
C	-2.287871	4.034282	0.660048
C	-1.294860	3.566587	1.522098
C	-0.925244	2.233610	1.417409
Tb	0.001735	-0.653721	-0.001723
H	-4.458187	-1.370799	0.564275
H	-3.966767	0.242153	1.067164
H	-3.276696	-1.871451	2.535556
H	-2.148645	-0.497909	2.350720
H	2.150932	-0.467057	-2.352577
H	3.287827	-1.831926	-2.547549
H	4.465996	-1.338298	-0.572421
H	3.964627	0.275115	-1.063929
H	-4.164911	0.978171	-1.282142
H	-2.614976	0.816468	-2.139745
H	4.157929	0.996048	1.290074
H	2.609157	0.818633	2.146654
H	0.781916	4.218136	-2.236954
H	2.570368	5.100223	-0.661990
H	3.680544	3.506387	0.913869
H	-3.704467	3.488518	-0.887638
H	-2.604730	5.078457	0.699433
H	-0.810092	4.197143	2.267785
N	-1.473303	1.414563	0.514824
N	1.463805	1.427495	-0.504088
C	-0.129776	1.590614	-2.296950

O	-0.255746	0.324450	-2.070331
O	-0.759472	2.251420	-3.096468
C	0.119065	1.575384	2.308964
O	0.252964	0.311616	2.073698
O	0.744669	2.234674	3.112936
H	2.494015	-2.725470	3.164840
H	1.889944	-1.036188	3.109525
H	4.153989	-1.451868	1.987862
H	3.317888	-2.547345	0.866501
H	-2.477475	-2.719623	-3.182445
H	-1.884511	-1.026862	-3.115648
H	-3.302125	-2.562714	-0.882852
H	-4.145531	-1.464995	-1.996527
H	0.293658	-1.977456	-3.472123
H	-0.337655	-3.652384	-3.359428
H	2.040071	-3.609069	-2.633407
H	0.971882	-4.005446	-1.259392
H	-0.281734	-2.004325	3.459409
H	0.360584	-3.674179	3.334417
H	-0.946596	-4.020455	1.231840
H	-2.017412	-3.641071	2.608578

MacropaTbΔ_λλλ_λλλ_opt.log

SCF (RwB97XD) = -1866.81904345
 E(SCF)+ZPE(0 K)= -1866.208900
 H(298 K)= -1866.174015
 G(298 K)= -1866.270905
 Lowest Frequency = 28.1350cm⁻¹

73

C	-3.693026	0.941849	0.399819
N	-2.631774	0.517383	1.325043
O	-1.988299	1.839936	-1.013860
C	-3.217451	1.123682	-1.034323
C	-2.483386	1.427754	2.461127
C	-1.872399	2.753017	2.043474
O	-0.528869	2.606361	1.597978
C	0.452083	2.708401	2.622014
C	1.790565	2.886975	1.950687
O	1.987891	1.840094	1.014397
O	0.528266	2.607038	-1.597183
C	-0.452708	2.709170	-2.621187
C	-1.791238	2.887174	-1.949805
N	2.631676	0.518467	-1.324931
C	2.483060	1.429174	-2.460718
C	1.871761	2.754157	-2.042626
C	3.217219	1.124134	1.034628
C	3.692832	0.942887	-0.399575
C	-2.786122	-0.870909	1.756161
C	2.786367	-0.869644	-1.756511
C	2.429816	-1.839206	-0.656885
C	-2.429325	-1.840020	0.656216
C	1.231227	-2.187690	1.297782
C	1.701277	-3.486648	1.427719
C	2.574188	-3.965656	0.451310
C	2.961309	-3.128604	-0.590967

C	-2.960490	-3.129532	0.589874
C	-2.573156	-3.966145	-0.452677
C	-1.700366	-3.486594	-1.428928
C	-1.230646	-2.187560	-1.298564
Tb	-0.000055	0.635934	0.000074
H	-4.119183	1.895187	0.747825
H	-4.527674	0.220148	0.400980
H	-3.973573	1.688623	-1.600667
H	-3.054395	0.161442	-1.540737
H	3.054398	0.161689	1.540727
H	3.973202	1.689077	1.601156
H	4.118754	1.896443	-0.747271
H	4.527654	0.221389	-0.400979
H	-3.814643	-1.078374	2.108548
H	-2.111837	-1.061898	2.605033
H	3.814937	-1.076736	-2.108972
H	2.112124	-1.060516	-2.605443
H	1.385307	-4.079760	2.286226
H	2.969823	-4.981436	0.513597
H	3.667820	-3.466128	-1.350856
H	-3.666917	-3.467485	1.349651
H	-2.968532	-4.982004	-0.515297
H	-1.384243	-4.079342	-2.287630
N	-1.560974	-1.409119	-0.260261
N	1.561357	-1.408825	0.259736
C	0.323193	-1.538618	2.334948
O	0.104692	-0.288368	2.109148
O	-0.135631	-2.205567	3.240910
C	-0.322771	-1.537925	-2.335516
O	-0.104566	-0.287698	-2.109302
O	0.136211	-2.204465	-3.241699
H	0.444623	1.793835	3.237113
H	0.244453	3.586872	3.255412
H	2.581952	2.880793	2.715064
H	1.825469	3.848670	1.412532
H	-0.445009	1.794817	-3.236600
H	-0.245302	3.587910	-3.254287
H	-1.826394	3.848684	-1.411336
H	-2.582620	2.881039	-2.714188
H	2.421298	3.204439	-1.204444
H	1.903275	3.466413	-2.882378
H	3.450601	1.624004	-2.964871
H	1.819422	0.945052	-3.190037
H	-1.904075	3.464987	2.883462
H	-2.422046	3.203450	1.205446
H	-3.450979	1.622191	2.965334
H	-1.819643	0.943554	3.190297