Supporting Information

Configuration Control in the Synthesis of Homo- and Heteroleptic Bis(oxazolinylphenolato/thiazolinylphenolato) Chelate Ligand Complexes of Oxorhenium(V): Isomer Effect on Ancillary Ligand Exchange Dynamics and Implications for Perchlorate Reduction Catalysis

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SUPPLEMENTAL TABLES AND FIGURES

Table S1. Crystal Data and Refinement Details

	N,N-*trans* Re(O)(*hoz*)$_2$Cl (2a)	**N,N-*cis* Re(O)(*hoz*)$_2$Cl•C_7H_8 (2b)**	**[Re(O)(*hoz*)$_2$(H_2O)] [OTf]**	**[H_2*hoz*] [Re(O)(*hoz*)Cl_3] (3)**
Formula	$C_{18}H_{16}ClN_2O_5Re$	$C_{25}H_{24}ClN_2O_5Re$	$C_{19}H_{18}F_3N_2O_9ReS$	$C_{18}H_{18}Cl_3N_2O_5Re$
Formula weight	561.98	654.11	693.61	634.89
Temperature (K)	193(2)	173(2)	188(2)	188(2)
Wavelength (Å)	0.71073	1.54178	0.71073	0.71073
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P\bar{1}$	$P2_1/c$
a (Å)	9.2210(9)	17.5402(6)	11.8818(3)	9.8742(8)
b (Å)	7.9281(8)	7.4270(2)	13.6186(4)	15.0566(12)
c (Å)	23.284(2)	19.3930(6)	14.7507(4)	3.6439(11)
α (deg)	90	90	108.1620(10)	90
β (deg)	95.854(4)	110.2000(10)	93.3860(10)	90.1360(10)
γ (deg)	90	90	99.3290(10)	90
V (Å^3)	1693.3(3)	2370.96(13)	2222.61(11)	2028.5(3)
Z	4	4	4	4
ρ_{calc} (g cm^{-3})	2.204	1.832	2.073	2.079
Absorption coefficient (mm^{-1})	7.370	11.399	5.642	6.419
F(000)	1080	1280	1344	1224
Crystal size (mm^3)	0.492 × 0.266 × 0.206	0.323 × 0.314 × 0.054	0.465 × 0.169 × 0.03	0.322 × 0.127 × 0.05
θ range (deg)	1.758 − 25.689	7.581 − 68.071	1.463 − 25.507	1.35 − 26.41
Index ranges	$-11 \le h \le 11$	$-20 \le h \le 21$	$-14 \le h \le 14$	$-12 \le h \le 12$
	$-9 \le k \le 9$	$-8 \le k \le 8$	$-16 \le k \le 16$	$-18 \le k \le 18$
	$-28 \le l \le 27$	$-23 \le l \le 18$	$-17 \le l \le 17$	$-17 \le l \le 17$
No. of reflections collected	23771	23318	31644	24087
No. of independent rflns, R_{int}	3209, 0.0239	4216, 0.0274	8247, 0.0252	4160, 0.0295
Completeness to θ = 25.69°	100.0 %	98.1 %	99.9 %	100.0 %
Absorption correction	integration	integration	integration	integration
Max. and min. transmission	0.4314 and 0.1966	0.6635 and 0.1665	0.8483 and 0.1558	0.7524 and 0.2258
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Data/restraints/parameters	3209 / 0 / 244	4216 / 0 / 309	8247 / 0 / 643	4160 / 0 / 269
Goodness-of-fit on F^2	1.379	1.138	1.041	1.052
R1/wR2 ($I > 2\sigma(I)$)	0.0285 / 0.0586	0.0214 / 0.0554	0.0166 / 0.0394	0.0152 / 0.0366
R1/wR2 (all data)	0.0299 / 0.0590	0.0217 / 0.0557	0.0189 / 0.0404	0.0164 / 0.0372
Largest diff. peak/hole (e Å^{-3})	1.643 and -1.197	0.905 and -0.865	1.419 and -0.567	0.820 and -0.508
Instrument	A[a]	B[b]	A	A

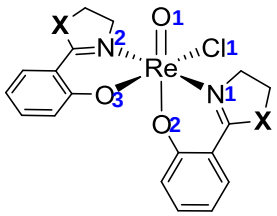
[a]Siemens Platform diffractometer equipped with an Apex II CCD detector using graphite-monochromatized Mo Kα radiation.
[b]Bruker X8 kappa diffractometer equipped with an Apex II CCD detector using graphite-monochromatized Cu Kα radiation.

Table S1 (continued). Crystal Data and Refinement Details

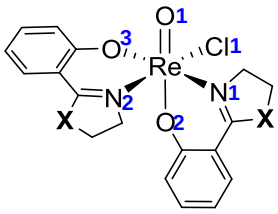
	N,N-*trans* Re(O)(*htz*)$_2$Cl (5a)	**N,N-*cis* Re(O)(*htz*)$_2$Cl (5b)**	**N,N-*trans* Re(O)(*hoz*)(*htz*)Cl (7a)**	**[H*t*Bu$_2$*Py*] [Re(O)(*htz*)Cl$_3$] (6)**
Formula	$C_{18}H_{16}ClN_2O_3S_2Re$	$C_{18}H_{16}ClN_2O_3S_2Re$	$C_{18}H_{16}ClN_2O_4SRe$	$C_{22}H_{30}Cl_3N_2O_2SRe$
Formula weight	594.10	594.10	578.04	679.09
Temperature (K)	100(2)	100(2)	173(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/c$	$P\bar{1}$
a (Å)	9.4422(8)	16.2996(6)	9.2555(8)	8.1795(4)
b (Å)	8.0051(7)	7.5281(2)	8.0421(7)	9.8471(4)
c (Å)	24.614(2)	16.4903(6)	24.075(2)	16.8728(8)
α (deg)	90	90	90	104.3792(17)
β (deg)	93.041(3)	111.7661(12)	94.944(4)	101.3449(18)
γ (deg)	90	90	90	98.7890(18)
V (Å^3)	1857.9(3)	1879.18(11)	1785.3(3)	1261.29(10)
Z	4	4	4	2
ρ_{calc} (g cm^{-3})	2.124	2.100	2.151	1.788
Absorption coefficient (mm^{-1})	6.932	6.853	7.101	5.239
F(000)	1144	1144	1112	668
Crystal size (mm^3)	0.223 × 0.157 × 0.067	0.201 × 0.165 × 0.081	0.174 × 0.10 × 0.049	0.163 × 0.075 × 0.029
θ range (deg)	2.652 − 27.244	2.215 – 28.311	1.698 – 28.432	2.185 – 25.373
Index ranges	$-12 \le h \le 12$ $-10 \le k \le 10$ $-31 \le l \le 31$	$-21 \le h \le 21$ $-10 \le k \le 10$ $-21 \le l \le 21$	$-12 \le h \le 12$ $-10 \le k \le 10$ $-32 \le l \le 32$	$-9 \le h \le 9$ $-11 \le k \le 11$ $-20 \le l \le 20$
No. of reflections collected	60050	51563	53422	29598
No. of independent rflns, R_{int}	4142, 0.0248	4657, 0.0469	4465, 0.0488	4612, 0.0352
Completeness to θ = 25.69°	99.9 %	100.0 %	100.0 %	99.9 %
Absorption correction	integration	integration	integration	integration
Max. and min. transmission	0.71771 and 0.41746	0.84296 and 0.62854	0.7459 and 0.3678	0.97943 and 0.86410
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Data/restraints/parameters	4142 / 0 / 244	4657 / 0 / 244	4465 / 0 / 244	4612 / 0 / 290
Goodness-of-fit on F^2	1.332	1.086	1.068	1.072
R1/wR2 ($I > 2\sigma(I)$)	0.0262 / 0.0551	0.0184 / 0.0371	0.0249 / 0.0496	0.0142 / 0.0308
R1/wR2 (all data)	0.0265 / 0.0552	0.0250 / 0.0388	0.0298 / 0.0511	0.0164 / 0.0314
Largest diff. peak/hole (e Å^{-3})	2.521 and -1.792	0.427 and -0.938	1.632 and -0.980	0.389 and -0.636
Instrument	C[c]	C	D[d]	C

[c]Burker D8 Venture equipped with a Photon 100 detector using multilayer optics to monochromatize Mo Kα radiation.
[d]Bruker X8 kappa diffractometer equipped with an Apex II CCD detector using graphite-monochromatized Mo Kα radiation.

Table S2. Selected Bond Distances (Å) for the Five Re(O)($L_{O\text{-}N}$)$_2$Cl Complexes



2a, **5a** and **7a**



2b and **5b**

	2a	**2b**	**5a**	**5b**	**7a**
Re(1)-O(1)	1.671(4)	1.6902(18)	1.692(3)	1.6927(17)	1.681(3)
Re(1)-O(2)	1.977(4)	1.9863(17)	1.979(3)	1.9933(17)	1.993(3)
Re(1)-O(3)	1.990(4)	2.0006(16)	1.990(3)	2.0036(16)	2.005(3)
Re(1)-N(2)	2.038(4)	2.099(2)	2.079(3)	2.102(2)	2.062(3)
Re(1)-N(1)	2.090(4)	2.113(2)	2.094(3)	2.108(2)	2.102(3)
Re(1)-Cl(1)	2.3824(14)	2.3700(6)	2.4175(10)	2.3650(6)	2.4061(10)

Table S3. Calculated Energy of Optimized Structures (B3LYP, Augmented LANL2DZ Basis Set for Re; 6-31G** for C, H, O, N; 6-311G* for S)

Structure	**B3LYP Energy**[a] **(Hartree)**	**298K (25 °C)**		**351K (78 °C)**	
		Total Gibbs free energy[a,b] **(Hartree)**	***ΔG*** **(kcal mol^{-1})**	**Total Gibbs free energy**[a,b] **(Hartree)**	***ΔG*** **(kcal mol^{-1})**
2a	-1720.688525	-1720.422307	0	-1720.437156	0
2b	-1720.687935	-1720.421373	+0.586	-1720.436212	+0.592
5a	-2366.67799	-2366.418359	0	-2366.433381	0
5b	-2366.678647	-2366.419179	-0.515	-2366.434217	-0.525
7a	-2043.686061	-2043.422091	0	-2043.436861	0
7b	-2043.681982	-2043.419053	+1.906	-2043.433963	+1.819
7c	-2043.683102	-2043.419643	+1.536	-2043.434525	+1.466
7d	-2043.681775	-2043.419211	+1.807	-2043.434217	+1.659
7a$^+$	-1716.086866	-1715.780738	0		
7b$^+$	-1716.083104	-1715.777755	+1.872		

[a]With solvent effect (ethanol for **2a** to **7d**, acetonitrile for **7a**$^+$ and **7b**$^+$) addressed using SMD model.

[b]With zero-point energy corrected.

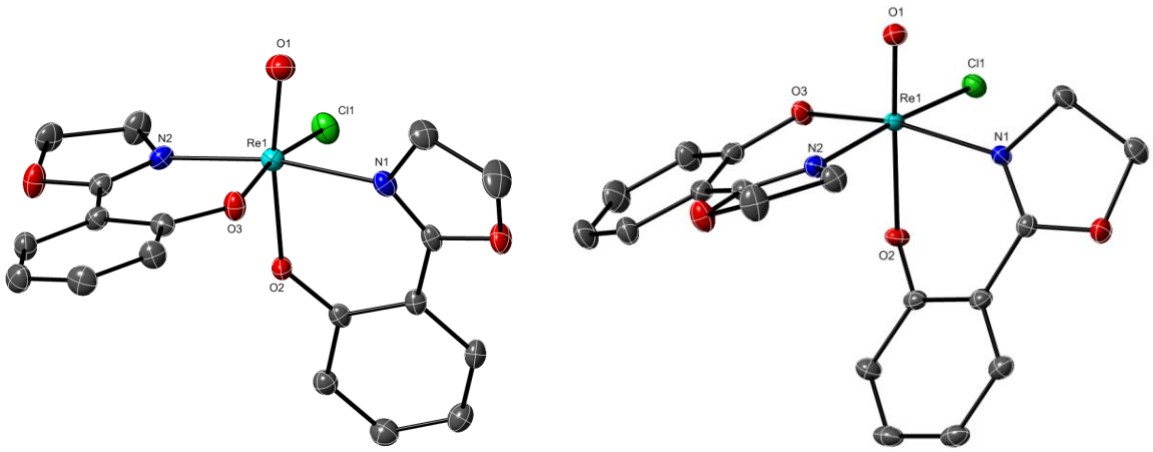


Figure S1. ORTEP diagrams (35% probability thermal ellipsoids) of **2a** and **2b**. Hydrogen atoms and co-crystallized toluene with **2b** are omitted for clarity.

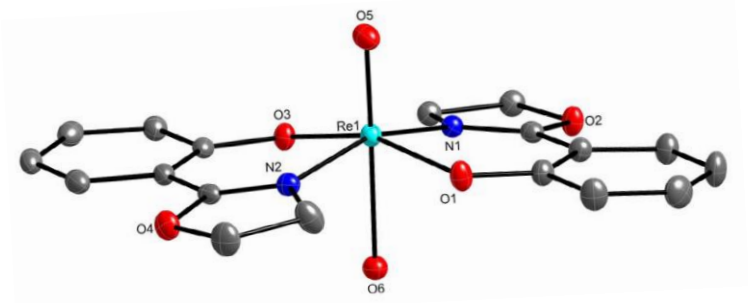


Figure S2. ORTEP diagram (35% probability thermal ellipsoids) of [Re(O)(*hoz*)$_2$(H$_2$O)][OTf] crystallized from the CH$_3$CN solution of **2a**$^+$. Only one of the two crystallographically independent molecules is shown. Hydrogen atoms and [OTf]$^-$ anion are omitted for clarity.

Additional note: Crystallization of **2b**$^+$ from CH$_3$CN solution also yielded this structure. Highly disordered yellow and orange crystals were also obtained as μ-oxo trimers and tetramers of C$_2$-symmetric Re(O)(*hoz*)$_2$ units. Since **2a**$^+$ and **2b**$^+$ do not interconvert appreciably in solution (i.e., <5% interconversion for both isomers at 80 °C for 4 h), this aqua complex should not be a dominant species for either **2a**$^+$ and **2b**$^+$ in CH$_3$CN. Attempts to crystallize **2a**$^+$ and **2b**$^+$ in anhydrous solvents were not successful.

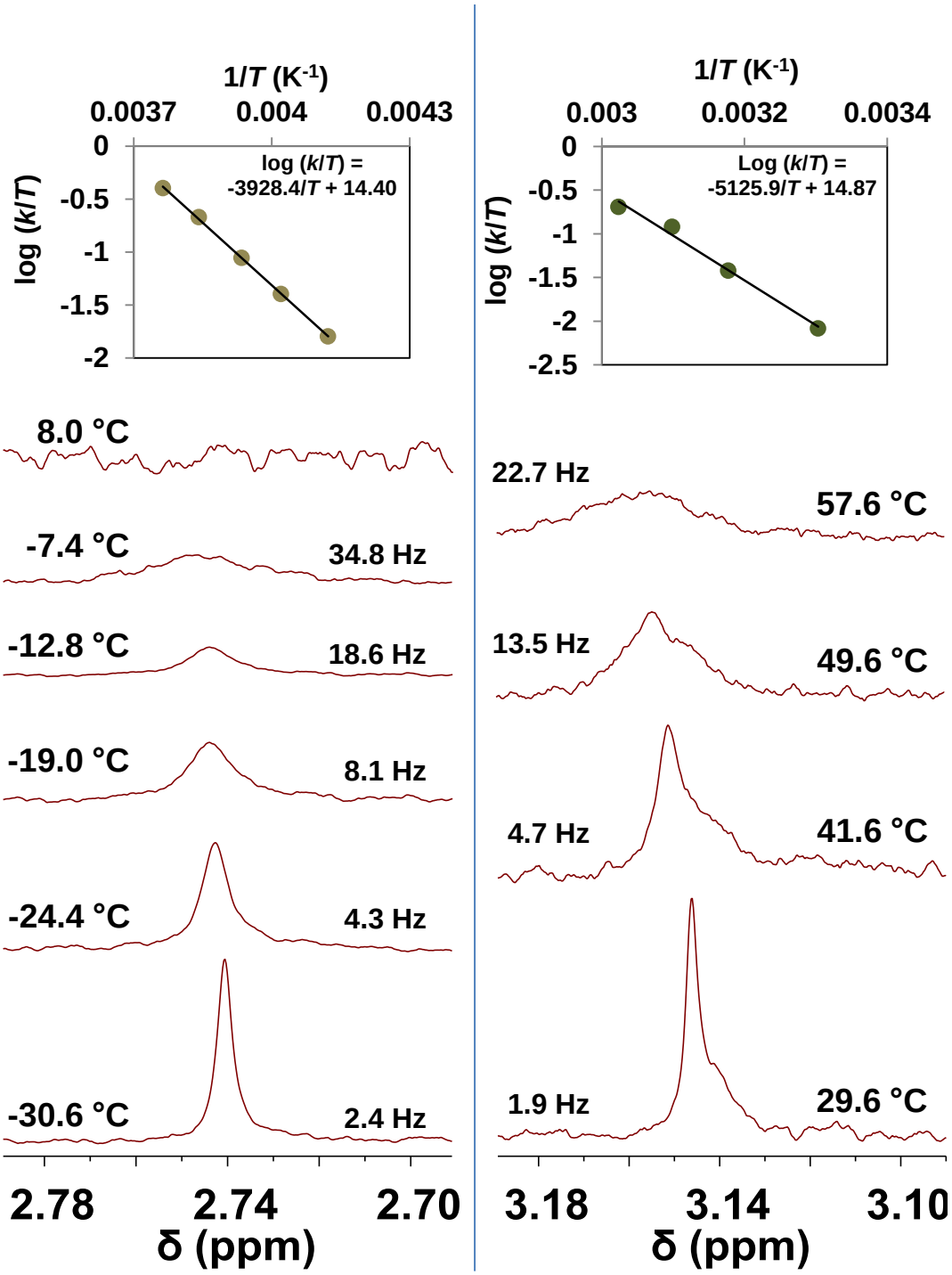


Figure S3. VT ^{1}H NMR (500 MHz, CD_3CN) spectra (half-height line width shown) of CH_3CN coordinated in **5a**$^{+}$ (left) and **5b**$^{+}$ (right). Inset plots: model fitting for measured solvent exchange rate (k_S) and temperature (T).

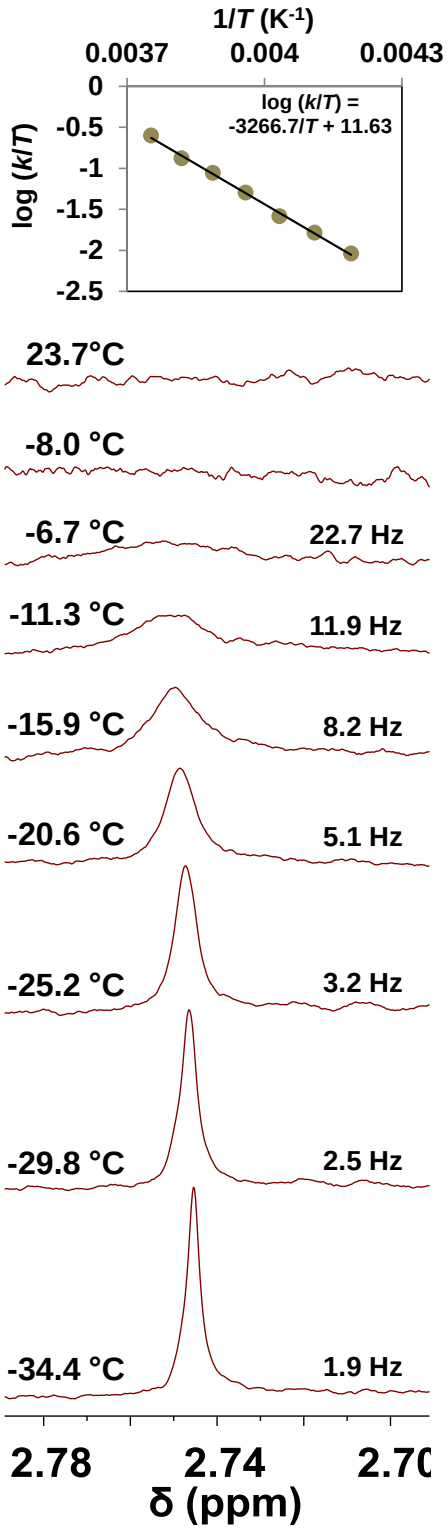


Figure S4. VT ^{1}H NMR (500 MHz, CD_3CN) spectra (half-height line width shown) of CH_3CN coordinated in **7a**$^{+}$. Inset plot: model fitting for measured solvent exchange rate (k_S) and temperature (T).

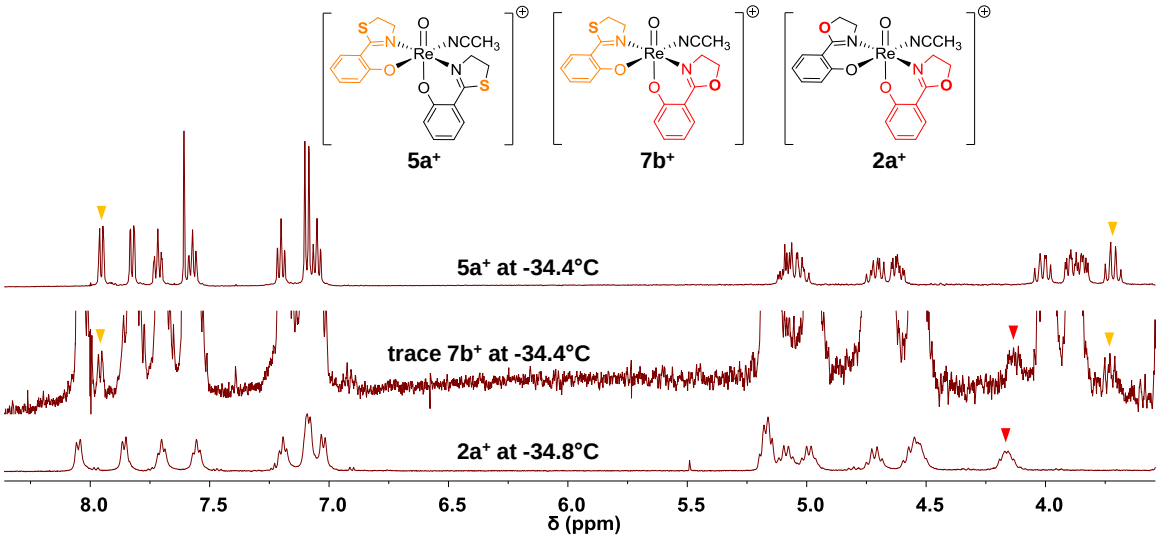


Figure S5. Comparative assignment of ^{1}H NMR (500 MHz, CD_3CN) resonances from equitorial *htz* and axial *hoz* ligands in the three N,N-*trans* cations at low temperature. The trace amount of **7b**$^{+}$ is identified in the zoomed-in spectrum of **7a**$^{+}$.

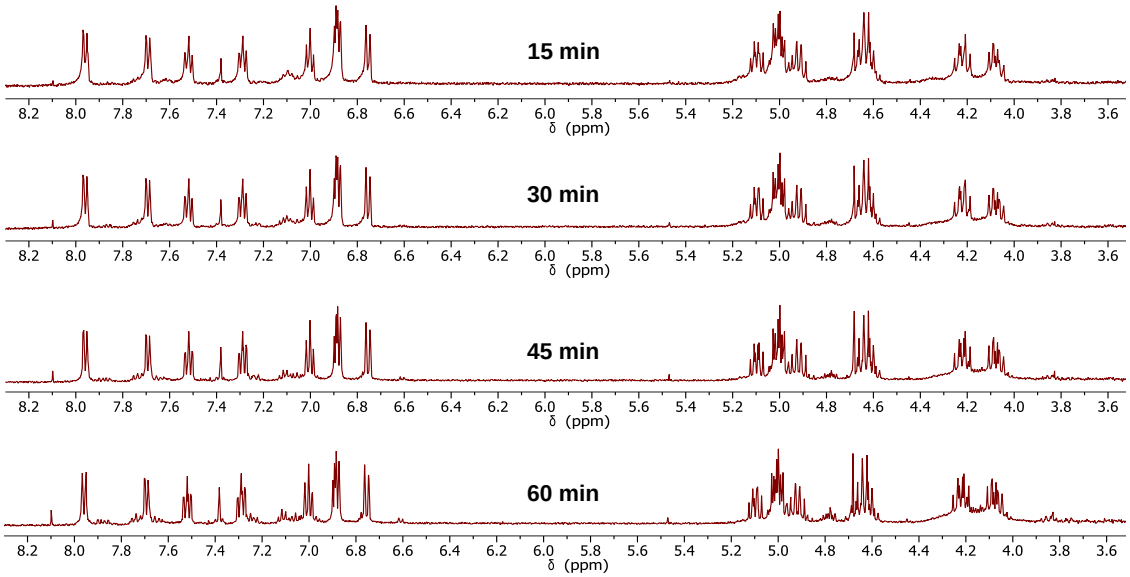


Figure S6. Partial ^{1}H NMR (500 MHz, 95/5 CD_3CN/D_2O) spectra of the homogeneous reaction mixture during ClO_4^- reduction using cation **2a**$^+$. Reaction conditions: Re (4 mM), $LiClO_4$ (100 mM) and Me_2S (400 mM) in 95/5 (v/v) CD_3CN/D_2O (corresponding to the data shown in **Figure 10a**).

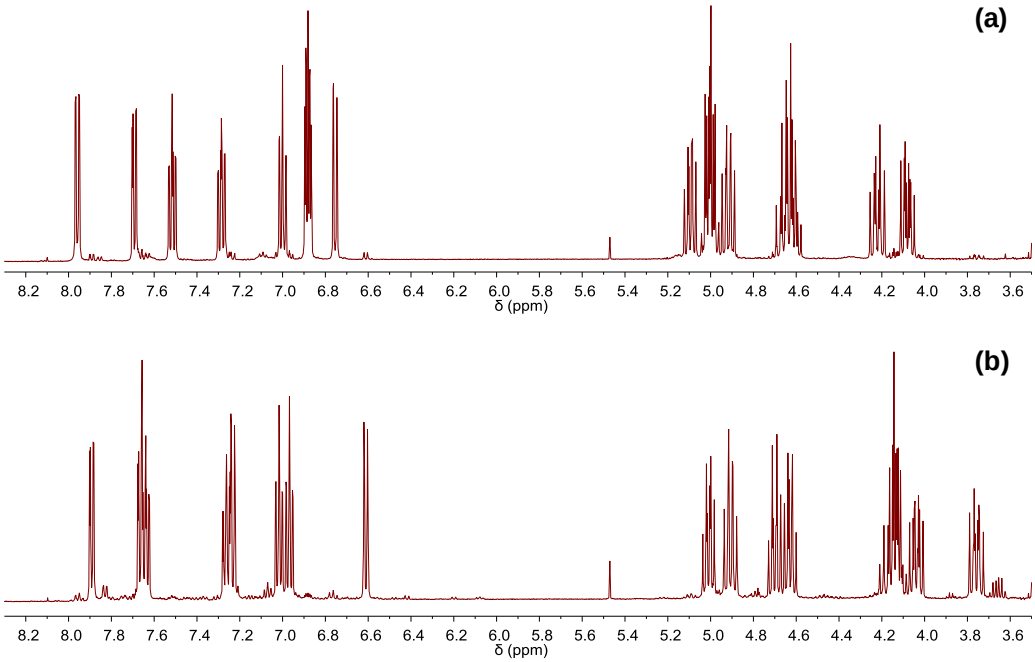


Figure S7. Partial ^{1}H NMR (500 MHz, 95/5 CD_3CN/D_2O) spectra of the homogeneous reaction mixture after ClO_4^- reduction was completed using (**a**) cation **2a**$^+$ and (**b**) **2b**$^+$. Reaction conditions: Re (16 mM), $LiClO_4$ (100 mM) and Et_2S (400 mM) in 95/5 (v/v) CD_3CN/D_2O.

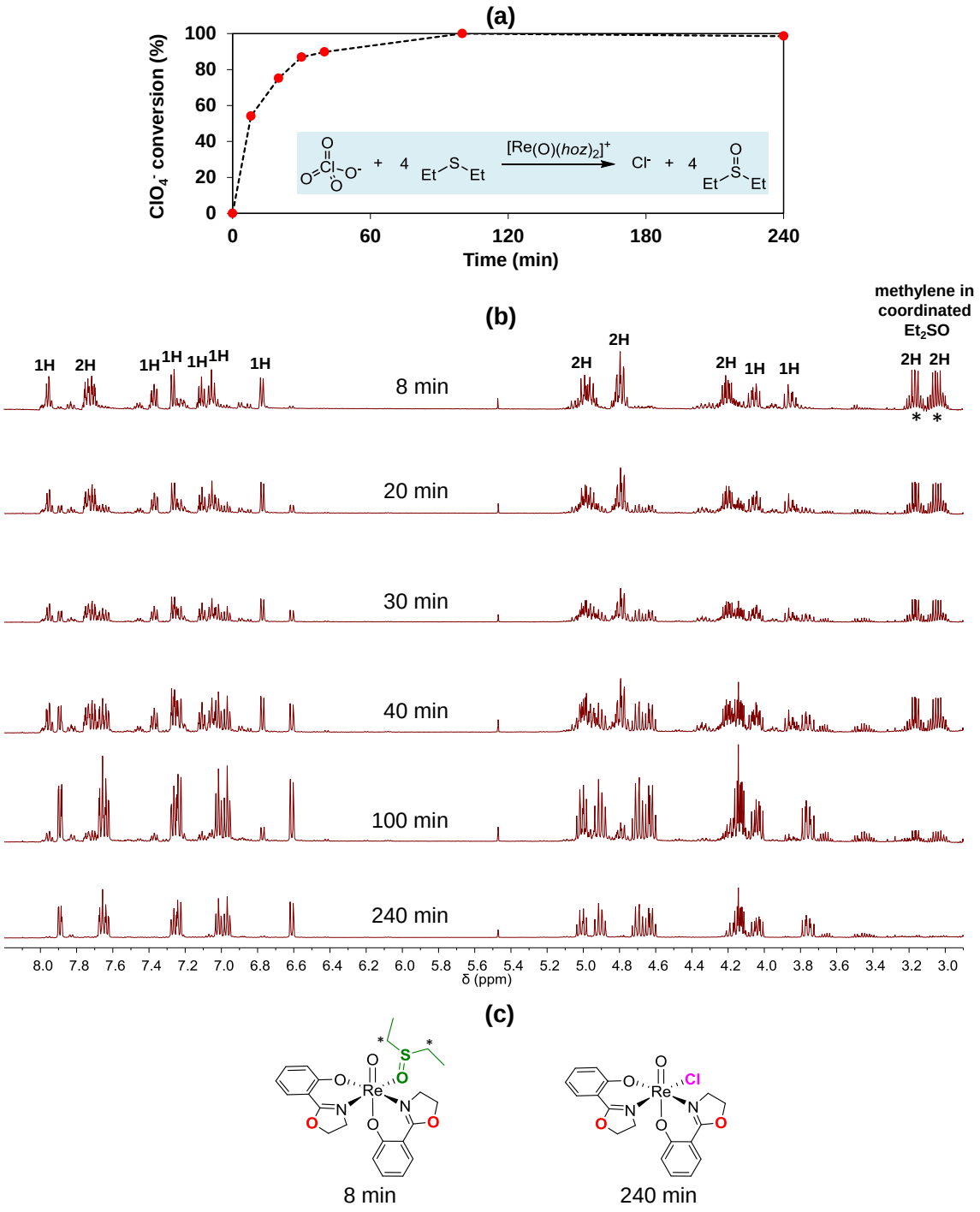


Figure S8. (a) Reaction profile and **(b)** partial ^{1}H NMR (500 MHz, 95/5 CD_3CN/D_2O) spectra of the homogeneous reaction mixture using **2b**$^{+}$ at corresponding time points. Reaction conditions: Re (16 mM), $LiClO_4$ (100 mM) and Et_2S (400 mM) in 95/5 (v/v) CD_3CN/D_2O. The dominant species at 8 min and 240 min are shown in **(c)**.

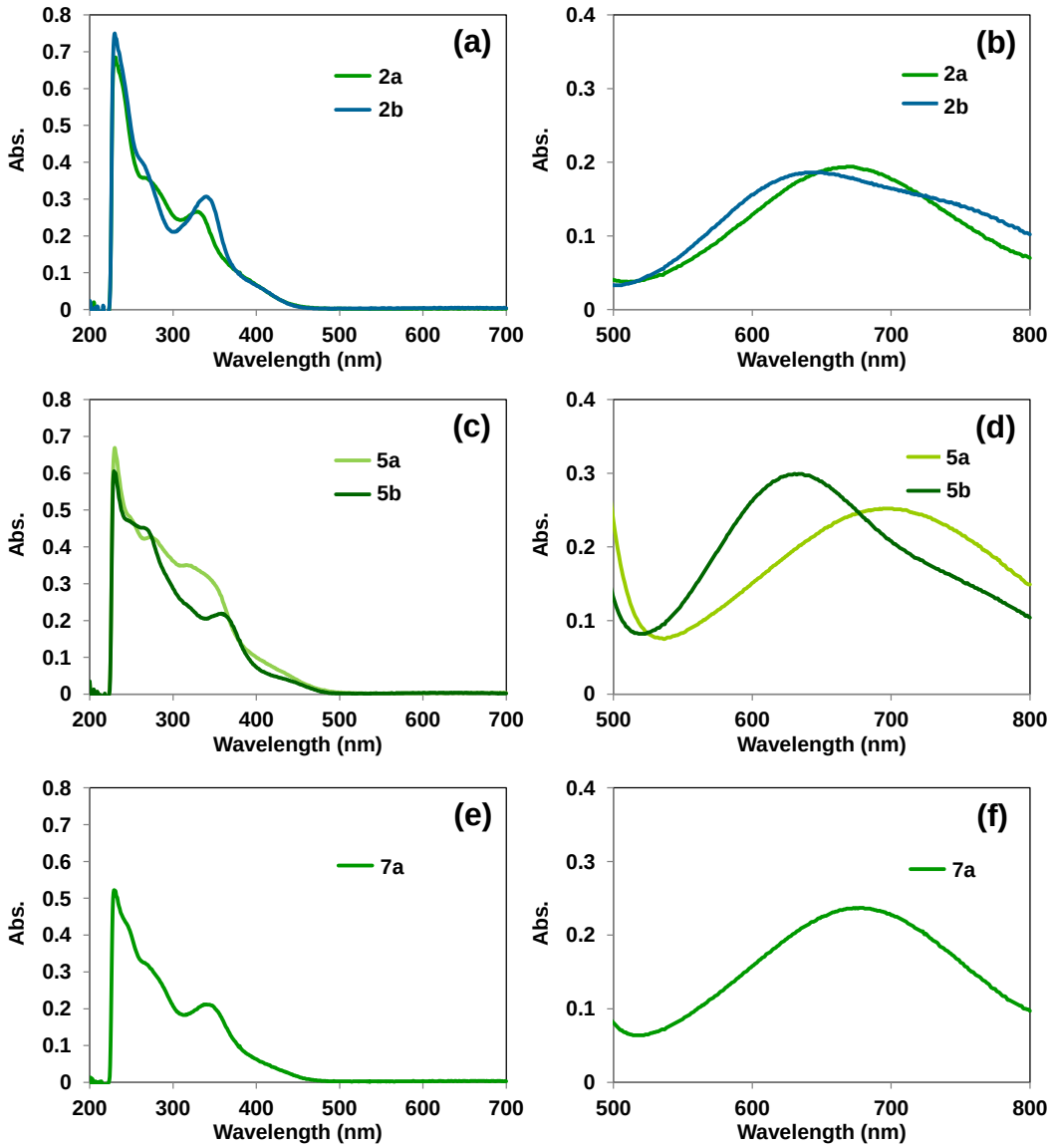


Figure S9. Ultraviolet and visible absorbance spectra of the five Re(O)($L_{O\text{-}N}$)$_2$Cl complexes in CH_2Cl_2 (1.78×10^{-5} M for UV and 1.78×10^{-3} M for visible).

Selected adsorption band assignment based on literature:[3]
2a 231 nm (ε = 38500 M^{-1} cm^{-1}, *IL*) 266 nm (ε = 20100, *IL*); 329 nm (ε = 14900, *LMCT*); 670 nm (ε = 109, *LF*/*MLLCT*)
2b 230 nm (ε = 42100); 264 nm (ε = 22300); 340 nm (ε = 17200); 649 nm (ε = 105)
5a 230 nm (ε = 37600); 273 nm (ε = 23900); 355 nm (ε = 15700); 696 nm (ε = 142)
5b 229 nm (ε = 34000); 263 nm (ε = 25400); 358 nm (ε = 12300); 632 nm (ε = 168)
7a 229 nm (ε = 29300); 266 nm (ε = 18300); 340 nm (ε = 11900); 676 nm (ε = 133)

(*IL* = inter-ligand transition; *LMCT* = ligand-metal charge transfer; *LF* = ligand field transition, *MLLCT* = metal-ligand-to-ligand charge transfer)

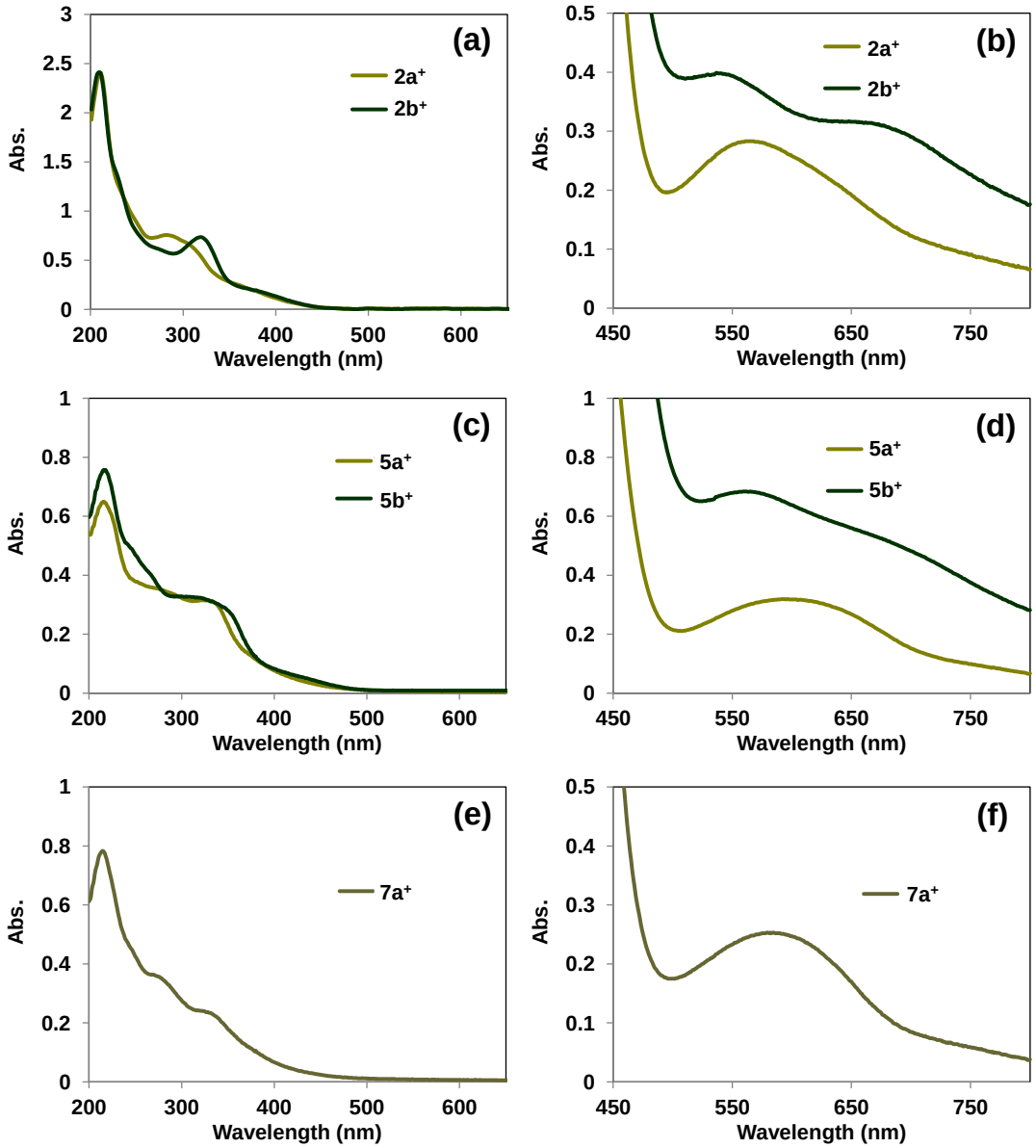


Figure S10. Ultraviolet and visible absorbance spectra of the five $[Re(O)(L_{O\text{-}N})_2]^+$ complexes in CH_3CN (concentration for UV: 5×10^{-5} M for (a) and 2.5×10^{-5} M for (c) and (e); concentration for visible: 2.5×10^{-3} M for all).

Selected adsorption band assignment based on literature:[3]

2a$^+$ 211 nm (ε = 48100 M^{-1} cm^{-1}, *LMCT*/*IL*); 283 nm (ε = 15100, *IL*); 309 nm (ε = 12900, *LMCT*); 565 nm (ε = 113, *LF*)

2b$^+$ 209 nm (ε = 48200); 319 nm (ε = 14700); 537 nm (ε = 160); 662 nm (ε = 126)

5a$^+$ 216 nm (ε = 26000); 325 nm (ε = 12600); 594 nm (ε = 128)

5b$^+$ 216 nm (ε = 30300); 316 nm (ε = 13000); 348 nm (ε = 11400); 561 nm (ε = 274); 698 nm (ε = 194)

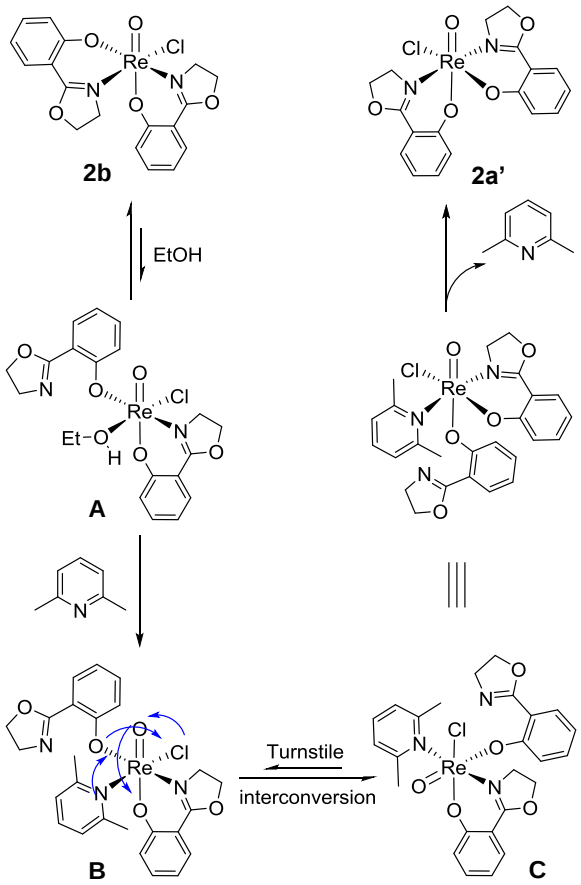
7a$^+$ 215 nm (ε = 31300); 266 nm (ε = 14600); 330 nm (ε = 9400); 582 nm (ε = 101)

PROPOSED MECHANISM FOR ISOMER INTERCONVERSION

Reflux in EtOH enables the conversion from **2b** to thermodynamically favored **2a**. **2b** did not convert to **2a** at room temperature either in nonpolar solvent (CH_2Cl_2 or $CHCl_3$) after weeks or in the solid state after 4 years. Therefore, a polar environment is favorable to facilitate the conversion. Scrutiny of ^{1}H NMR spectra of **2a** and **2b** in CD_3CN identifies several slightly broadened resonances, while all resonances are sharp in $CDCl_3$. This supports a conclusion that certain dynamic processes are favored in polar solution environments. The possibility of thermodynamically driven isomer conversion via cationic $[Re(O)(hoz)_2]^+$ species upon chloride dissociation is excluded, because heating CH_3CN solutions of $\mathbf{2a}^+$ and $\mathbf{2b}^+$ at 80 °C for 4 h only resulted in ~5% interconversion in both directions.

Therefore, we propose a mechanism whereby either EtOH or pyridines act to replace one of the oxazoline N in **2b** to open the chelate ring,[1] and the resulting intermediate (**A** or **B**) undergoes an interconversion such as a turnstile mechanism shown in **Scheme S1**, where the two isomers (**B** and **C**) could equilibrate based on their respective stabilities. Coordination with a relatively bulky and electron-rich pyridine might further lower the conversion energy barrier than with EtOH. A moderate steric hindrance on the pyridine is also needed to ensure that the oxazoline N pendant in **C** could readily exchange with the substituted pyridine to yield **2a'** (the enantiomer of **2a**).

Scheme S1. Proposed Mechanism for Pyridine-facilitated Conversion of **2b** to **2a**



NMR SPECTRA

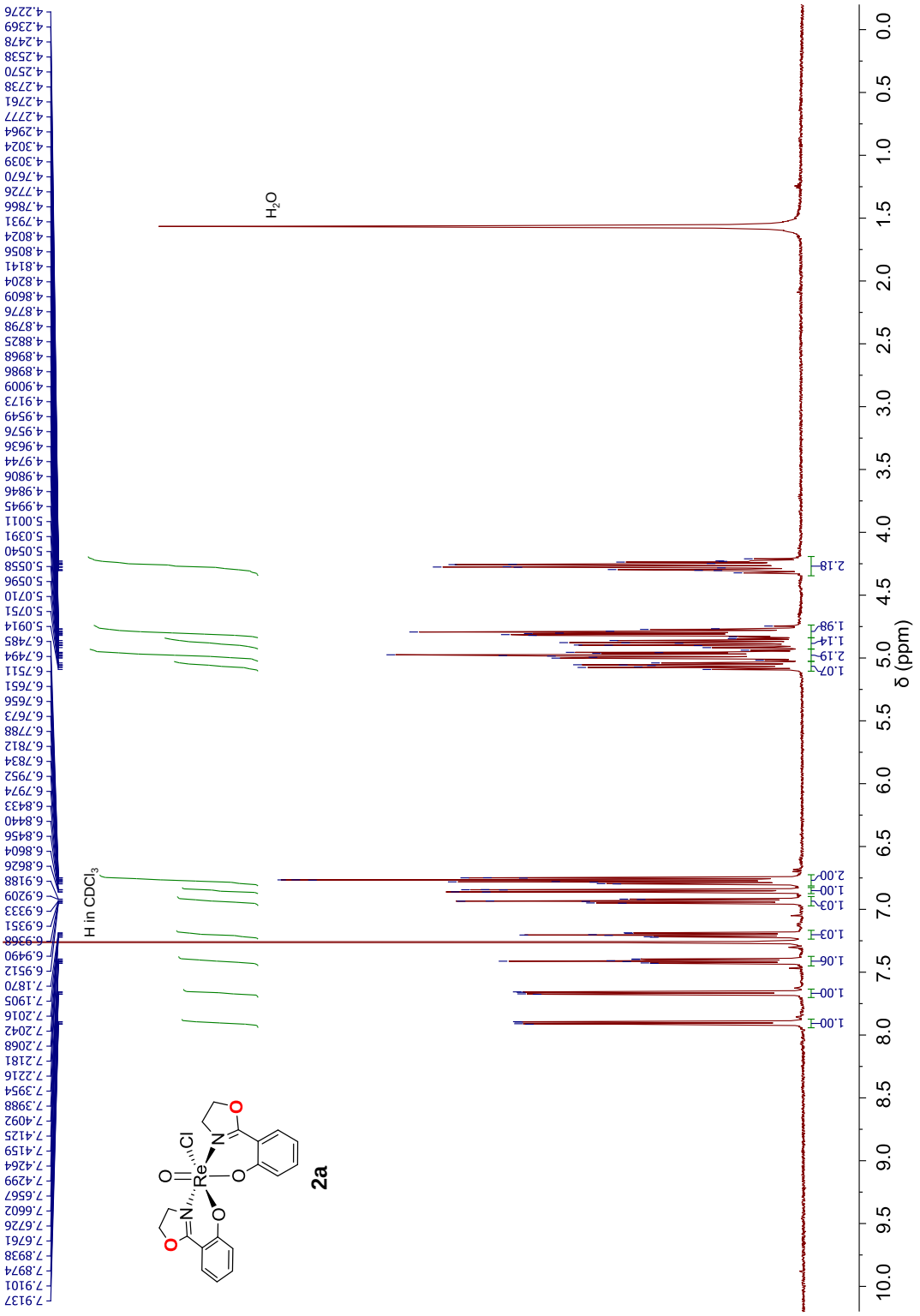


Figure A1. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of N,N-*trans* Re(O)(*hoz*)$_2$Cl (**2a**). Solvent impurity peaks are assigned based on literature.[2]

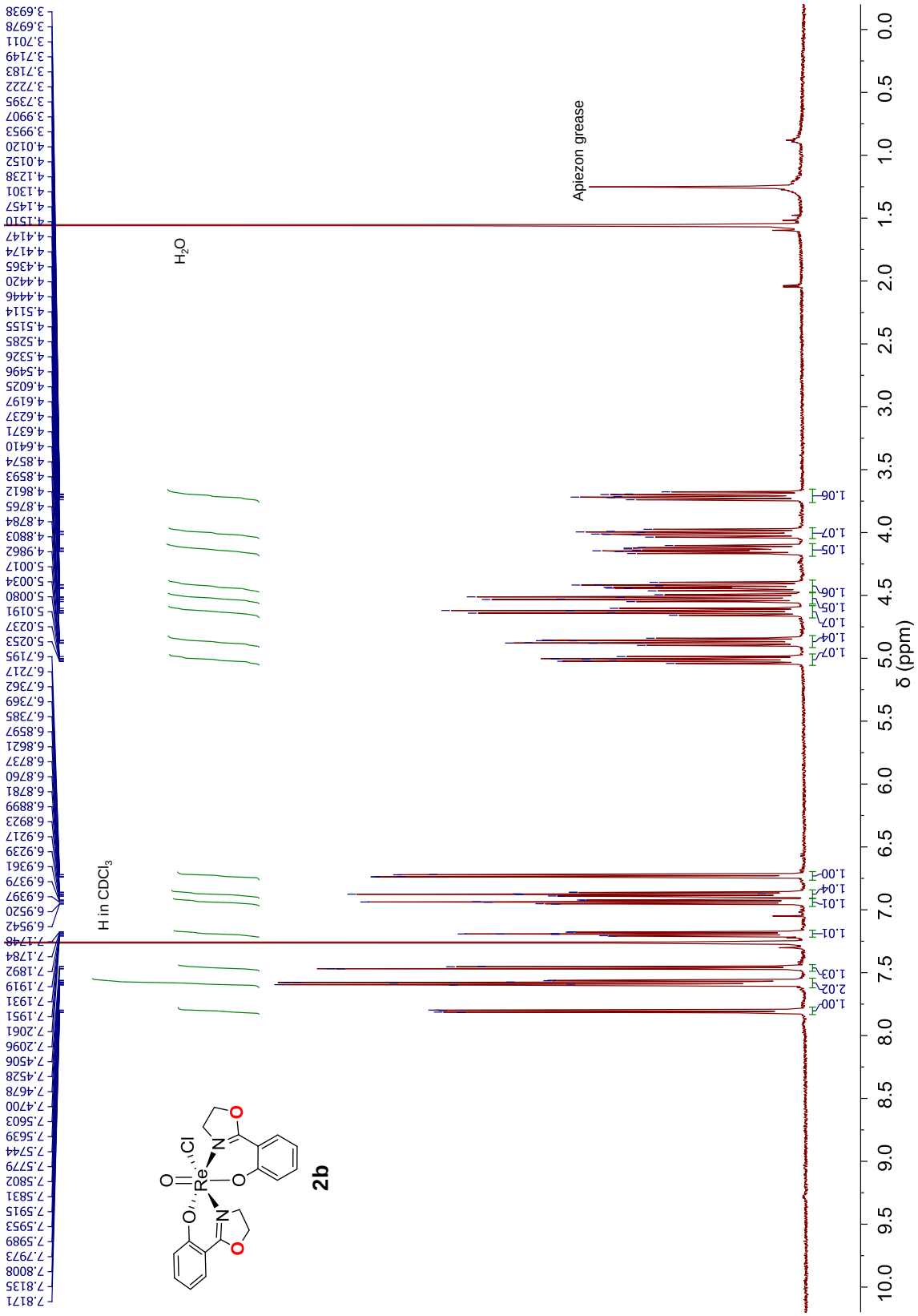


Figure A2. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of N,N-*cis* Re(O)(*hoz*)$_2$Cl (**2b**).

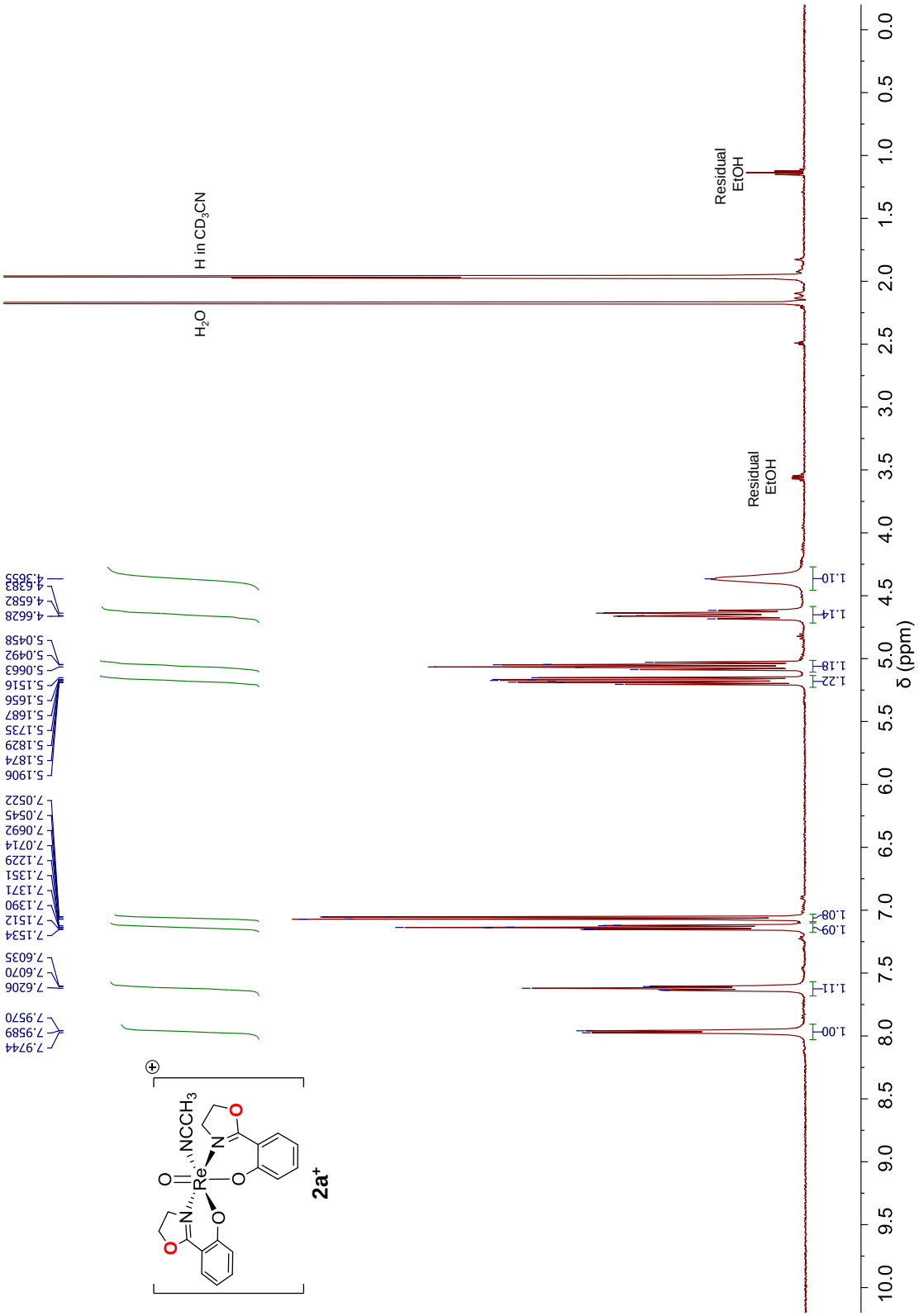


Figure A3. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of N,N-*trans* [Re(O)(*hoz*)$_2$(NCMe)][OTf] (**2a**$^{+}$) at room temperature.

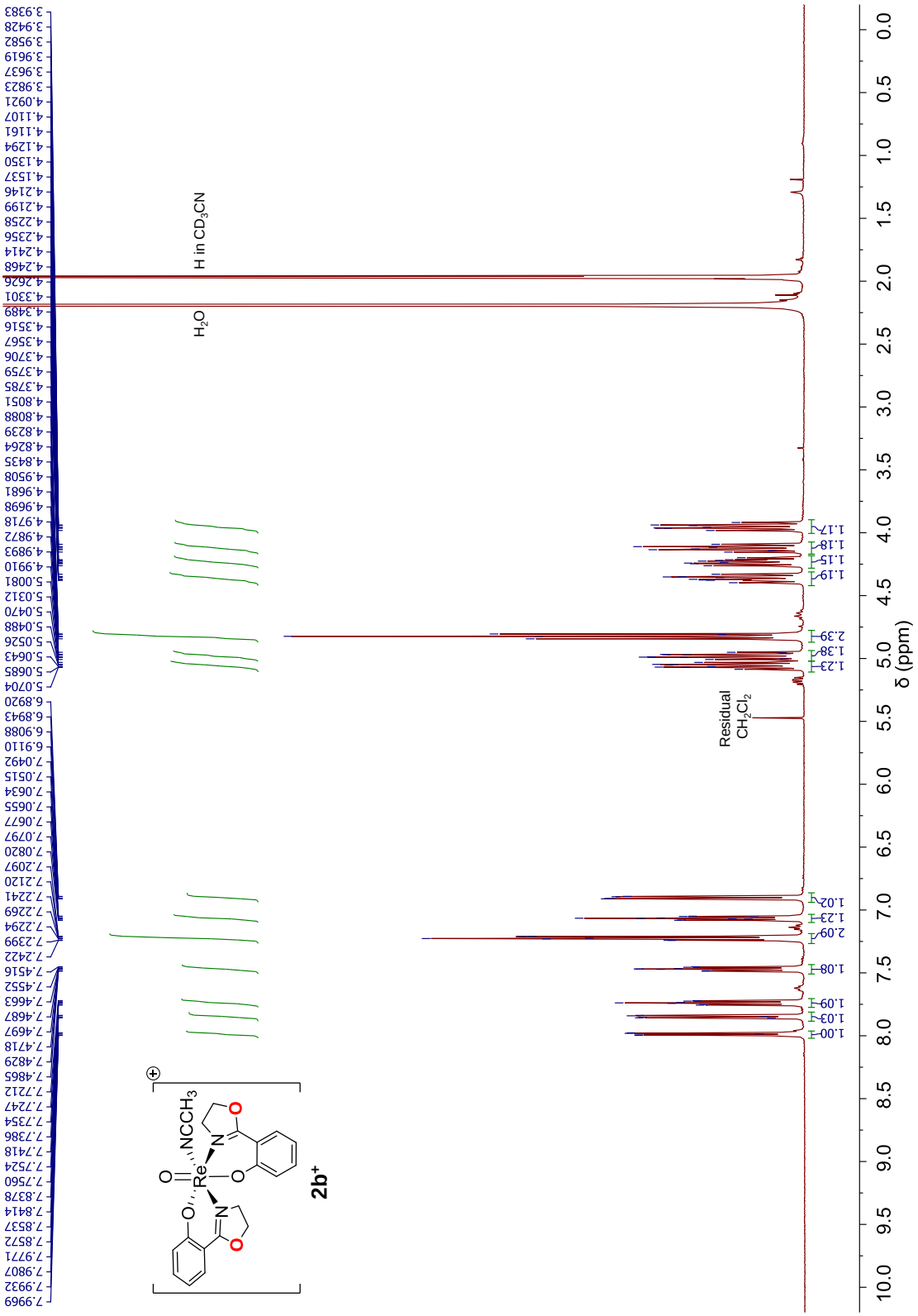


Figure A4. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of N,N-*cis* [Re(O)(*hoz*)$_2$(NCMe)][OTf] (**2b**$^{+}$) at room temperature.

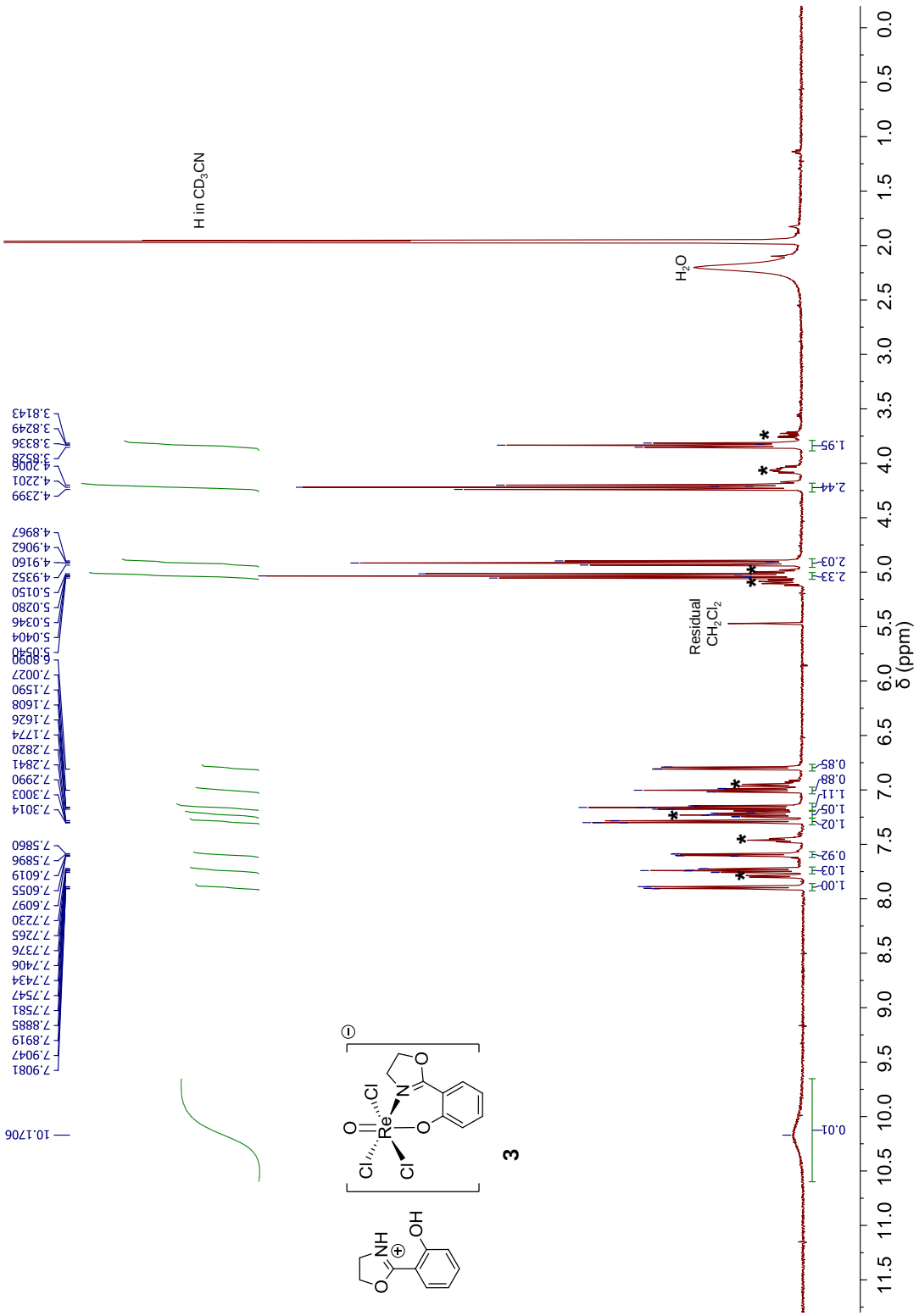


Figure A5. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of [H_2*hoz*][Re(O)(*hoz*)Cl_3] (**3**). Asterisks indicate an uncharacterized impurity containing one Re-coordinated *hoz* or two *hoz* ligands showing symmetry.

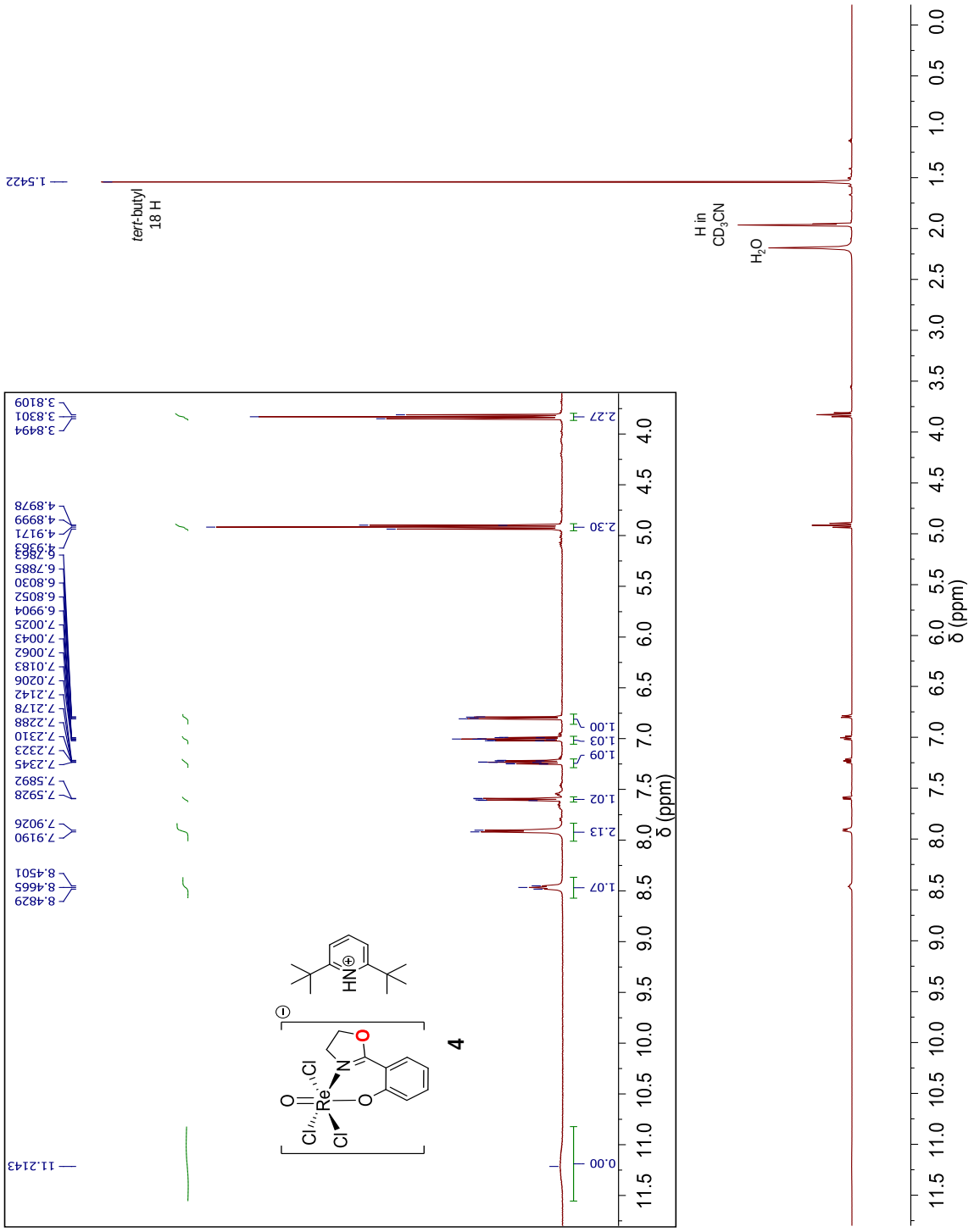


Figure A6. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of [H*t*Bu$_2$*Py*][Re(O)(*hoz*)Cl$_3$] (**4**).

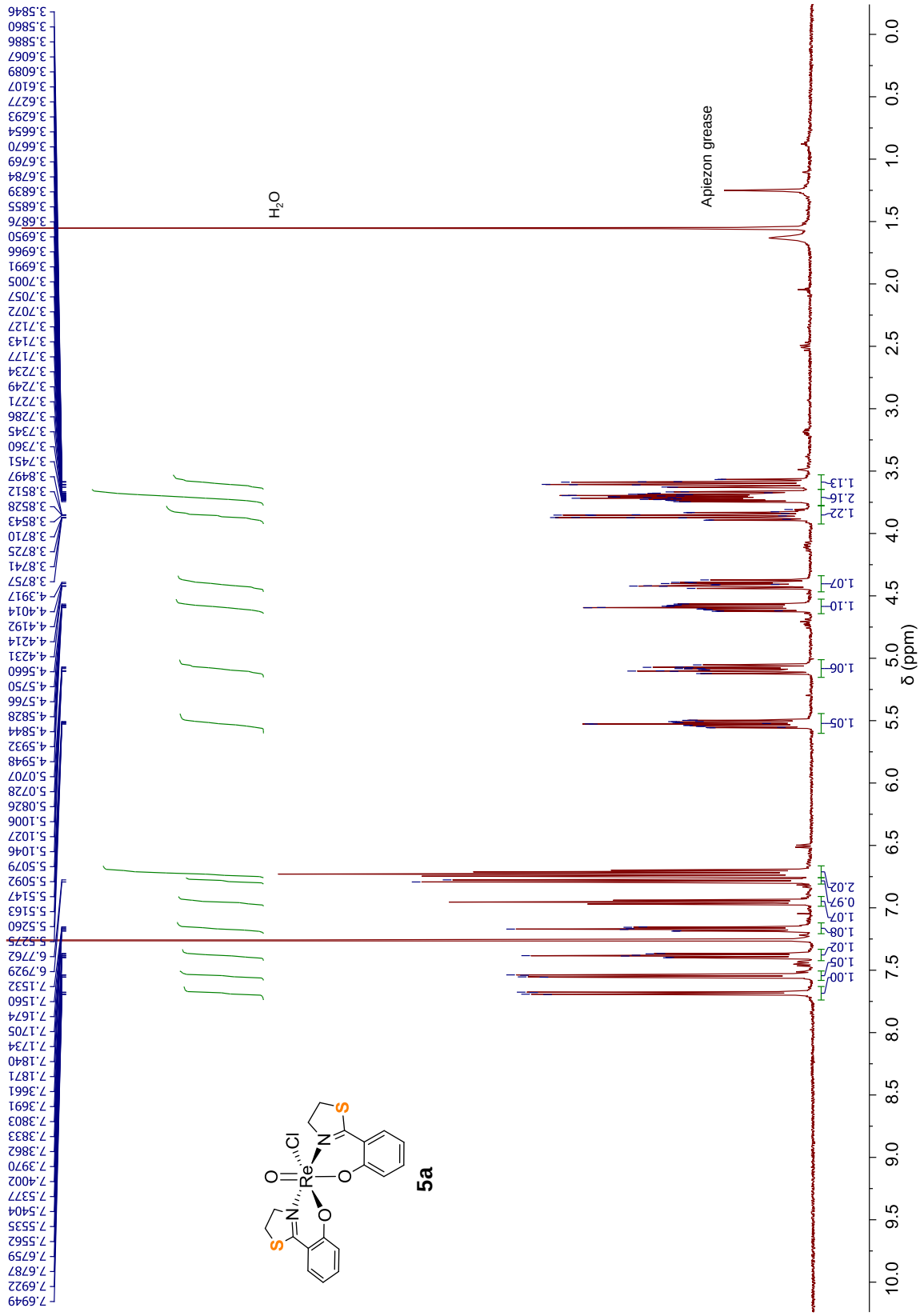


Figure A7. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of N,N-*trans* Re(O)(*htz*)$_2$Cl (**5a**).

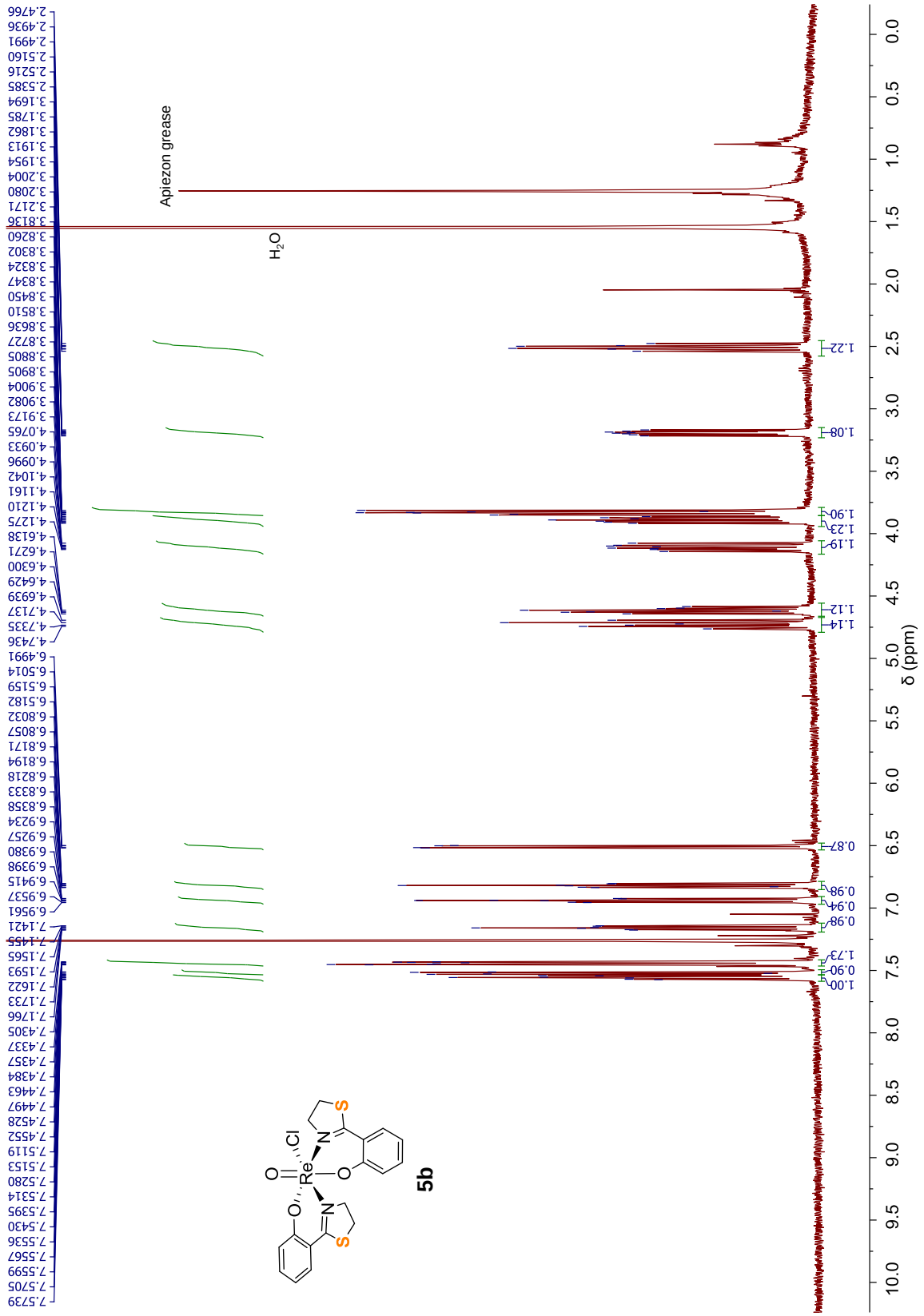


Figure A8. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of N,N-*cis* Re(O)(*htz*)$_2$Cl (**5b**).

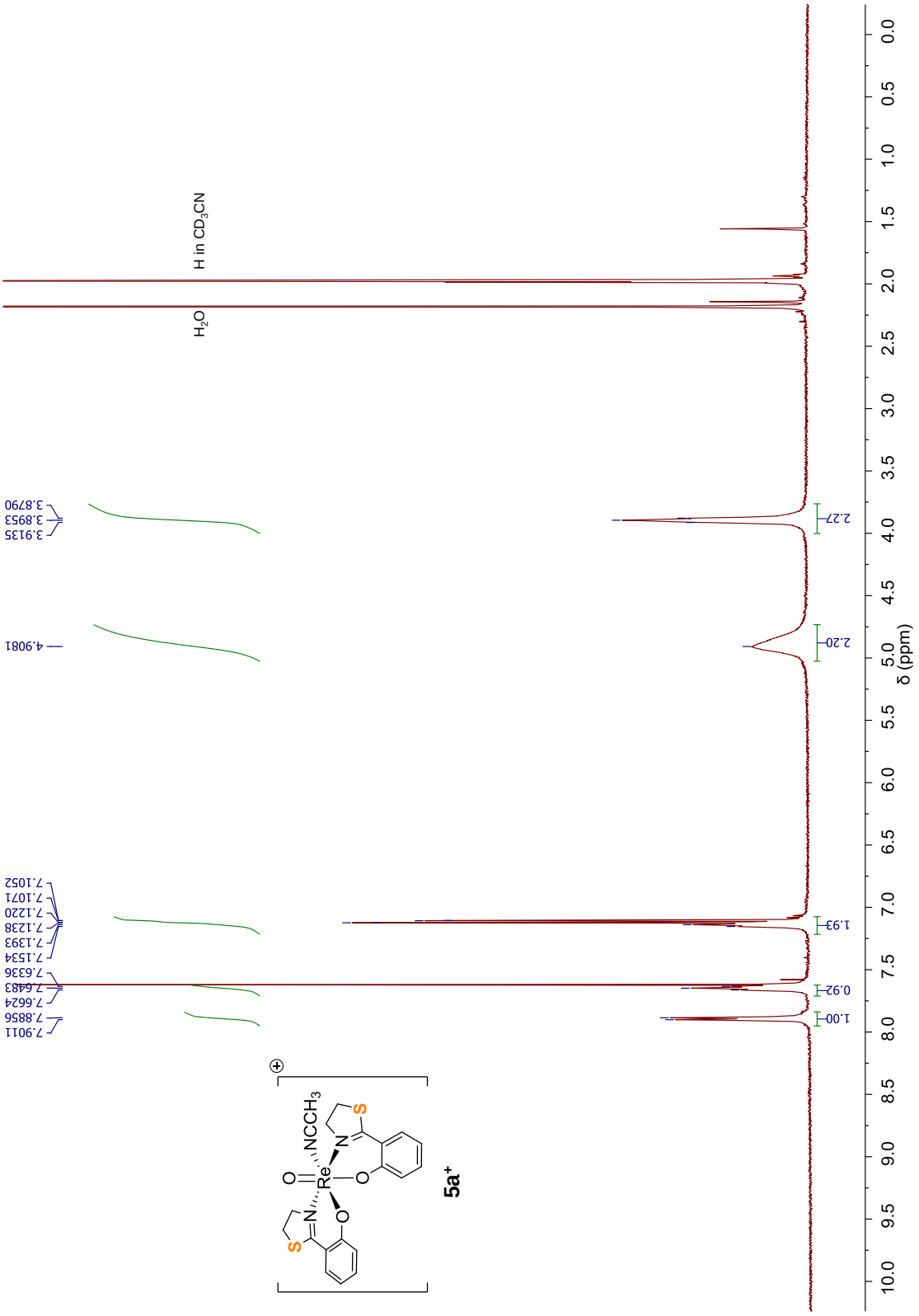


Figure A9. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of N,N-*trans* [Re(O)(*htz*)$_2$(NCMe)][OTf] (**5a**$^{+}$) at room temperature.

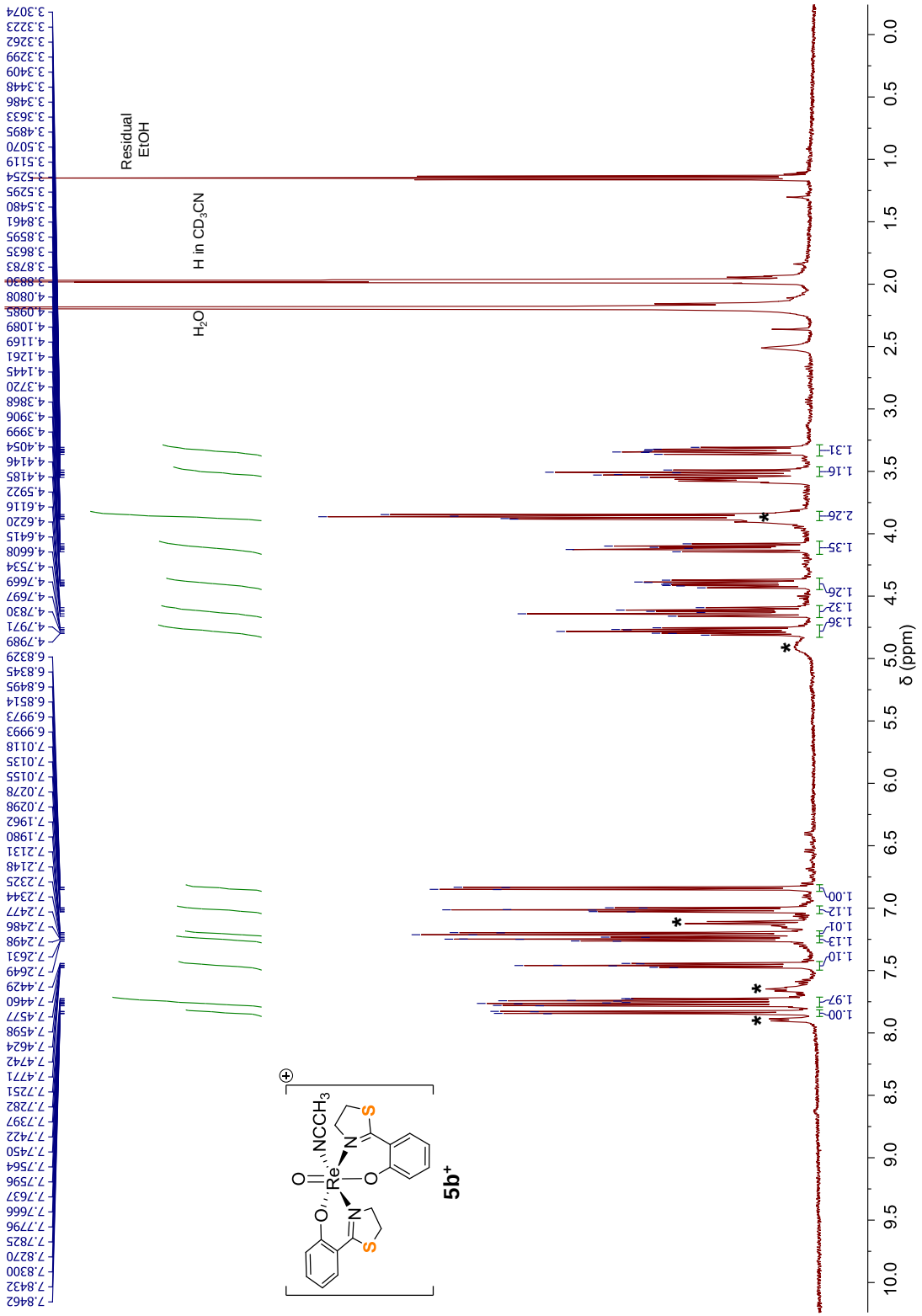


Figure A10. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of N,N-*cis* [Re(O)(*htz*)$_2$(NCMe)][OTf] (**5b**$^{+}$) at room temperature. Impurities marked with asterisks represent **5a**$^{+}$ formed during the chloride abstraction from **5b** under reflux temperature.

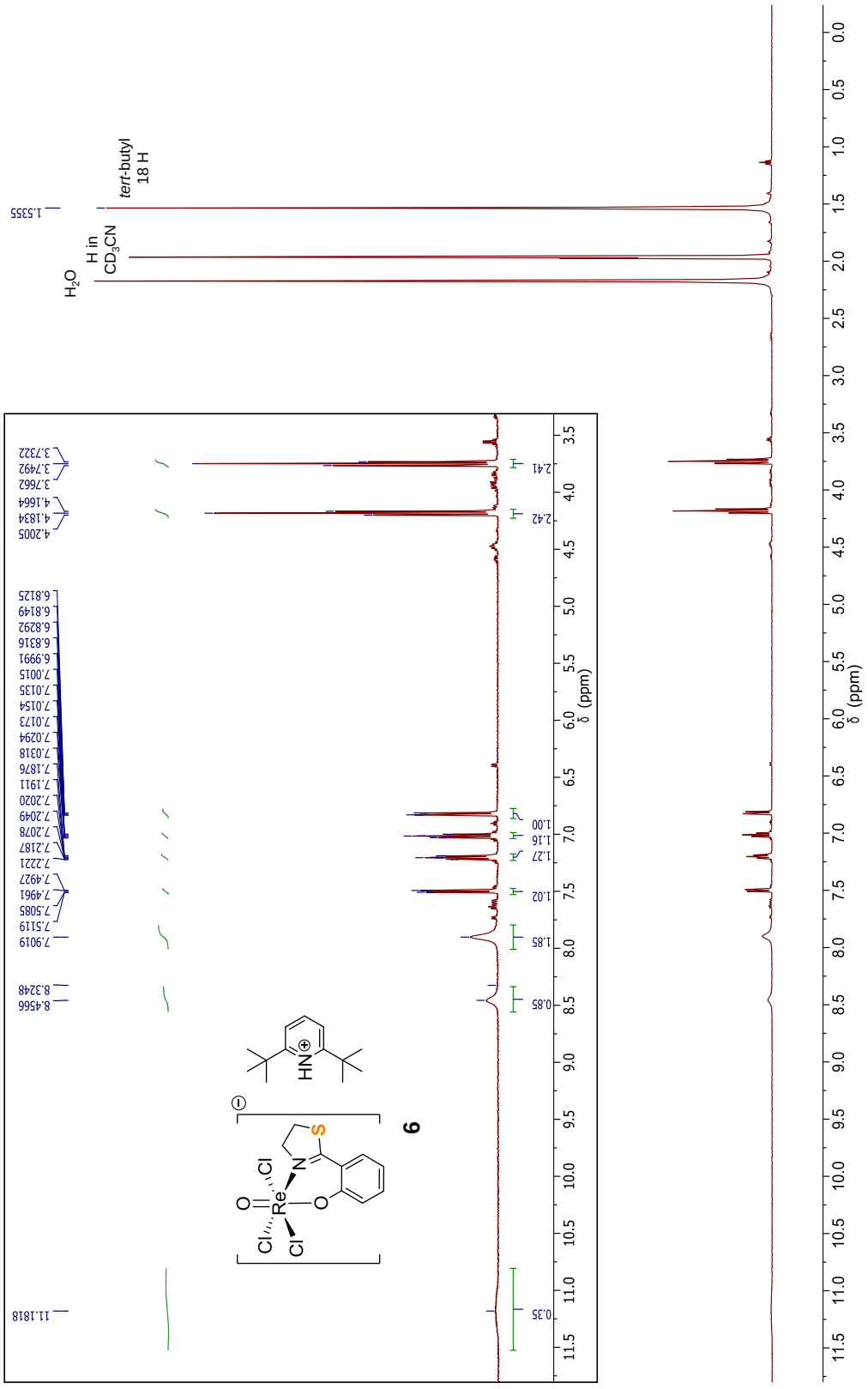


Figure A11. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of [H*t*Bu$_2$*Py*][Re(O)(*htz*)Cl$_3$] (**6**).

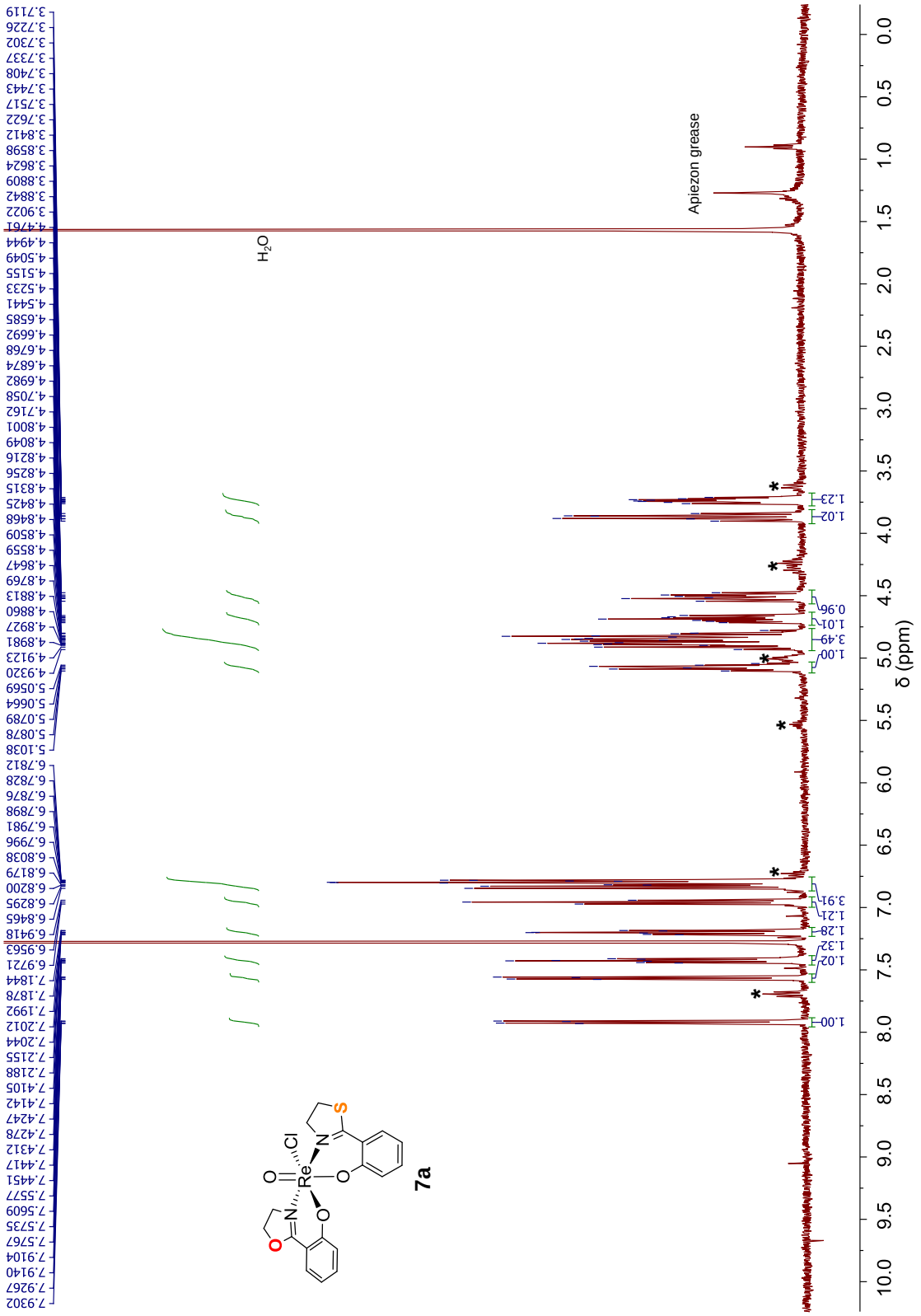


Figure A12. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of N,N-*trans* Re(O)(*hoz*)$_{eq}$(*htz*)$_{ax}$Cl (**7a**). Asterisks indicate an uncharacterized isomer upon dissolution in $CDCl_3$.

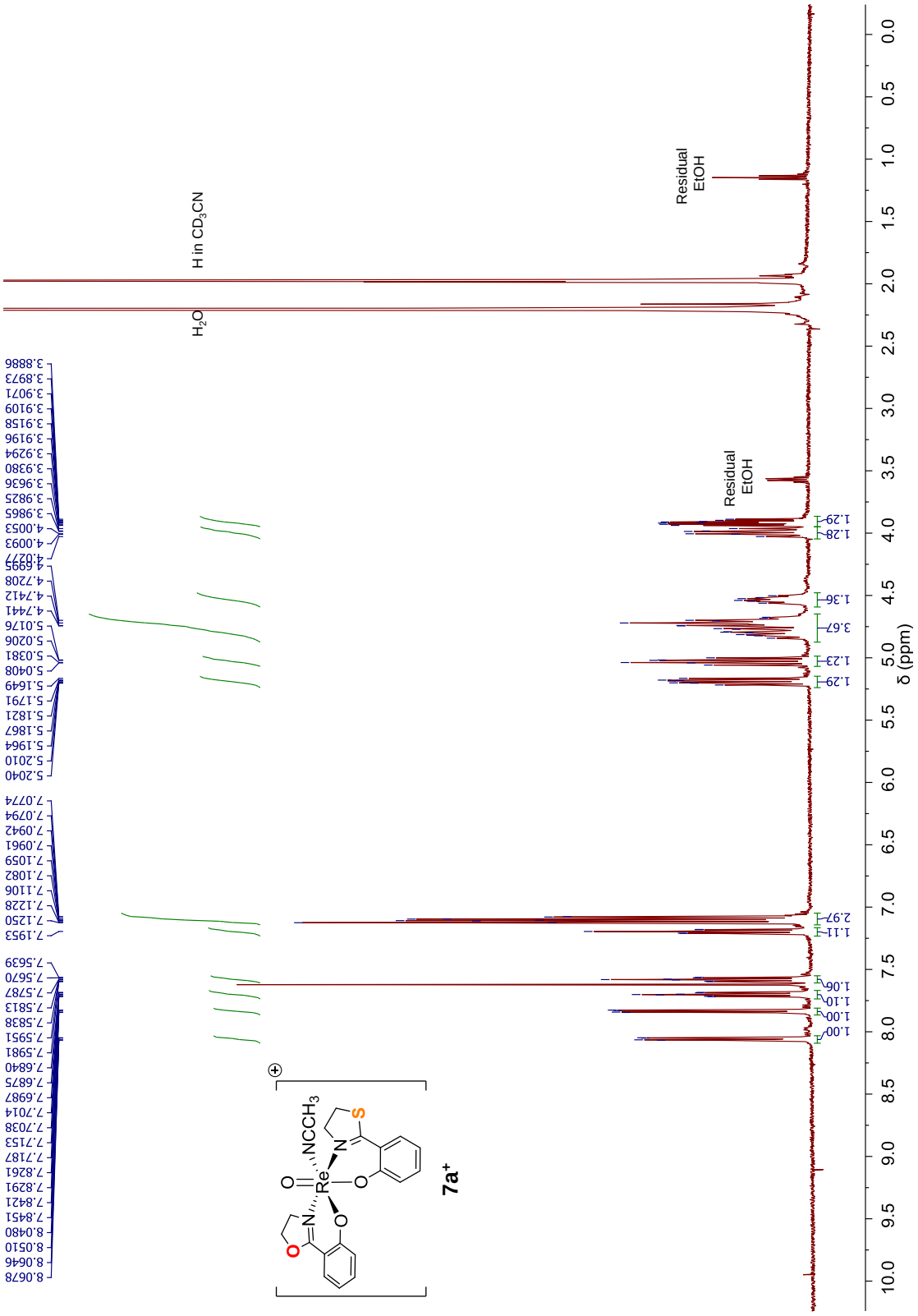


Figure A13. ^{1}H NMR (CD_3CN, 500 MHz) spectrum of N,N-*trans* [Re(O)(*hoz*)$_{eq}$(*htz*)$_{ax}$(NCMe)][OTf] (**7a**$^{+}$) at room temperature.

COORDINATES OF DFT-OPTIMIZED STRUCTURES (corresponding to Table S3)

2a

Atom	X	Y	Z
Re	-0.067682	-0.027931	-0.778052
Cl	1.313178	-1.852678	-1.809258
O	-0.406236	0.522387	-2.345479
O	0.73359	-0.716511	0.909764
O	3.675339	2.028856	-0.129489
O	-0.958095	1.375294	0.355773
O	-3.690636	-1.913242	0.313679
N	1.673166	1.206249	-0.696516
N	-1.678772	-1.281657	-0.418634
C	1.960348	-0.826662	1.420052
C	3.011979	0.028641	1.001691
C	4.287574	-0.098922	1.583224
H	5.084252	0.560141	1.255327
C	4.527126	-1.057821	2.557813
H	5.515875	-1.154398	2.994677
C	3.48275	-1.8963	2.974698
H	3.663351	-2.645621	3.740399
C	2.213082	-1.781471	2.419831
H	1.398586	-2.423865	2.740582
C	2.747093	1.068433	0.025106
C	3.239297	2.878415	-1.236212
H	3.864749	2.639678	-2.100596
H	3.390755	3.915877	-0.939029
C	1.771097	2.486001	-1.43471
H	1.072184	3.208116	-0.999876
H	1.512742	2.33754	-2.484337
C	-2.224015	1.434805	0.772921
C	-3.161284	0.367072	0.698085
C	-4.477013	0.559625	1.183009
H	-5.181881	-0.261372	1.11641
C	-4.868741	1.767056	1.73177
H	-5.882855	1.898956	2.094451
C	-3.938632	2.816752	1.814288
H	-4.233209	3.76922	2.246246
C	-2.643832	2.653461	1.34746
H	-1.91997	3.46037	1.408168
C	-2.800398	-0.932675	0.174675
C	-3.190462	-3.089741	-0.401532
H	-3.78835	-3.19088	-1.310444
H	-3.339131	-3.953573	0.245522
C	-1.725445	-2.744352	-0.672428
H	-1.038822	-3.249344	0.013154
H	-1.421757	-2.960805	-1.695762

2b

Atom	X	Y	Z
Re	-0.070718	-1.008473	-0.067034
Cl	0.701985	-2.378377	-1.963501
O	-0.187705	-2.28877	1.044044
O	0.447749	0.596035	-1.114915
O	4.100428	-0.086187	0.763265
O	-1.831861	-0.892531	-1.021409
O	-2.174593	1.791917	2.327888
N	1.992232	-0.813939	0.544957
N	-0.764739	0.382706	1.330614
C	1.414427	1.511896	-1.169641
C	2.639392	1.332881	-0.481166
C	3.636564	2.321834	-0.564054
H	4.569498	2.176556	-0.030249
C	3.429744	3.472212	-1.314942
H	4.202259	4.232648	-1.368538
C	2.219078	3.641831	-2.001194
H	2.052389	4.538503	-2.591632
C	1.221691	2.674203	-1.935411
H	0.282042	2.796404	-2.465458
C	2.85991	0.118022	0.283639
C	4.050605	-1.280542	1.60139
H	4.114972	-0.954853	2.643066
H	4.910765	-1.901328	1.350727
C	2.697627	-1.909532	1.252552
H	2.787892	-2.76795	0.579799
H	2.136281	-2.215985	2.13561
C	-2.924457	-0.190829	-0.704172
C	-3.050256	0.68015	0.414618
C	-4.275437	1.35155	0.636395
H	-4.36175	2.007443	1.49517
C	-5.352549	1.184079	-0.216347
H	-6.284152	1.707903	-0.028511
C	-5.223199	0.332349	-1.324711
H	-6.059307	0.194128	-2.004776
C	-4.033975	-0.339403	-1.562686
H	-3.925601	-1.001926	-2.416023
C	-1.959153	0.916416	1.341878
C	-1.00663	1.786058	3.209588
H	-1.312892	1.31954	4.148578
H	-0.720655	2.823528	3.3819
C	0.031179	0.965777	2.43409
H	0.83283	1.583014	2.020045
H	0.473569	0.171441	3.038404

5a

Atom	X	Y	Z
Re	0.04995	0.085208	-0.731476
Cl	-1.21791	-1.747875	-1.923682
S	4.229236	-1.822636	0.112581
S	-4.19525	1.905366	0.196558
O	0.826596	1.449814	0.508366
O	-0.611863	-0.870233	0.878157
O	0.317033	0.748597	-2.2709
N	1.814718	-1.048951	-0.500996
N	-1.803959	1.110409	-0.485313
C	3.064669	-3.145609	-0.396891
H	3.575836	-3.843085	-1.061156
H	2.724184	-3.669655	0.498923
C	1.939376	-2.399105	-1.100907
H	2.157766	-2.264405	-2.167463
H	0.99132	-2.92676	-1.011864
C	2.920192	-0.623072	0.069298
C	3.148716	0.689541	0.651844
C	2.101271	1.635023	0.850105
C	2.398038	2.864695	1.476288
H	1.578916	3.560796	1.628455
C	3.686869	3.176634	1.872982
H	3.885935	4.134573	2.345308
C	4.731765	2.261124	1.666328
H	5.745293	2.501352	1.969718
C	4.454907	1.042133	1.077343
H	5.271741	0.342461	0.931826
C	-3.377594	2.843964	-1.153839
H	-3.783983	2.508486	-2.110507
H	-3.567527	3.909841	-1.024075
C	-1.900085	2.496691	-1.000111
H	-1.37476	2.56746	-1.953613
H	-1.403834	3.157687	-0.279243
C	-2.858833	0.728872	0.18378
C	-2.978519	-0.498518	0.956032
C	-1.816959	-1.23806	1.308569
C	-1.932708	-2.355448	2.152841
H	-1.029128	-2.893625	2.422397
C	-3.179031	-2.763566	2.609951
H	-3.254469	-3.638498	3.24943
C	-4.336655	-2.060518	2.244716
H	-5.311064	-2.389112	2.591269
C	-4.230516	-0.939525	1.434959
H	-5.13064	-0.405113	1.147188

5b

Atom	X	Y	Z
Re	-0.04101	-1.173121	0.100736
S	-4.429038	0.603951	0.214373
S	2.35034	2.213994	2.265251
Cl	-0.836848	-2.909859	-1.427613
O	-0.154241	-2.038225	1.561118
O	-0.137009	0.181999	-1.341113
O	1.776134	-1.528672	-0.644561
N	-2.092281	-0.565519	0.326854
N	0.758999	0.430091	1.238769
C	-0.798786	1.32196	-1.533713
C	-2.055235	1.556841	-0.915827
C	-2.702702	2.788248	-1.150167
H	-3.650353	2.996512	-0.663248
C	-2.140295	3.749911	-1.977642
H	-2.652547	4.692991	-2.138162
C	-0.910892	3.494745	-2.601818
H	-0.468106	4.240703	-3.255693
C	-0.247447	2.293101	-2.386768
H	0.706165	2.081531	-2.860638
C	-2.68417	0.50754	-0.125181
C	-4.265089	-0.773669	1.415847
H	-4.123364	-0.354792	2.414757
H	-5.168169	-1.384549	1.39646
C	-3.040729	-1.538384	0.9262
H	-2.55116	-2.07062	1.741661
H	-3.304261	-2.262597	0.147106
C	2.865567	-0.757164	-0.579182
C	3.002929	0.428194	0.205877
C	4.224703	1.141924	0.129219
H	4.338736	2.060527	0.695645
C	5.281399	0.714155	-0.653811
H	6.20225	1.287061	-0.685328
C	5.143182	-0.462652	-1.404732
H	5.96312	-0.814825	-2.024304
C	3.957075	-1.177565	-1.36799
H	3.831892	-2.085723	-1.949617
C	1.971487	0.901582	1.120932
C	0.576765	2.344985	2.722889
H	0.493021	2.589488	3.782308
H	0.117772	3.133698	2.122406
C	0.01649	0.966422	2.400283
H	0.162812	0.270564	3.236302
H	-1.048081	1.010704	2.171153

7a

Atom	X	Y	Z
Re	-0.169743	-0.014384	-0.753542
Cl	1.132534	-1.844326	-1.884666
S	3.969671	2.081985	0.132518
O	-0.444475	0.627602	-2.300849
O	0.546583	-0.878634	0.886769
O	-1.010009	1.341787	0.474646
O	-3.890689	-1.801024	0.176148
N	1.635879	1.119821	-0.53875
N	-1.852673	-1.210444	-0.515313
C	1.767439	-1.154706	1.340169
C	2.887096	-0.360032	0.972136
C	4.156827	-0.703013	1.48291
H	5.026054	-0.123501	1.187286
C	4.321229	-1.782811	2.337789
H	5.309047	-2.034834	2.709656
C	3.204438	-2.542772	2.715103
H	3.324425	-3.385764	3.389706
C	1.941826	-2.230796	2.227448
H	1.069592	-2.813404	2.507722
C	2.703522	0.828604	0.152351
C	3.108597	2.926273	-1.251966
H	3.230204	4.005359	-1.152901
H	3.544946	2.589788	-2.19499
C	1.654287	2.491177	-1.100835
H	1.109378	3.143648	-0.407831
H	1.136909	2.498345	-2.060955
C	-2.28506	1.442694	0.857424
C	-3.271137	0.430858	0.691092
C	-4.589056	0.660134	1.152634
H	-5.331235	-0.118253	1.016334
C	-4.937505	1.851393	1.762948
H	-5.954461	2.013059	2.105033
C	-3.960197	2.845656	1.933998
H	-4.220046	3.784499	2.415294
C	-2.661259	2.644529	1.493456
H	-1.900994	3.408653	1.623302
C	-2.961024	-0.850998	0.094796
C	-3.434322	-2.955504	-0.600974
H	-4.036766	-2.989499	-1.511732
H	-3.611983	-3.845822	0.001456
C	-1.957473	-2.650269	-0.86004
H	-1.287819	-3.224282	-0.213339
H	-1.667429	-2.813428	-1.897284

7b

Atom	X	Y	Z
Re	0.044966	0.115146	-0.760817
Cl	1.409401	-1.672725	-1.925384
O	3.849041	1.944796	0.065787
O	-0.266673	0.71192	-2.319429
O	0.806353	-0.76536	0.862072
O	-0.77348	1.445185	0.499976
S	-3.915242	-2.050995	0.391925
N	1.8186	1.260056	-0.571924
N	-1.630096	-1.119283	-0.449295
C	2.037924	-0.99207	1.318636
C	3.124449	-0.149449	0.965871
C	4.404462	-0.400221	1.496298
H	5.226544	0.250814	1.218601
C	4.615512	-1.469578	2.354938
H	5.60742	-1.661851	2.751146
C	3.538009	-2.296134	2.708131
H	3.697111	-3.132132	3.383535
C	2.264205	-2.060065	2.204237
H	1.424917	-2.692695	2.476515
C	2.893139	1.002841	0.1179
C	3.430583	2.936846	-0.9234
H	3.614747	3.924597	-0.501543
H	4.042539	2.788214	-1.81685
C	1.949643	2.614791	-1.154063
H	1.274987	3.30056	-0.631461
H	1.681902	2.597958	-2.212137
C	-2.059223	1.582814	0.823999
C	-3.059159	0.58344	0.636907
C	-4.393369	0.88874	1.009205
H	-5.173355	0.15514	0.833144
C	-4.73642	2.105479	1.5677
H	-5.767913	2.311155	1.833748
C	-3.736803	3.068807	1.779947
H	-3.990152	4.027353	2.224123
C	-2.425922	2.810525	1.415195
H	-1.645886	3.550739	1.56441
C	-2.743461	-0.745343	0.144733
C	-2.968099	-3.139997	-0.740945
H	-3.406252	-3.069799	-1.738827
H	-3.024035	-4.169073	-0.384312
C	-1.552079	-2.582727	-0.682035
H	-0.985834	-3.021149	0.1487
H	-1.006974	-2.773465	-1.605053

7c

Atom	X	Y	Z
Re	-0.15859	-1.010463	-0.073798
Cl	0.541556	-2.472549	-1.921238
O	-0.226002	-2.227197	1.109825
O	0.245361	0.548068	-1.213741
S	4.409929	0.075512	0.724745
O	-1.967434	-1.007852	-0.927995
O	-2.24762	1.759647	2.367667
N	1.939299	-0.737134	0.408437
N	-0.818798	0.417266	1.308459
C	1.119079	1.552476	-1.261484
C	2.370001	1.467771	-0.598659
C	3.254445	2.561461	-0.69177
H	4.217074	2.523047	-0.191055
C	2.918742	3.701941	-1.408739
H	3.614296	4.533244	-1.459674
C	1.684888	3.766193	-2.070049
H	1.419256	4.651204	-2.641194
C	0.79468	2.701131	-2.002372
H	-0.16338	2.731839	-2.512055
C	2.733946	0.258263	0.133618
C	4.097257	-1.703157	1.04002
H	4.642576	-2.021078	1.929423
H	4.437966	-2.275174	0.17409
C	2.58798	-1.79001	1.232456
H	2.212805	-2.76963	0.940338
H	2.308421	-1.607763	2.277207
C	-3.057026	-0.305124	-0.596421
C	-3.149301	0.618947	0.482706
C	-4.371628	1.291435	0.715877
H	-4.430447	1.993803	1.539495
C	-5.480352	1.068109	-0.081932
H	-6.40906	1.593781	0.114831
C	-5.386697	0.157632	-1.145837
H	-6.248632	-0.027261	-1.781024
C	-4.198921	-0.51198	-1.397886
H	-4.117572	-1.218329	-2.218436
C	-2.031888	0.902643	1.365665
C	-0.977489	1.986148	3.058792
H	-1.161597	1.878733	4.127595
H	-0.664242	3.00774	2.831533
C	-0.049205	0.918666	2.468863
H	0.908636	1.328769	2.14761
H	0.13383	0.089444	3.159922

7d

Atom	X	Y	Z
Re	0.059212	-1.091469	0.094131
Cl	1.047407	-2.721829	-1.464179
O	0.004747	-2.119595	1.446577
O	0.455113	0.325611	-1.232253
O	4.12243	0.318184	0.742829
O	-1.662925	-1.315322	-0.9015
S	-2.402896	2.351297	2.076548
N	2.081678	-0.603129	0.671425
N	-0.811378	0.48662	1.201268
C	1.359912	1.271633	-1.485568
C	2.587852	1.324318	-0.782201
C	3.520598	2.332801	-1.085499
H	4.457829	2.365901	-0.540758
C	3.247117	3.274839	-2.069423
H	3.971372	4.050792	-2.295318
C	2.033327	3.213951	-2.768264
H	1.81618	3.945375	-3.541636
C	1.098098	2.224121	-2.484165
H	0.156673	2.165715	-3.021757
C	2.881738	0.318498	0.224203
C	4.15215	-0.683327	1.804535
H	4.187889	-0.150463	2.758407
H	5.056182	-1.278523	1.675241
C	2.850094	-1.466468	1.600484
H	3.00897	-2.441654	1.130493
H	2.296846	-1.613287	2.528765
C	-2.784457	-0.597728	-0.820869
C	-3.013414	0.490751	0.074465
C	-4.275683	1.135218	0.029928
H	-4.480865	1.952561	0.713677
C	-5.268749	0.754764	-0.853267
H	-6.22086	1.274868	-0.858218
C	-5.030042	-0.312601	-1.732654
H	-5.79991	-0.627301	-2.43159
C	-3.81295	-0.972362	-1.712227
H	-3.613293	-1.802114	-2.383304
C	-2.016222	0.965114	1.024757
C	-0.936098	1.985984	3.116952
H	-1.253037	1.36976	3.961178
H	-0.508129	2.920545	3.481077
C	0.005121	1.244559	2.17544
H	0.63673	1.942711	1.613331
H	0.649568	0.555827	2.723056

7a$^+$

Atom	X	Y	Z
Re	0.207111	0.105675	-0.662175
N	-1.080936	1.70604	-1.225891
S	-3.629461	-2.584636	-0.130919
O	0.465516	-0.114231	-2.32413
O	-0.533456	0.55307	1.111161
O	1.240414	-1.407183	0.084581
O	3.827236	1.963854	0.46181
N	-1.452856	-1.246667	-0.660881
N	1.794895	1.351428	-0.220766
C	-1.768784	0.617571	1.61208
C	-2.807131	-0.213947	1.110097
C	-4.094055	-0.102146	1.678512
C	-4.348308	0.788094	2.711367
C	-3.308651	1.584956	3.212639
C	-2.030885	1.498875	2.673687
C	-2.520478	-1.214374	0.090908
C	-2.728211	-3.067432	-1.657582
C	-1.329911	-2.488927	-1.460165
C	2.521329	-1.478641	0.459552
C	3.407099	-0.369886	0.542232
C	4.74373	-0.575293	0.957898
C	5.202243	-1.838604	1.286011
C	4.322285	-2.930849	1.210318
C	3.006808	-2.754561	0.807439
C	2.969589	0.975568	0.241136
C	3.224276	3.218406	0.001496
C	1.770482	2.832866	-0.296192
C	-1.789272	2.56307	-1.545437
H	-4.904668	-0.709987	1.288939
H	-5.347821	0.865034	3.126189
H	-3.500633	2.279453	4.025243
H	-1.217497	2.110914	3.050501
H	-2.716513	-4.154214	-1.743524
H	-3.240343	-2.632341	-2.51829
H	-0.681834	-3.177597	-0.906074
H	-0.856807	-2.260782	-2.416316
H	5.409545	0.278182	1.015084
H	6.23093	-1.981121	1.599717
H	4.670627	-3.926579	1.469407
H	2.320172	-3.592993	0.748125
H	3.779283	3.537028	-0.882935
H	3.339543	3.948407	0.80213
H	1.070105	3.222174	0.447945
H	1.449599	3.150974	-1.289203
C	-2.674475	3.639639	-1.942567
H	-2.18929	4.603534	-1.763338
H	-3.60085	3.58166	-1.363839
H	-2.906946	3.540775	-3.007142

7b$^+$

Atom	X	Y	Z
Re	0.006416	-0.04683	-0.688147
N	-1.311894	1.517194	-1.299677
O	-3.561361	-2.376433	-0.135727
O	0.303427	-0.267449	-2.34243
O	-0.76397	0.436185	1.071745
O	1.024434	-1.543213	0.094831
S	3.851508	2.185683	0.673621
N	-1.638627	-1.384959	-0.692357
N	1.590309	1.229291	-0.196971
C	-1.995196	0.45607	1.590383
C	-3.008584	-0.414074	1.109946
C	-4.285297	-0.389795	1.703865
C	-4.561381	0.484002	2.746061
C	-3.554183	1.337266	3.221478
C	-2.283374	1.322747	2.657292
C	-2.703153	-1.370213	0.061891
C	-3.089985	-3.135368	-1.296139
C	-1.660321	-2.620921	-1.507923
C	2.317973	-1.623565	0.409944
C	3.211853	-0.514856	0.469023
C	4.569791	-0.765028	0.7939
C	5.030835	-2.037247	1.074338
C	4.133403	-3.117141	1.039314
C	2.802688	-2.911786	0.713405
C	2.76821	0.850545	0.257854
C	2.754363	3.375243	-0.190824
C	1.388868	2.699348	-0.161486
C	-2.058648	2.326411	-1.654838
H	-5.05226	-1.060177	1.331661
H	-5.55051	0.503111	3.191593
H	-3.765247	2.018641	4.040598
H	-1.496927	1.97473	3.024067
H	-3.152627	-4.194125	-1.046967
H	-3.755274	-2.904364	-2.131692
H	-0.897097	-3.311442	-1.137016
H	-1.447123	-2.386123	-2.552197
H	5.273345	0.060805	0.807119
H	6.076689	-2.195907	1.3144
H	4.481327	-4.121803	1.261293
H	2.099002	-3.737163	0.674835
H	3.129702	3.517794	-1.206241
H	2.759146	4.325214	0.34398
H	0.843252	2.939861	0.758795
H	0.786496	3.004025	-1.016683
C	-2.988127	3.34569	-2.099778
H	-2.466253	4.30053	-2.210777
H	-3.790026	3.450769	-1.363067
H	-3.418098	3.049542	-3.061144

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