Supporting Information

Cationic Heteroleptic Ni(II) Complexes of Dithiocarbamate and Phosphine Ligands: Synthesis, Characterization and Proton Reduction Study

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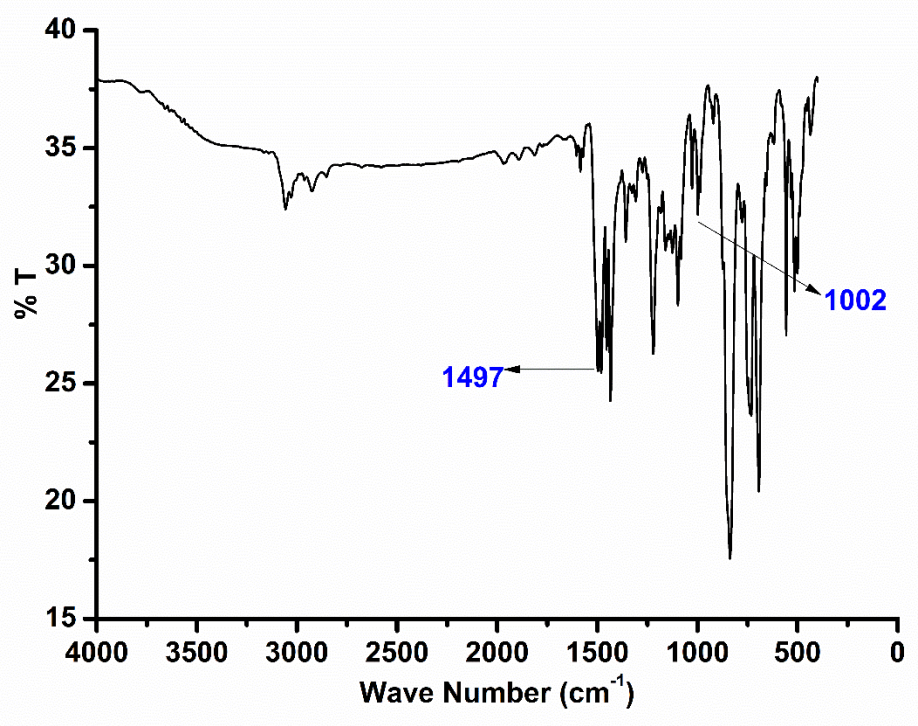


Fig. S1a: IR Spectrum of Complex **1**.

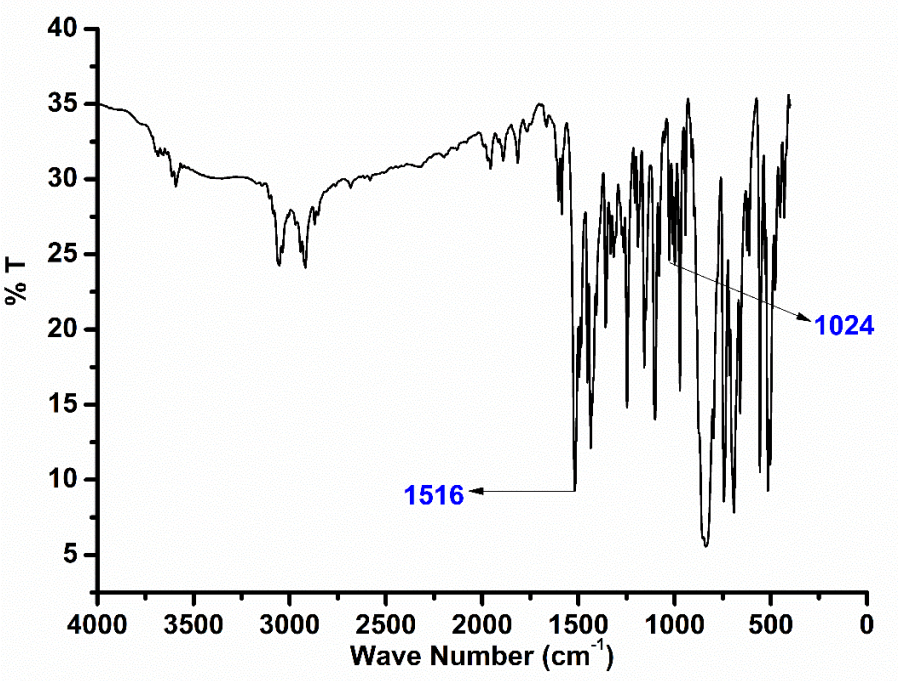


Fig. S1b: IR Spectrum of Complex **3**.

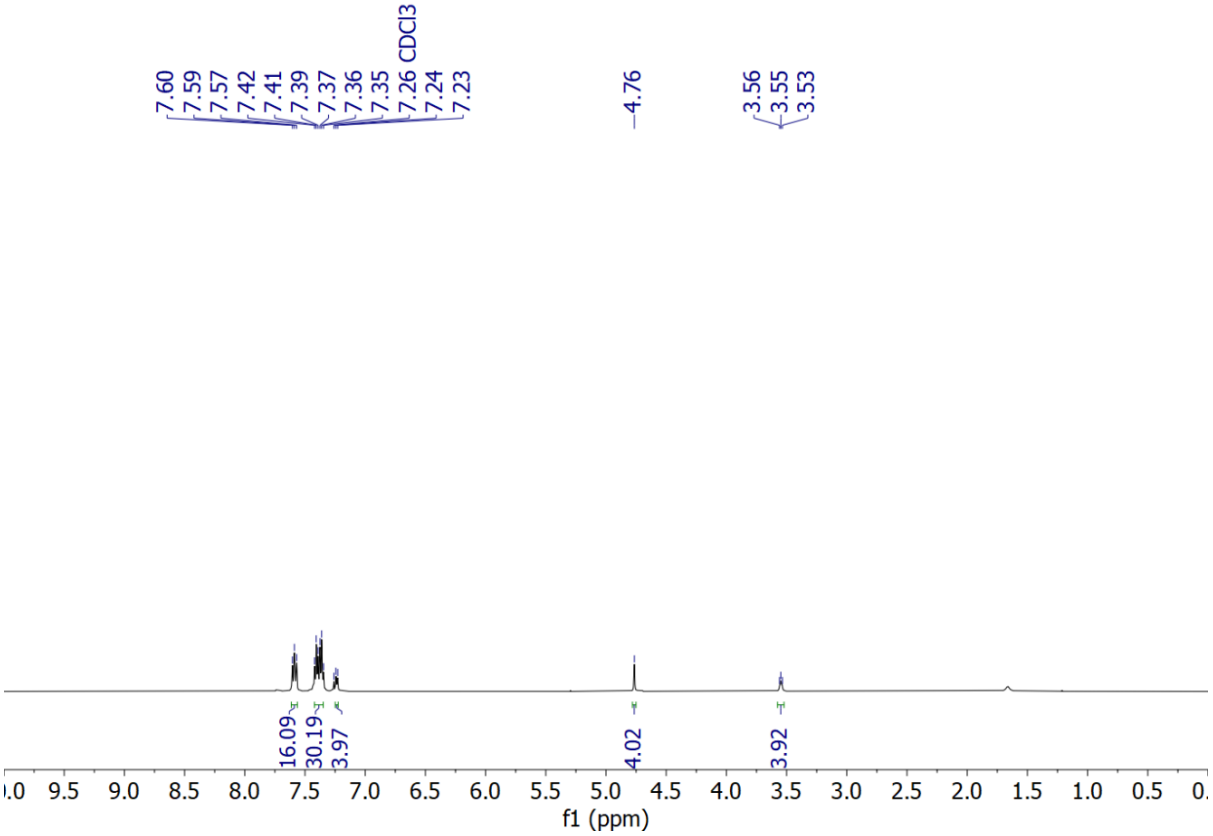


Fig. S2a: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of complex **1**.

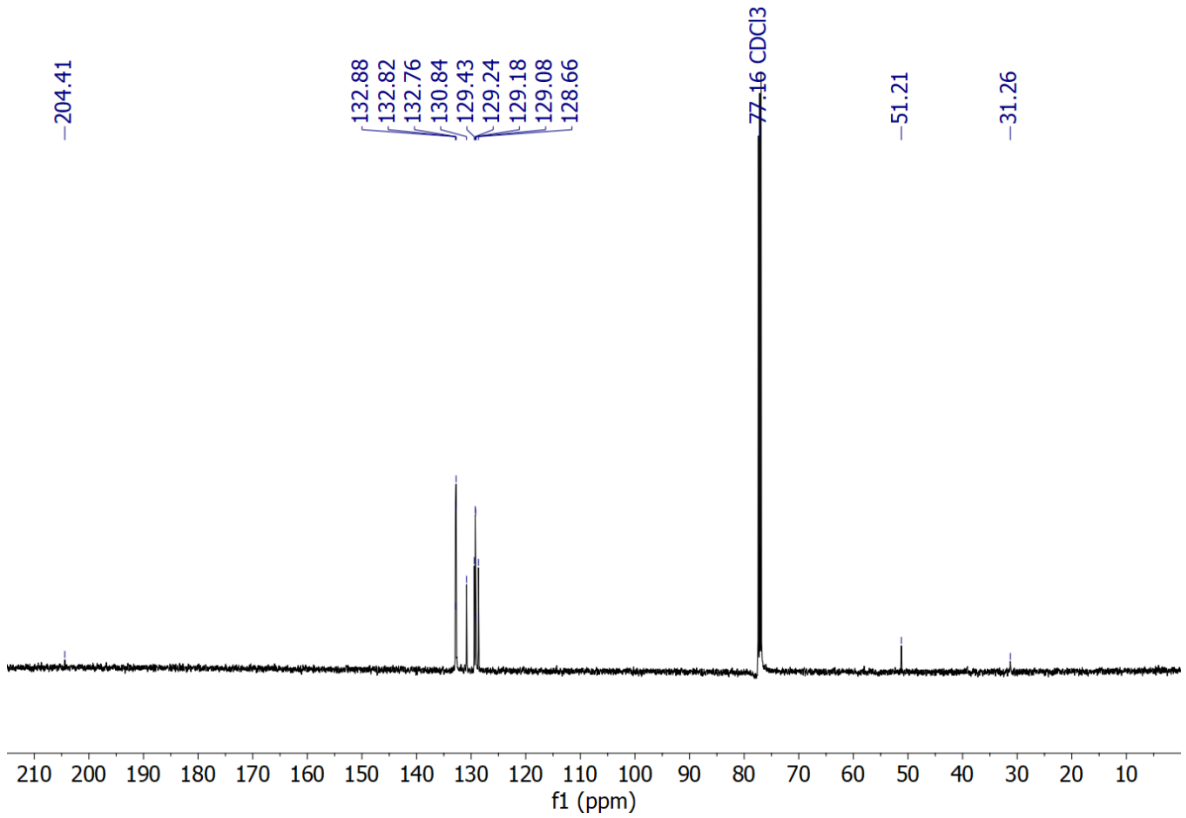


Fig. S2b: $^{13}C\{^{1}H\}$ NMR spectrum (500 MHz, $CDCl_3$) of complex **1**.

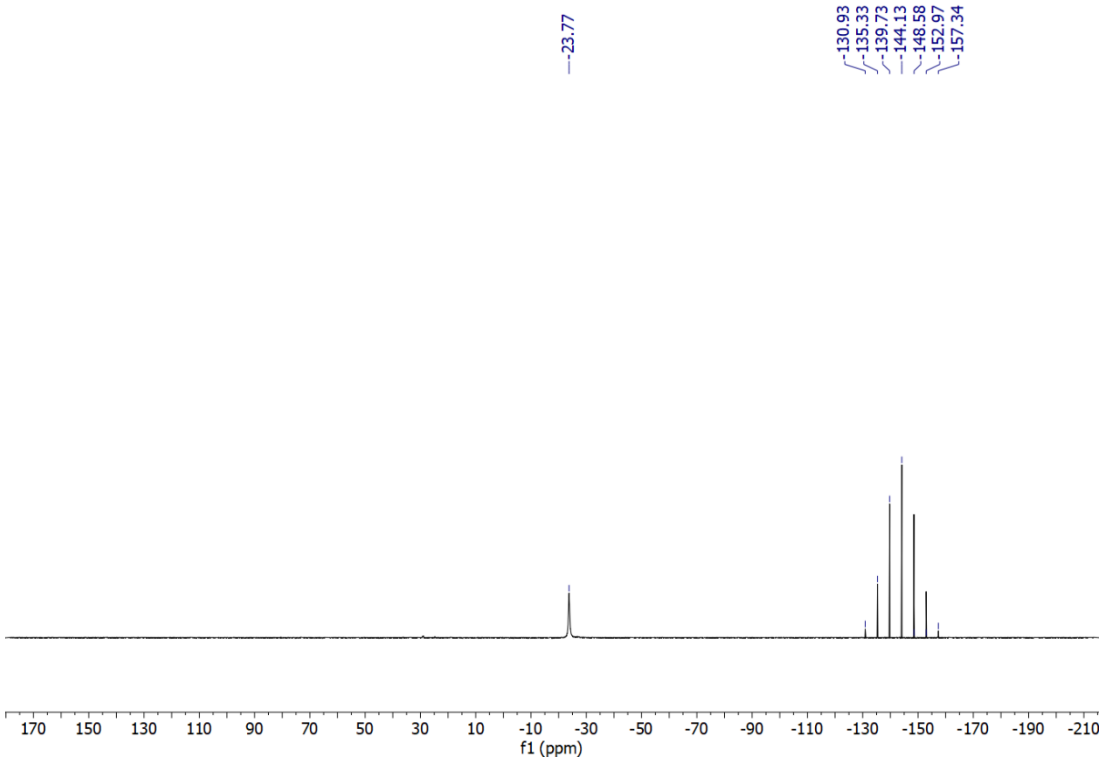


Fig. S2c: $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, $CDCl_3$) of complex **1**.

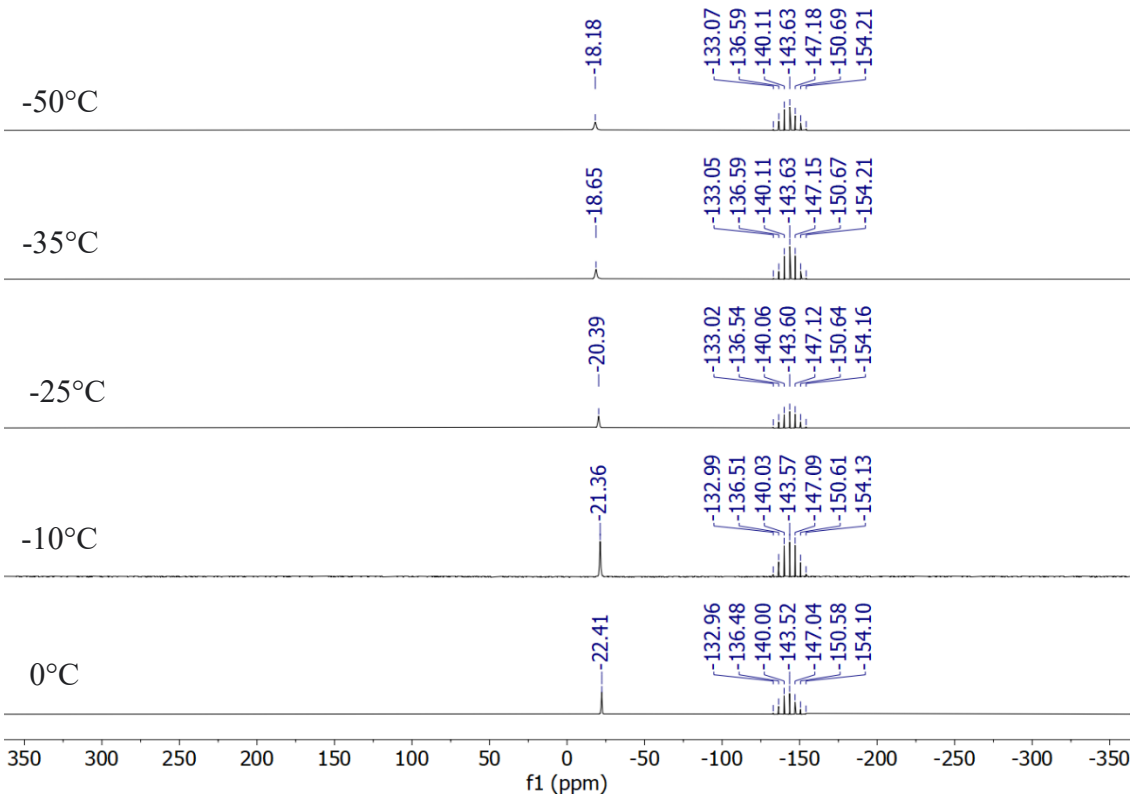


Fig. S2d: $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, $CDCl_3$) of complex **1** at -50°C.

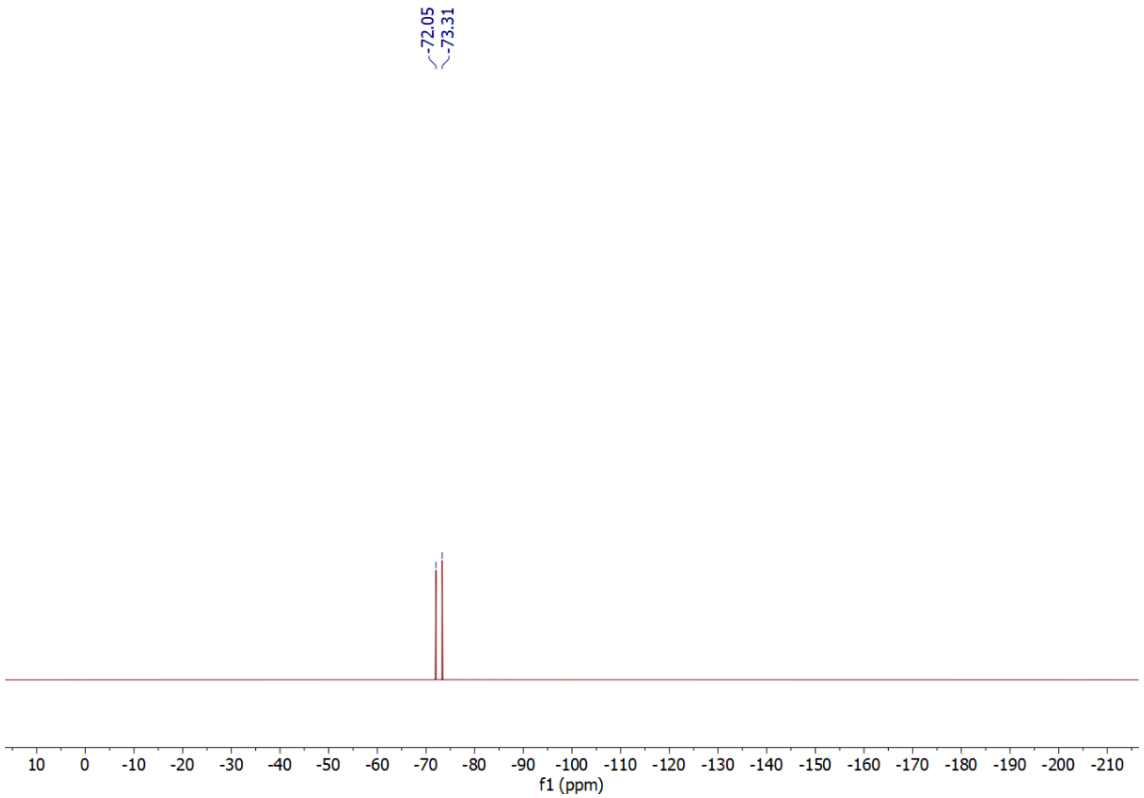


Fig. S2e: $^{19}F\{^{1}H\}$ NMR spectrum (470 MHz, $CDCl_3$) of complex **1**.

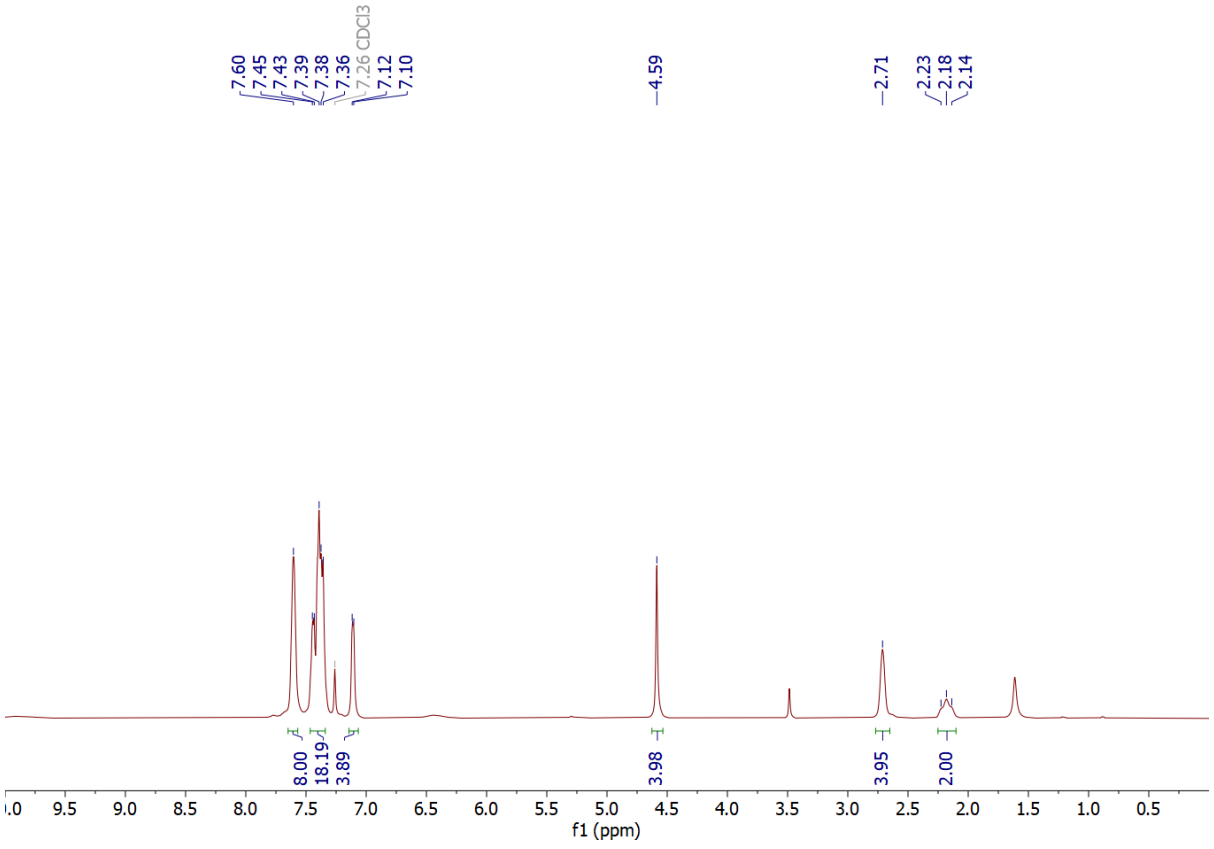


Fig. S2f: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of complex **3**.

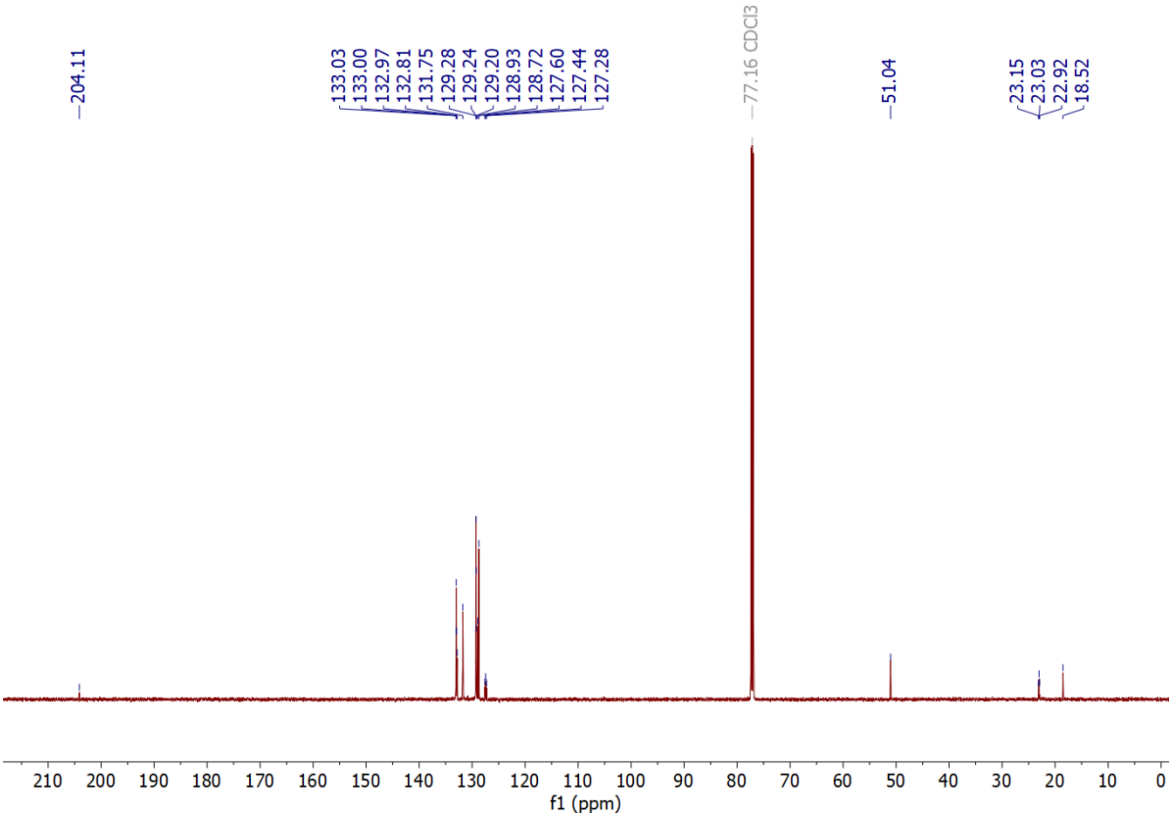


Fig. S2g: $^{13}C\{^{1}H\}$ NMR spectrum (500 MHz, $CDCl_3$) of complex **3**.

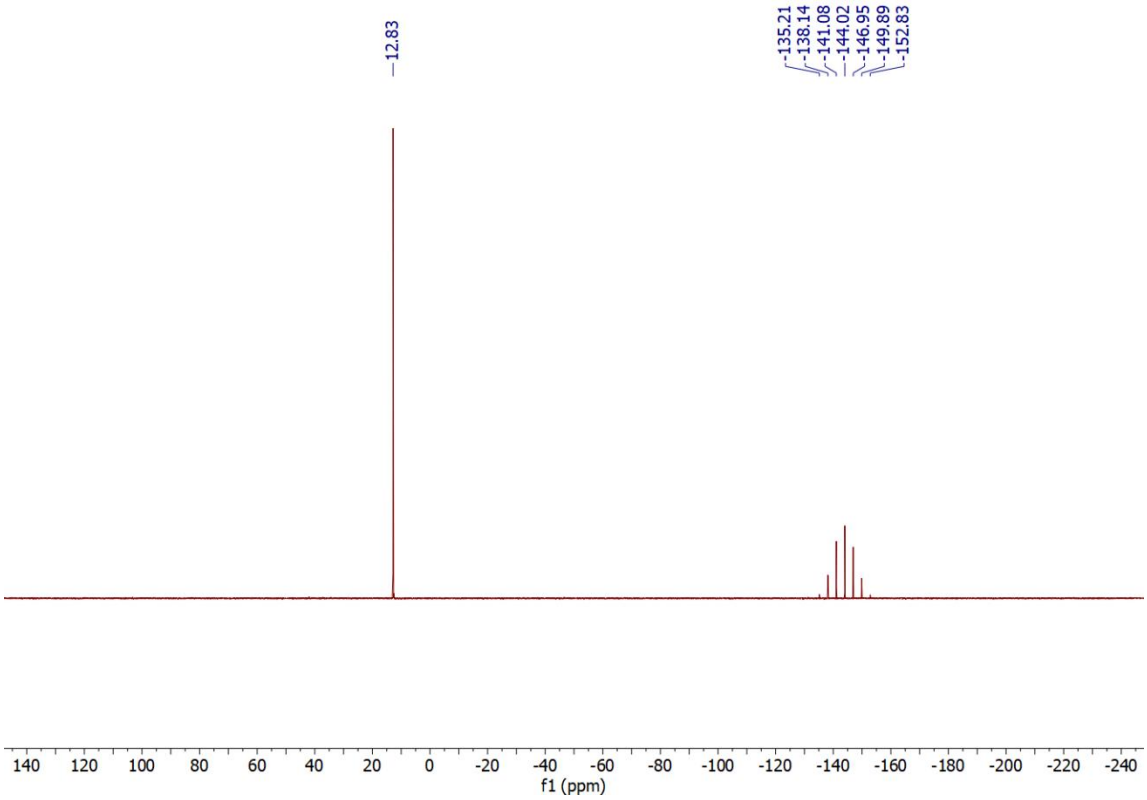


Fig. S2h: $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, $CDCl_3$) of complex **3**.

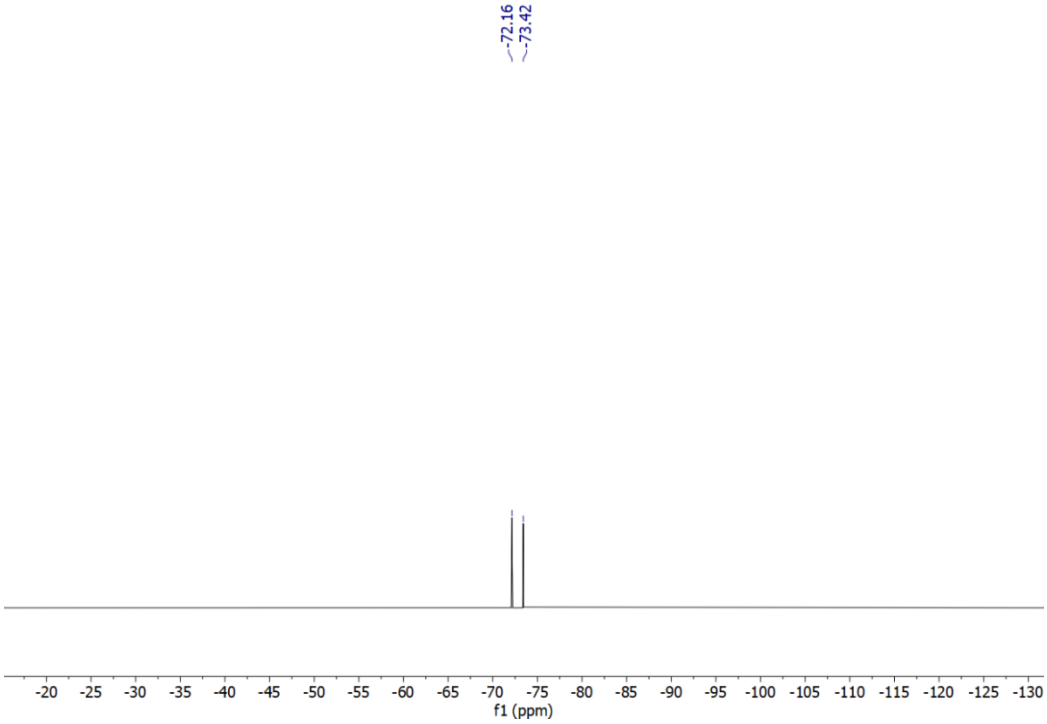
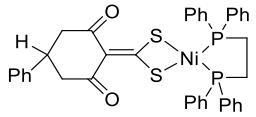
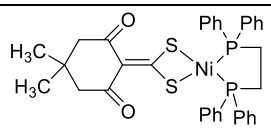
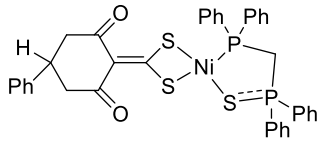
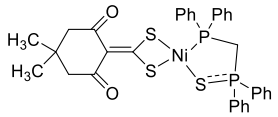
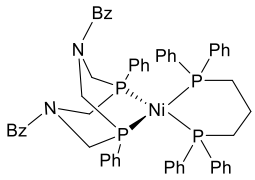
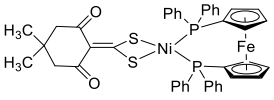
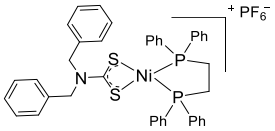
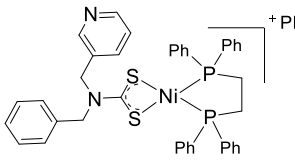
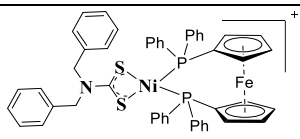
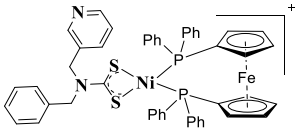
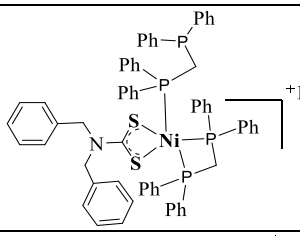
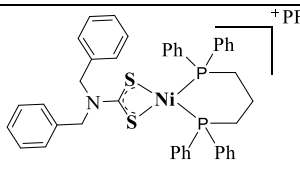


Fig. S2i: $^{19}F\{^{1}H\}$ NMR spectrum (470 MHz, $CDCl_3$) of complex **3**.

Table S1: Comparison of Spectroscopic Parameters from Analogous Ni-Based Complexes.

S. No.	Complexes	^{1}H NMR Spectra	^{13}C NMR Spectra	31p	^{19}F	References
1.		*δ* 7.87–7.27 (m, 25H, Ar–H), 2.81–2.68 (m, 4H, –$(CH_2)_2$–), 3.41–3.36 (m, 1H, –CH–), 2.36 (d, *J* = 16.1 Hz, 4H, P–$(CH_2)_2$–P).	*δ* 210.89 (–CS_2), 195.34 (C=O), 122.34(C=CS_2), 143.00, 132.85 – 126.42, (Ar–C), 25.59, 25.41 (P–$(CH_2)_2$–P), 46.81, 36.80 (–$(CH_2)_2$–,CH–).	δ 53.34 (s, dppe).	–	Anamika et al.,[1]
2.		*δ* 7.79–7.43 (m, 20H, Ar–H), 2.31 (s, 4H, –$(CH_2)_2$–), 0.99 (s, 6H, –$(CH_3)_2$), 2.26 (d, 4H, *J*=10.0 Hz, P– $(CH_2)_2$–P).	*δ* 208.52 (–CS_2), 196.22 (C=O), 121.75 (C=CS_2), 132.89–128.29 (Ar–C), 25.45, 25.26 (P–$(CH_2)_2$–P), 53.38, 30.32 (–$(CH_2)_2$–,–C–), 28.33 (–$(CH_3)_2$).	δ 53.62 (s, dppe).	–	Anamika et al.,[1]
3.		*δ* 7.77–7.22 (m, 25H, Ar–H), 2.79–2.61 (m, 4H, –$(CH_2)_2$–), 3.37–3.32 (m, 1H, –CH–), 3.52 (t, *J* = 9.6 Hz, 2H, P–(CH_2)–P).	–	δ 58.32 (s, dppm).	–	Anamika et al.,[1]
4.		*δ* 7.73–7.29 (m, 25H, Ar–H), 2.34 (s, 2H, –(CH_2)–), 2.28 (s, 2H,	–	δ 58.07 (s, dppm).	–	Anamika et al.,[1]

		–(CH_2)–), 1.00 (s, 6H, –(CH_3)$_2$), 3.49 (t, *J* = 8.6 Hz, 2H, P–(CH_2)–P).				
5.		*δ* 7.62-6.96 (m, 40H), 3.45 (s, 4H), 3.07 (d, *J* = 11 Hz, 4H), 2.61 (d, *J* = 11 Hz, 4H), 2.33 (s, 4H), 1.7 (bs, 2H).	–	δ 19.77 (s, dppp), 0.18 (s, $P^{Ph}{}_2N^{Bz}{}_2$).	–	DuBois et al.,[2]
6.		δ 7.87–7.31(m, 20H, Ar–H), 4.35–4.30 (d, 8H, Cp-H), 2.22 (s, 4H, –(CH_2)$_2$–), 0.93 (s, 6H, –(CH_3)$_2$).	–	δ 29.11	–	Anjali et al.,[3]
7.		δ 7.76 (s, 8H), 7.57 (dd, *J* = 17.0, 6.2 Hz, 12H), 7.38 (s, 6H), 7.18 (s, 4H), 4.71 (d, *J* = 15.3 Hz, 4H), 2.70 (d, *J* = 17.6 Hz, 4H).	δ 204.3, (–CS_2), 132.9 -127.0, (Ar–C), 51.2 Ph–CH_2, 26.3, 25.9 (P–(CH_2)$_2$–P).	δ 61.6 (s, dppe), -144.2 (sept, PF_6).	δ -73.1 (d, PF_6)	Kamlesh et al.,[4]
8.		δ 8.58 (d, *J* = 4.2 Hz, 1H), 8.43 (s, 1H), 7.76 (q, *J* = 7.4 Hz, 9H), 7.57 (dd, *J* = 17.2, 8.3, Hz, 15H), 7.37–7.35 (m, 3H), 7.31 (dd, J = 7.7, 4.9 Hz, 1H), 7.18–7.15 (m, 2H), 4.78 (s, 4H), 2.71 (d, J = 18.3 Hz, 4H).	δ 205.5, (–CS_2), 150.2-124.1 (Ar–C), 51.8, Ph–CH_2, 49.0, C_5H_4N–CH_2, 29.8, 26.3 (P–(CH_2)$_2$–P).	δ 62.6, (s, dppe), -143.6, (sept, PF_6)	δ -73.0 (d, PF_6)	Kamlesh et al.,[4]
9.		δ 7.81 (s, 8H), 7.59 (s, 4H), 7.50 (s, 8H), 7.36 (s, 6H), 7.07 (s, 4H), 4.61 (s, 4H), 4.54 (s, 4H), 4.45 (s, 4H).	δ 202.0 (–CS_2), 134.2-128.8 (Ar–C), 76.4,74.9, 71.2 (Fc), 51.4 Ph–CH_2,	δ 31.6 (s, dppf), -144.2, (sept, PF_6).	δ -73.5, (d, PF_6).	Kamlesh et al.,[4]
10.		δ 8.53 (s, 1H), 8.26 (s, 1H), 7.80 (d, *J* = 6.7 Hz, 8H), 7.54 (dt, *J* = 44.0, 8.0 Hz, 14H), 7.32 (d, *J* = 6.7 Hz, 4H), 7.07 (d, *J* = 6.7 Hz, 2H), 4.60 (d, *J* = 8.0 Hz, 8H), 4.45 (s, 4H).	δ 202.6 (–CS_2), 149.8 – 128.6 (Ar–C), 76.2, 74.5, 71.0 (Fc), 74.5, 71.0 (Cp), 51.9, Ph–CH_2, 48.9. C_5H_4N-CH_2.	δ 32.2 (s, dppf), -143.5 (sept, PF_6).	δ -73.1 (d, PF_6)	Kamlesh et al.,[4]
11.		δ 7.61 – 7.56 (m, 16H), 7.42 – 7.39 (m, 30H), 7.24 (d, *J* = 8.0 Hz, 4H), 4.76 (s, 4H), 3.55 (s, 4H).	δ 204.4, (–CS_2), 132.8–128.6 (Ar–C), 51.2 Ph–CH_2, 31.2 (*P*–CH_2–*P*).	δ -23.77, (*P*–CH_2–*P*), -144.13 (sept, PF_6).	δ -72.58 (d, PF_6).	This Work
12.		δ 7.60 (s, 8H), 7.46 – 7.34 (m, 18H), 7.11 (d, *J* = 6.7 Hz, 4H), 4.59 (s, 4H), 2.71 (s, 4H), 2.18 (t, *J* = 25 Hz, 2H).	δ 204.1 (–CS_2), 133.0-127.2 (Ar–C), 51.0 Ph–CH_2, 23.1, 23.0, 22.9, 18.5 (*P*–CH_2–CH_2–CH_2–*P*).	δ 12.83, (*P*–CH_2–CH_2–CH_2–*P*), -144.02, (sept, PF_6).	δ -72.79 (d, PF_6).	This Work

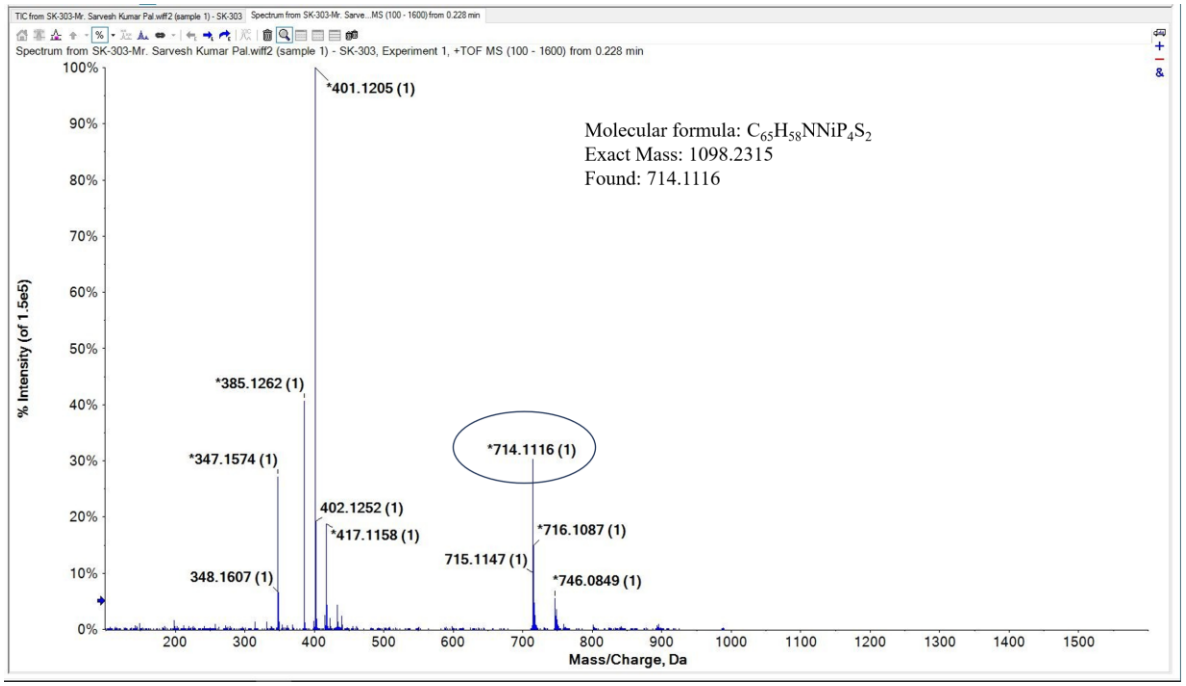


Fig. S3a: MS spectrum of complex **1** positive ion mode.

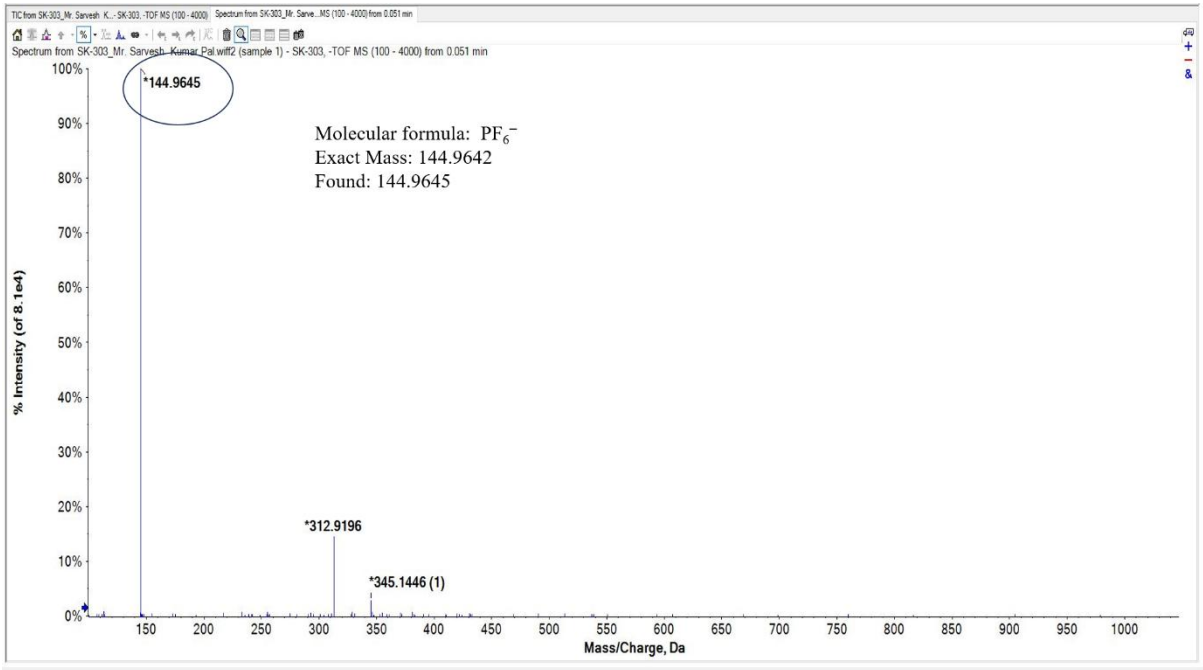


Fig. S3b: MS spectrum of complex **1** negative ion mode.

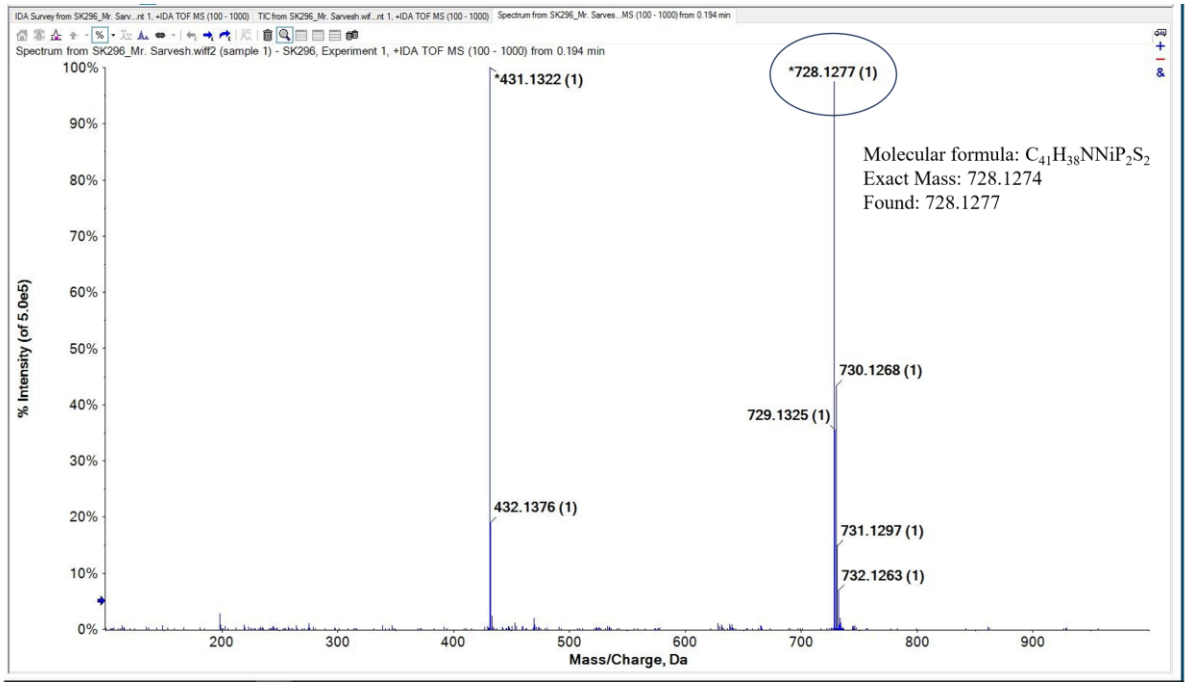


Fig. S3c: MS spectrum of complex **2** positive ion mode.

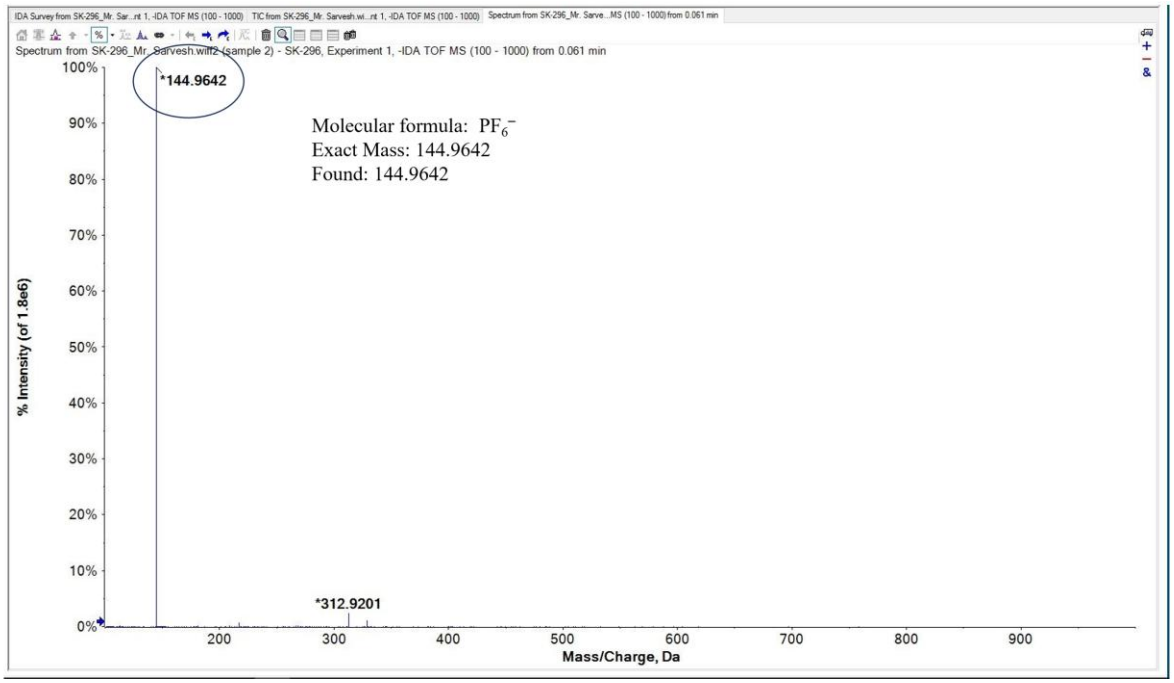


Fig. S3d: MS spectrum of complex **2** negative ion mode.

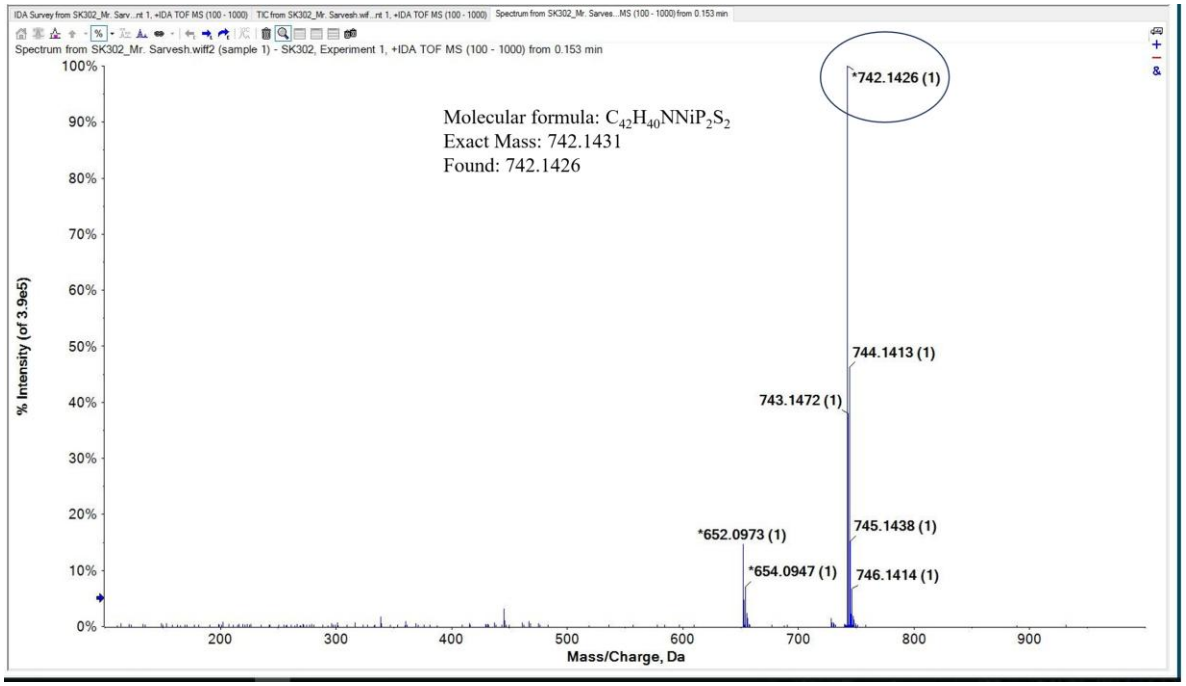


Fig. S3e: MS spectrum of complex **3** positive ion mode.

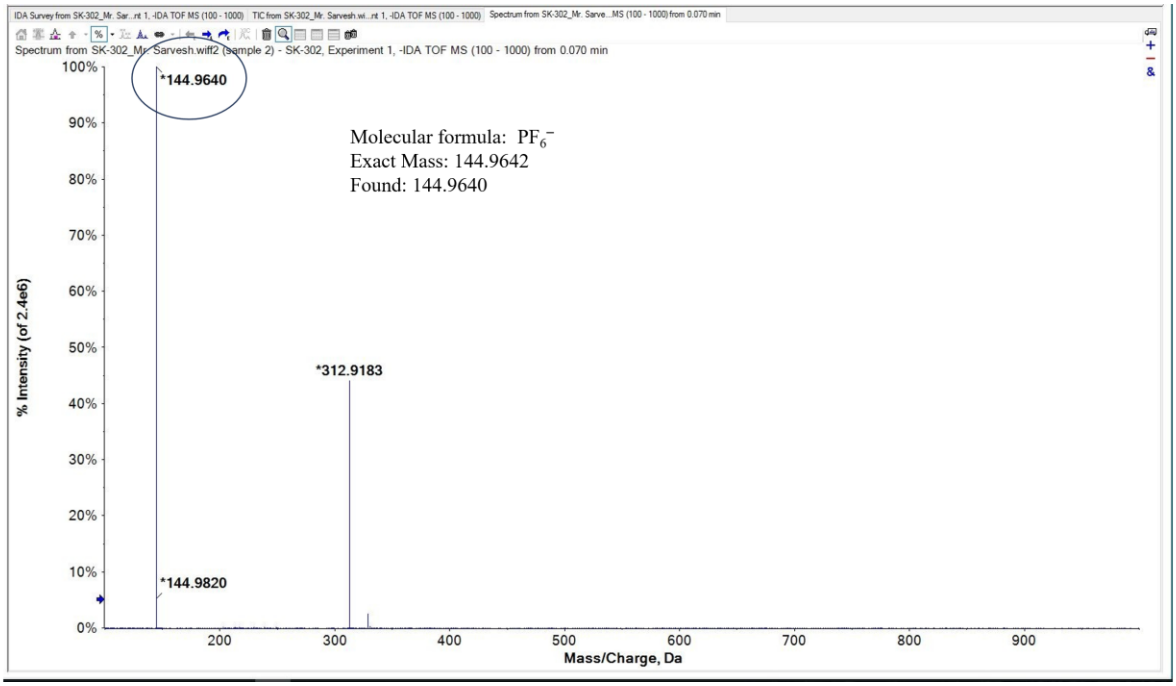


Fig. S3f: MS spectrum of complex **3** negative ion mode.

Table S2: Crystal data and refinement parameters for complexes **1** and **3.**

Complex	**1**	**3**
Empirical formula	$C_{65}H_{58}F_6NNiP_5S_2$	$C_{42}H_{40}F_6NNiP_3S_2{\cdot}CH_3OH$
Formula weight	1244.80	920.53
Temperature/K	298(2)	298(2)

Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	14.2266(7)	11.2659(3)
b/Å	14.5459(6)	13.1885(5)
c/Å	17.7323(8)	15.7690(4)
α/°	79.054(4)	68.936(3)
β/°	70.147(4)	84.682(2)
γ/°	61.742(5)	89.924(2)
Volume/Å^3	3038.2(3)	2175.70(12)
Z	2	2
ρ_{calc}g/cm^3	1.361	1.405
μ/mm^{-1}	2.840	0.712
F(000)	1288.0	952.0
Crystal size/mm^3	0.220 × 0.190 × 0.180	0.210 × 0.180 × 0.160
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.904 to 144.294	4.832 to 49.996
Index ranges	-17 ≤ h ≤ 16, -17 ≤ k ≤ 14, -19 ≤ l ≤ 21	-13 ≤ h ≤ 13, -15 ≤ k ≤ 15, -18 ≤ l ≤ 18
Reflections collected	21537	26232
Independent reflections	11747 [R_{int} = 0.0333, R_{sigma} = 0.0475]	7504 [R_{int} = 0.0493, R_{sigma} = 0.0580]
Data/restraints/parameters	11747/0/771	7504/2/510
Goodness-of-fit on F^2	1.042	1.083
Final R indexes R_1[a], wR_2[b] [I>=2σ (I)]	0.0551, 0.1510	0.0539, 0.1442
R_1[a], wR_2[b] [all data]	0.0698, 0.1661	0.0771, 0.1610
Largest diff. peak/hole / e Å^{-3}	0.47/-0.35	0.91/-0.85

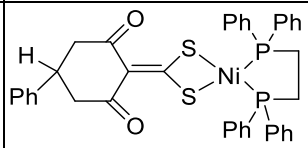
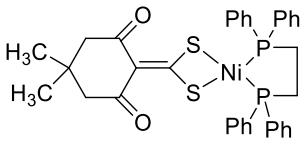
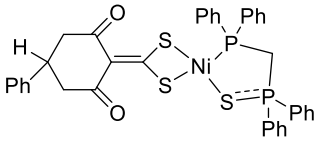
[a]$R1 = \Sigma \| |Fo| - |Fc| \| / \Sigma |Fo|$, [b]$wR_2 = \{[\Sigma w (Fo^2 - Fc^2)/ \Sigma w (Fo^2)^2]\}^{/2}$,
[c]GOF= S= $\{\Sigma [w(Fo^2-Fc^2)^2]/(n-p)\}^{/2}$, where n is the number of reflections, and p is the number of the refined parameters.

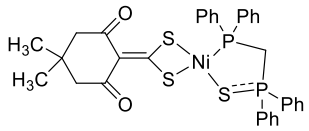
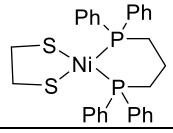
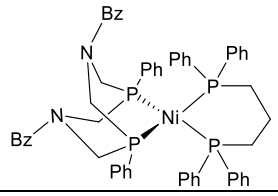
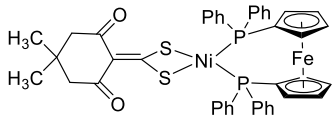
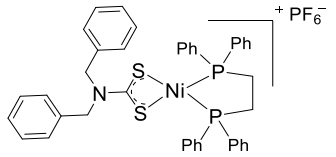
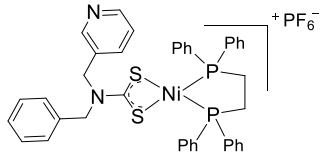
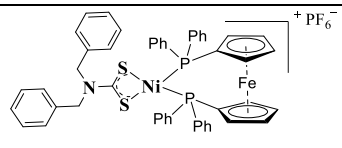
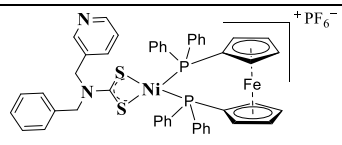
Table S3: Selected Bond Lengths (Å) & Angles (°) for Complexes **1** and **3.**

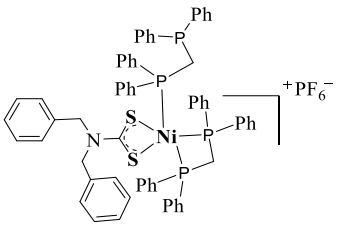
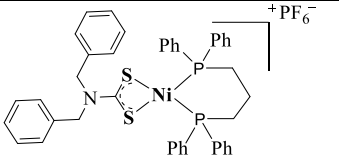
Bonds distance	**1**	**3**
Ni1–S1	2.3895(9)	2.2151(10)

Ni1–S2	2.2550(8)	2.2135(10)
Ni1–P1	2.2127(8)	2.1747(10)
Ni1–P2	2.1818(8)	2.1826(11)
Ni1–P3	2.2356(8)	
Bond angles **(°)**		
S1–Ni1–S2	76.13(3)	79.05(4)
P1–Ni1–S1	101.47(3)	95.32(4)
P1–Ni1–S2	92.00(3)	169.43(4)
P1–Ni1–P3	143.67(3)	
P2–Ni1–S1	100.96(3)	172.26(4)
P2–Ni1–S2	166.20(4)	94.00(4)
P2–Ni1–P1	75.24(3)	92.07(4)
P2–Ni1–P3	103.14(3)	
P3–Ni1–S1	114.23(3)	
P3–Ni1–S2	90.22(3)	

Table S4: Comparison of Selected Bond Lengths (Å) and Bond Angles (°) from Analogous Ni-Based Complexes.

	Selected bond lengths and angles of the complexes					
S. No.		Bond distances		Bond angles		References
1.		Ni1–S11	2.1963(11)	S13–Ni1–S11	77.66(4)	Anamika et al.,[1]
		Ni1–S13	2.1937(9)	P1–Ni1–P2	86.97(4)	
		Ni1–P1	2.1867(11)	P1–Ni1–S11	176.67(4)	
		Ni1–P2	2.1636(9)	P2–Ni1–S11	96.18(4)	
		C12–S11	1.734(3)	P1–Ni1–S13	99.17(4)	
		C12–S13	1.733(4)	P2–Ni1–S13	173.82(4)	
		C12–C14	1.394(4)			
2.		Ni1–S11	2.2004(8)	S13–Ni1–S11	77.80(3)	Anamika et al.,[1]
		Ni1–S13	2.1938(8)	P1–Ni1–P2	87.76(3)	
		Ni1–P1	2.1837(8)	P1–Ni1–S11	174.44(4)	
		Ni1–P2	2.1782(8)	P2–Ni1–S11	96.20(3)	
		C12–S11	1.740(3)	P1–Ni1–S13	98.72(3)	
		C12–S13	1.734(3)	P2–Ni1–S13	170.89(4)	
		C12–C14	1.387(4)			
3.		Ni1–S11	2.1962(14)	S13–Ni1–S11	77.49(5)	Anamika et al.,[1]
		Ni1–S13	2.1670(13)	P1–Ni1–S2	94.07(5)	
		Ni1–P1	2.1763(14)	P1–Ni1–S11	173.03(6)	
		Ni1–S2	2.2390(14)	S2–Ni1–S11	91.93(5)	
		C12–S11	1.732(5)	P1–Ni1–S13	96.39(5)	
		C12–S13	1.709(5)	S2–Ni1–S13	169.27(6)	
		C12–C14	1.411(6)			

4.		Ni1–S11	2.1991(13)	S13–Ni1–S11	76.87(5)	Anamika et al.,[1]
		Ni1–S13	2.1838(13)	P1–Ni1–S2	95.81(5)	
		Ni1–P1	2.2096(13)	P1–Ni1–S11	174.60(5)	
		Ni1–S2	2.2597(13)	S2–Ni1–S11	89.55(5)	
		C12–S11	1.720(5)	P1–Ni1–S13	97.78(5)	
		C12–S13	1.719(5)	S2–Ni1–S13	166.39(5)	
		C12–C14	1.409(6)			
5.		Ni1-P1	2.1787 (10)	P1-Ni1-P2	92.00 (4)	Pei-Hua Zhao et al.,[5]
		Ni1-P2	2.1761 (10)	S1-Ni1-S2	91.24 (4)	
		Ni1-S1	2.1660 (11)			
		Ni1-S2	2.1839 (10)			
6.		Ni1-P1	2.1238(8)	P1-Ni1-P2	85.63(3)	DuBois et al.,[2]
		Ni1-P2	2.1397(7)	P1-Ni1-P4	108.97(3)	
		Ni1-P4	2.1401(8)	P2-Ni1-P4	118.87(3)	
		Ni1-P3	2.1502(8)	P1-Ni1-P3	117.00(3)	
		Ni1 · · · N8	3.399	P2-Ni1-P3	124.19(3)	
		Ni1· · ·N18	3.762	P4-Ni1-P3	101.66(3)	
7.		Ni1–S1	2.2009(5)	S1–Ni–S2	76.93(2)	Anjali et al.,[3]
		Ni1–S2	2.2105(6)	S1–Ni–P1	94.50(2)	
		Ni1–P1	2.2108(6)	S1–Ni–P2	161.95(2)	
		Ni1–P2	2.2082(6)	S2–Ni–P1	166.02(2)	
		S1–C1	1.733(2)	S2–Ni–P2	90.02(2)	
		S2–C1	1.7317(19)	P2–Ni–P1	100.54(2)	
		C1–C2	1.386(3)			
8		Ni1–S1	2.2110(13)	S1–Ni1–S2	79.68(6)	Kamlesh et al.,[4]
		Ni1–S2	2.2126(13)	P1–Ni1–S1	96.61(5)	
		Ni1–P1	2.1638(13)	P1–Ni1–S2	174.36(5)	
		Ni1–P2	2.1647(13)	P2–Ni1–S1	175.13(5)	
		S1–C	1.718(5)	P2–Ni1–S2	97.13(5)	
		S2–C	1.725(4)	P2–Ni1–P1	86.84(6)	
		N1–C(CS_2)	1.303(8)	C–S1–Ni1	84.87(18)	
				C–S2–Ni1	84.65(18)	
9.		Ni1–S1	2.209(2)	S1–Ni1–S2	79.91(9)	Kamlesh et al.,[4]
		Ni1–S2	2.209(2)	P1–Ni1–S1	97.03(9)	
		Ni1–P1	2.159(2)	P1–Ni1–S2	176.12(7)	
		Ni1–P2	2.154(2)	P2–Ni1–S1	174.92(7)	
		S1–C	1.718(6)	P2–Ni1–S2	96.04(9)	
		S2–C	1.714(6)	P2–Ni1–P1	87.14(9)	
		N1–C(CS_2)	1.338(8)	C–S1–Ni1	84.2(2)	
				C–S2–Ni1	84.3(2)	
10.		Ni1–S1	2.2094(7)	S1–Ni1–S2	78.60(3)	Kamlesh et al.,[4]
		Ni1–S2	2.2258(8)	P1–Ni1–S1	91.67(3)	
		Ni1–P1	2.2015(8)	P1–Ni1–S2	170.26(3)	
		Ni1–P2	2.2099(7)	P2–Ni1–S1	167.69(3)	
		S1–C	1.724(3)	P2–Ni1–S2	89.23(3)	
		S2–C	1.718(3)	P2–Ni1–P1	100.50(3)	
		N1–C(CS_2)	1.314(3)	C–S1–Ni1	86.13(9)	
				C–S2–Ni1	85.74(9)	
11.		Ni1–S1	2.2386(9)	S1–Ni1–S2	78.25(3)	Kamlesh et al.,[4]
		Ni1–S2	2.2063(9)	P1–Ni1–S1	90.93(3)	
		Ni1–P1	2.2105(9)	P1–Ni1–S2	168.34(4)	
		Ni1–P2	2.2076(9)	P2–Ni1–S1	167.07(4)	
		S1–C	1.718(3)	P2–Ni1–S2	90.07(3)	
		S2–C	1.713(3)	P2–Ni1–P1	101.09(3)	

		N1–C(CS_2)	1.318(4)	C–S1–Ni1	85.41(12)	
				C–S2–Ni1	86.56(11)	
12.		Ni1–S1	2.3895(9)	S1–Ni1–S2	76.13(3)	This Work
		Ni1–S2	2.2550(8)	P1–Ni1–S1	101.47(3)	
		Ni1–P1	2.2127(8)	P1–Ni1–S2	92.00(3)	
		Ni1–P2	2.1818(8)	P1–Ni1–P3	143.67(3)	
		Ni1–P3	2.2356(8)	P2–Ni1–S1	100.96(3)	
				P2–Ni1–S2	166.20(4)	
				P2–Ni1–P1	75.24(3)	
				P2–Ni1–P3	103.14(3)	
				P3–Ni1–S1	114.23(3)	
				P3–Ni1–S2	90.22(3)	
13.		Ni1–S1	2.2151(10)	S1–Ni1–S2	79.05(4)	This Work
		Ni1–S2	2.2135(10)	P1–Ni1–S1	95.32(4)	
		Ni1–P1	2.1747(10)	P1–Ni1–S2	169.43(4)	
		Ni1–P2	2.1826(11)	P1–Ni1–P3		
				P2–Ni1–S1	172.26(4)	
				P2–Ni1–S2	94.00(4)	
				P2–Ni1–P1	92.07(4)	
				P2–Ni1–P3		
				P3–Ni1–S1		
				P3–Ni1–S2		
				S1–Ni1–S2		
				P1–Ni1–S1		

Description of weak non covalent interaction in complex 3

In the crystal structure of complex **3**, the presence of Ni···H–C anagostic/preagostic interactions,[6, 7] between the metal center and the ortho protons of the dppp phenyl groups can be observed. The ortho-phenyl hydrogen atoms (H36 and H23) of the dppp ligand interact with the nickel center at a distance of 2.98 Å and 3.08 Å, with ∠C–H···Ni angles of 116.75° and 104.73°, respectively (**Fig. S4**).

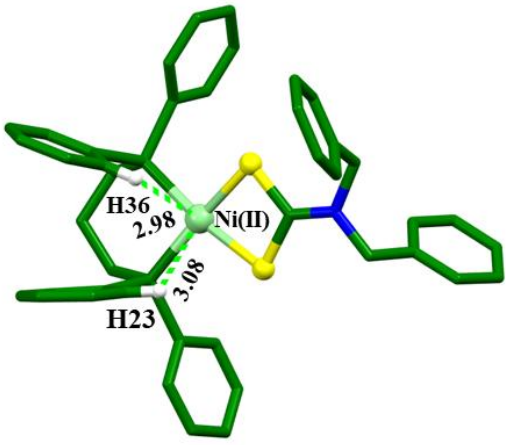


Fig. S4. Intramolecular Ni···H–C an anagostic/preagostic interaction in complex **3.**

Close examination of the X-ray structures of **1** and **3** revealed weak non-covalent intermolecular interactions, like C–H···S and C–H···F. These interactions lead to the formation

of one-dimensional (1D) supramolecular architectures. Complex **1** exhibits C–H···S hydrogen bonding interactions as well as weak π···π stacking interactions between two molecules of complex **1**, resulting in a 1D non-bonding supramolecular chain (**Fig. S5**).[8]

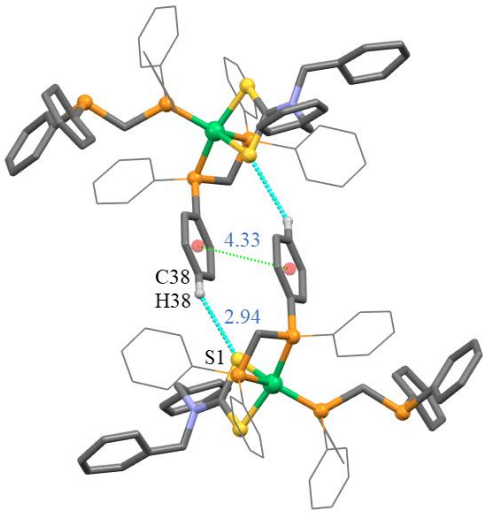


Fig. S5. 1D non-covalent bond polymeric chain network constructed via intermolecular C–H···S and weak π···π stacking interactions (hydrogen atoms omitted for clarity) in the crystal structure of complex **1**.

In complex **3**, the cationic part of the complex is connected through weak C–H···F hydrogen bonding interactions, resulting in a 1D hydrogen-bonded polymeric chain (**Fig. S6**).

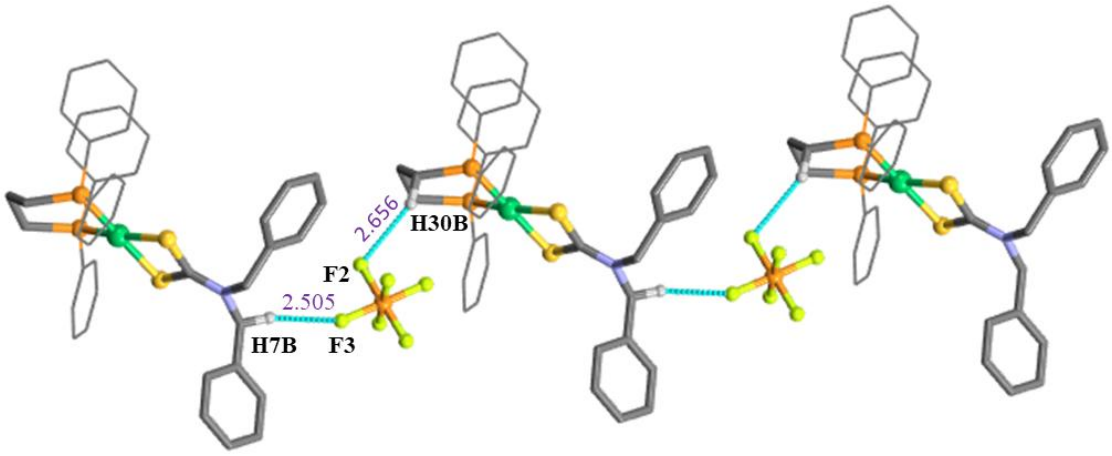


Fig. S6. 1D hydrogen bonding polymeric chain network constructed via intermolecular C–H···F interactions (hydrogen atoms omitted for clarity) in complex **3**.

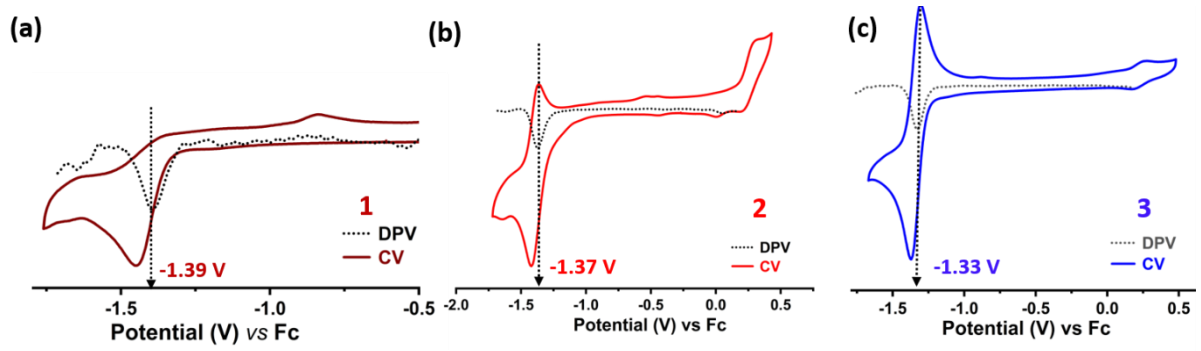


Fig. S7: CVs and DPV plots for complexes (a) **1**, (b) **2** and (c) **3** in CH_3CN containing 0.1 M $TBAPF_6$ at 100 mV/s scan rate.

Estimation of bulk chronocoulometric

The number of electrons transferred during the redox process of complex **3** was estimated from chronocoulometric measurements (**Fig. S8a**). A solution of 3 mL of 20 mM complex **3** was employed, and the chronocoulometric measurement was performed at -1.31 V for 6000 s. **Fig. S8a** exhibited a charge saturation value of 4.27 C at 6000 s. After subtracting the background contribution of the blank (0.049 C at 6000 s), the net charge was determined as 4.22 C. Further, the number of moles of complex used is determined as,

$n_{mol} = C \times V = 20.0 \times 10^{-3}$ (mol L^{-1}) $\times$ 3.0×10^{-3} (L) = 6.00×10^{-5} mole

Theoretical charge (Q_{Th}) required to complete the reduction of complex **3** with *n* number of electron transfer is given by,

$Q_{Th} = n \times F \times n_{mol} = n \times 96485 \times 6 \times 10^{-5}$ C

$= n \times 5.789$ C

The number of experimental electron transfer is obtained by equating the theoretical charge with obtained experimental charge, given as

$$n = \frac{Q_{net}}{Q_{Th}} = \frac{4.221}{5.789} = 0.73 \approx 1$$

This corresponds to the transfer of approximately one electron per molecule of complex **3**, confirming the one electron reduction process at -1.31 V. Due to similar nature of ligands, the other complexes are also likely to exhibit one electron reduction process.

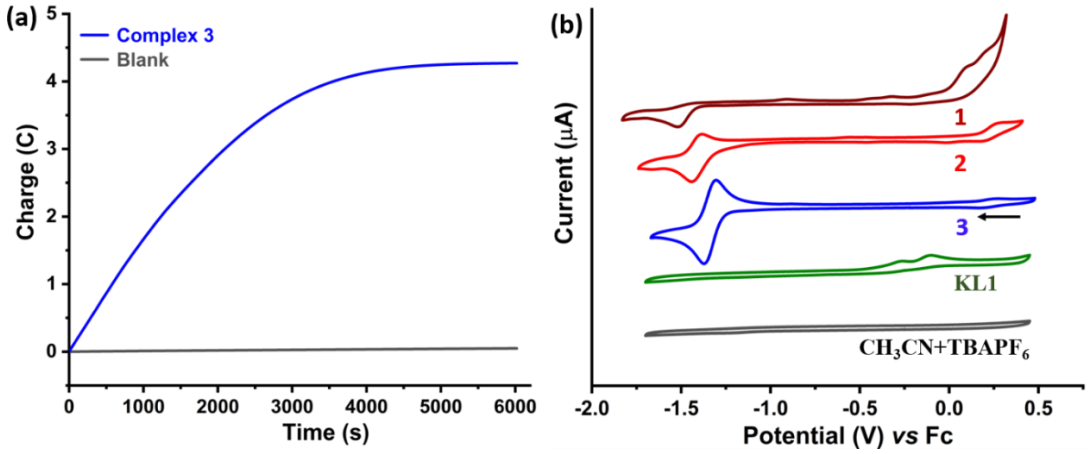


Fig. S8: (a) Bulk chronocoulometric response recorded at –1.4 V for 3 mL solution of 0.1 M $TBAPF_6$ in CH_3CN containing 20 mM of complex **3** (blue curve) and for the blank solution without the complex (black curve). (b) Comparison of CVs of the potassium salt of dithiocarbamate ligand (KL) with complexes **1-3** in CH_3CN containing 0.1 M $TBAPF_6$ at 100 mV/s scan rate.

Randles–Ševčík Equation

A direct correlation between peak currents and the square root of the scan rate signifies diffusion-controlled phenomena. The analysis of the best-fit equation's slope, as per the Randles- Ševčík equation, provides the diffusion coefficient of the catalyst.

$$i_p = 0.4463nFA[C]\left(\frac{nF\nu D_{cat}}{RT}\right)^{1/2} \text{.....} \quad \text{(S1)}$$

where, I_p = peak current, n = 1 (number of electron transferred),

A = 0.07 cm^2 (Electrode area), F = 96500 C/mole (Faraday constant),

R = 8.314 J/K/mole (Gas constant), T = 295 K (Temperature),

D_{cat} = diffusion coefficient of catalyst, ν = Scan rate (V/s)

Overpotential Calculations

For overpotential estimation, $E^T_{1/2}$ (= E_{ref}) is calculated using $E^0_{H^+/H_2}$, pKa, ε_D and $C^0_{H_2}$ by applying the Fourmond's approach[9], given by

$$E^T_{1/2} = E^0_{H^+/H_2} - 2.303\frac{RT}{F}pK_a + \varepsilon_D - \frac{RT}{2F} ln \frac{c_0}{C^0_{H_2}} \text{.....} \quad \text{(S2)}$$

$E^T_{1/2}$ in 4 mM AcOH in CH_3CN is estimated as,

$$E^{T}_{1/2} = (-0.07) - 2.303 \frac{8.314 \times 295}{96485} 22.3 + 0.040 - \frac{8.314 \times 295}{2 \times 96485} ln \frac{4}{3.3}$$

$$E^{T}_{1/2} = -1.33 \text{ V versus } Fc^{+/0}$$

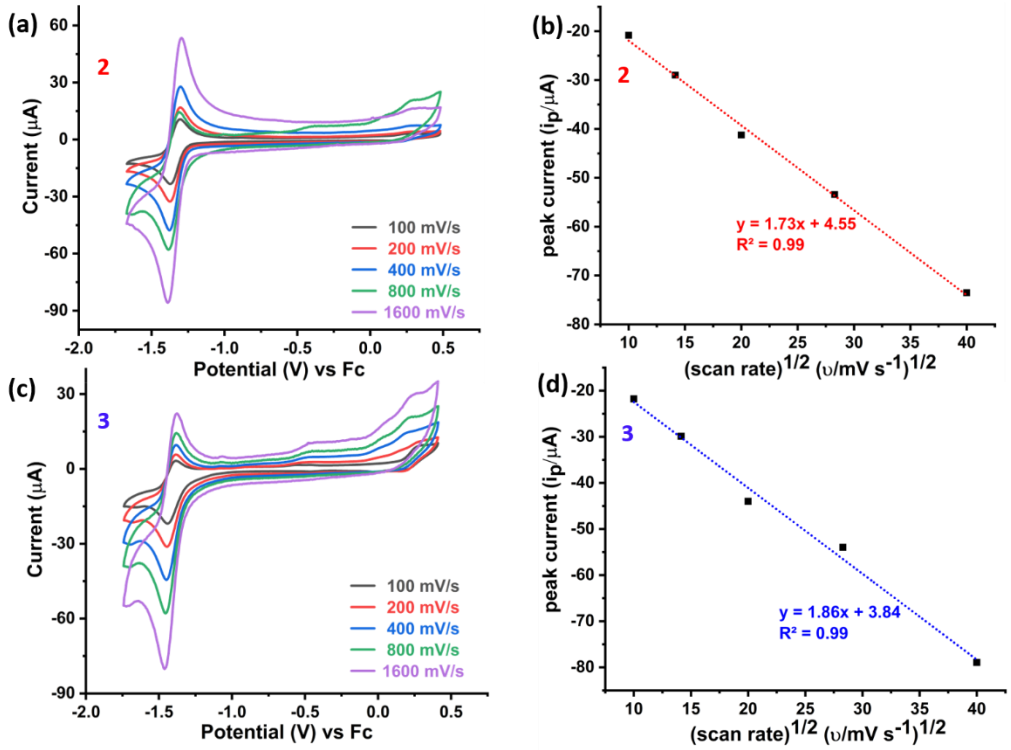


Fig. S9: (a) Effect of variation of scan rate from 100 mV/s to 1600 mV/s on cyclic voltammogram of 1 mM complex **2** (a) and **3** (c) in CH_3CN containing 0.1 M $TBAPF_6$. Fig. (b) and (d) show the variation of peak current with the square root of scan rate for complexes **2** and **3**, respectively. The calculated value of diffusion coefficient (D_{cat}) from the slope (using eq S1), is listed.

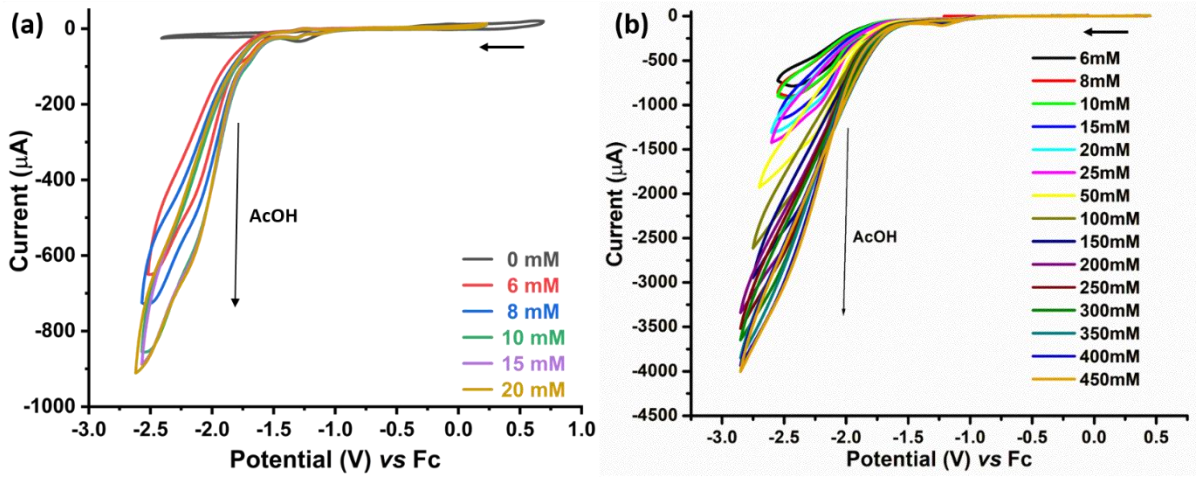


Fig. S10: Variation of the catalytic peak current of complexes **2** and **3** on increasing the concentration of AcOH. CVs was recorded for 1 mM of **2** and **3** in CH_3CN containing 0.1 M $TBAPF_6$ at a scan rate of 100 mV/s vs $Fc^{+/0}$.

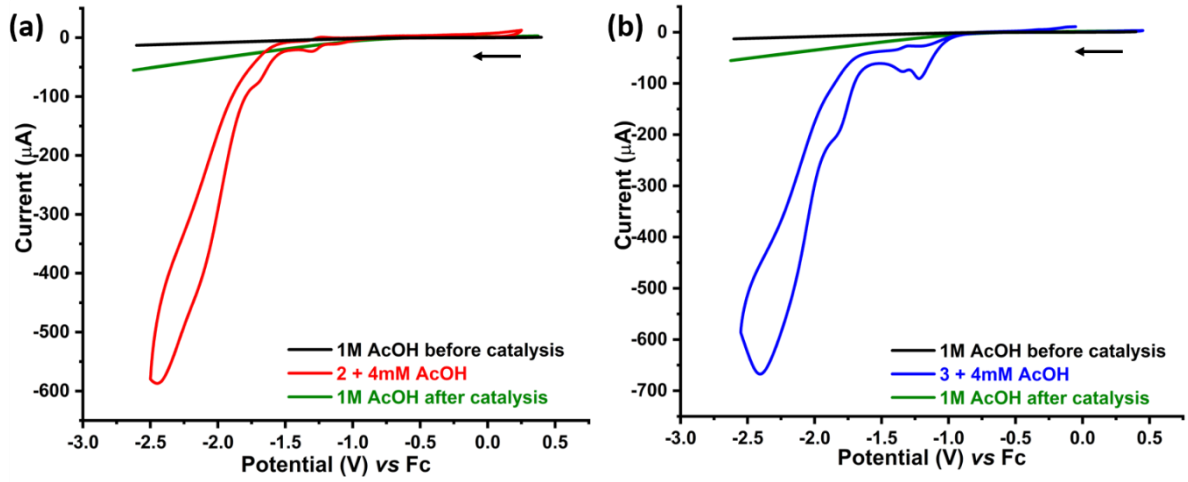


Fig. S11: Rinse test analysis after electrocatalytic proton reduction by complexes (a) 2 and (b) 3 using a glassy carbon working electrode. The black and green lines correspond to CVs recorded in 1 M AcOH at a scan rate of 100 mV/s before and after the catalysis experiment, respectively. The red and blue curves correspond to CVs of 1 mM complexes 2 and 3, respectively, in the presence of 4 mM AcOH. The minor variations in current observed before and after the catalysis experiments (black and green curves), compared with the currents obtained for 1 mM complex in the presence of 4 mM AcOH (red and blue curves), suggest that the molecular integrity of the catalyst is preserved during the electrocatalytic measurements.

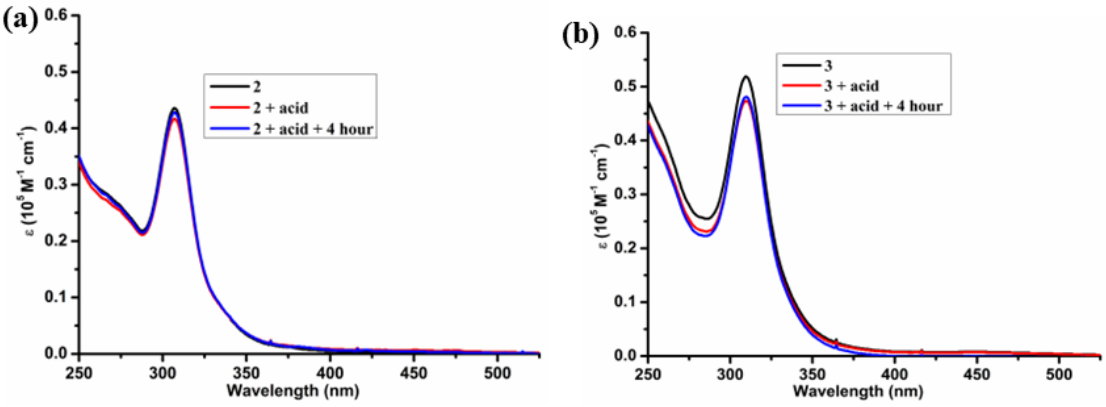


Fig. S12: UV-Vis, spectra of complexes **2** and **3** in dichloromethane solution at 10^{-5} molar concentration in the presence of 25 equivalents of acetic acid.

Detection and Quantification of the H_2 gas

The generated gas during bulk electrolysis were analysed using an gas chromatography (Agilent 7890B) equipped with a thermal conductivity detector using PoraPak-Q (for analysing O_2, N_2, CO_2 and other hydrocarbons) and molecular sieve (for analysing H_2). The generated H_2 gas was confirmed by injecting an authentic H_2 gas sample into the GC-TCD (gas chromatography equipped with a thermal conductivity detector) and by comparing both the chromatograms with the retention time (RT) of H_2 gas under the specified method. The amount of generated H_2 gas was confirmed by taking the gas sample from the head-space of Tedlar bag (0.5 L) with a 1 mL gas-tight syringe and injected into the GC-TCD. The amount of H_2 gas was quantified by multiplying the percentage of H_2 with volume of gas collected in the Tedlar bag. The gas volume collected in the Tedlar bag was measured using airtight gas chromatography (GC) syringes of 10 mL capacities. A small oxygen peak (retention time ≈ 7.6 min) was observed in the GC chromatogram. To confirm whether this O_2 signal originated from the bulk electrolysis or from external contamination during gas transfer with the syringe, the electrochemical cell was directly connected to the GC instrument. The N_2 pressure was increased to ensure sufficient *in situ* generated gas from the electrochemical cell was passed through the GC-TCD detector. Under these conditions, the GC chromatogramme showed no O_2 peak, while a low H_2 signal (0.4%), attributed to high N_2 pressure, and a prominent N_2 peak were observed. These results confirm the absence of O_2 generation during bulk electrolysis. Therefore, the contribution of the O_2 peak area was neglected in the Faradaic efficiency (FE) calculation.

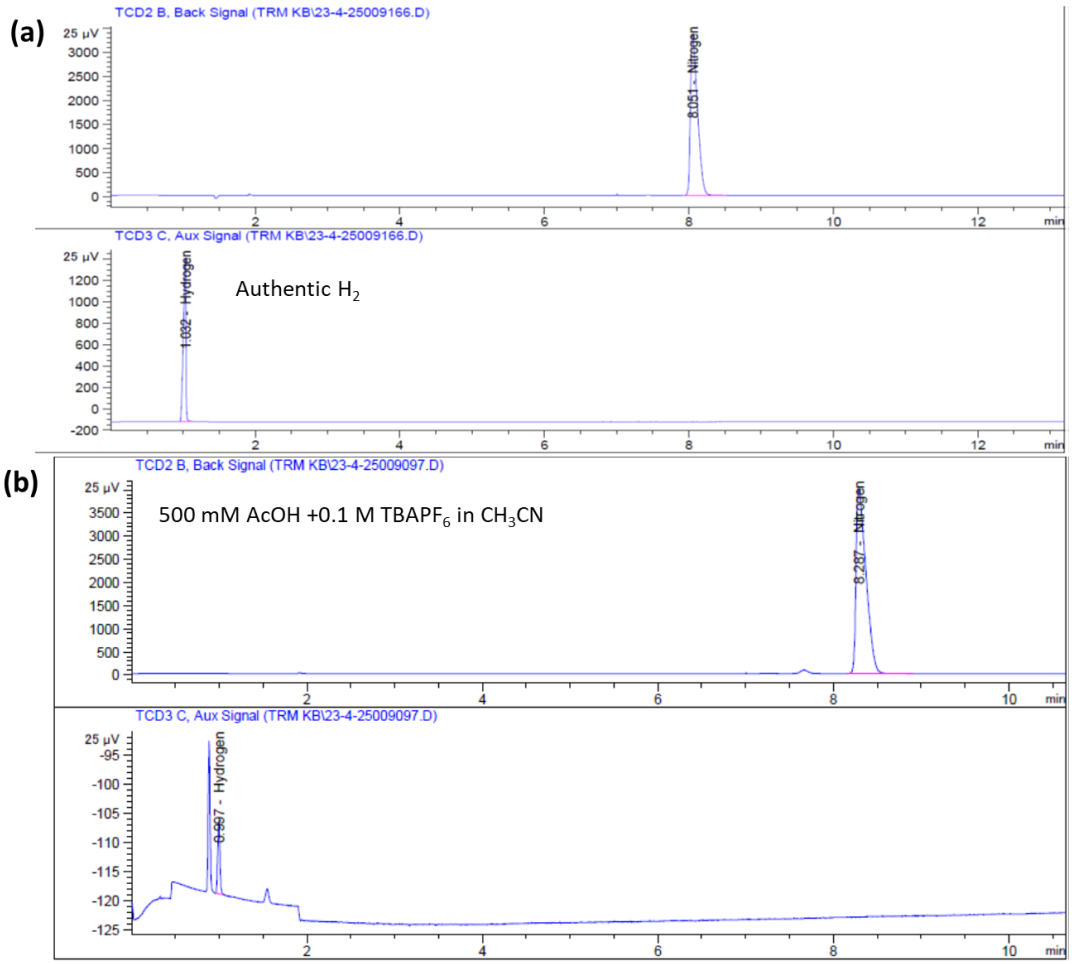


Fig. S13: GC chromatograms for (a) H_2 and N_2 gas in RGA gas standard. (b) Blank (Without catalyst) recorded at potential of -2.3 V in 500 mM AcOH containing 0.1 M $TBAPF_6$ in acetonitrile.

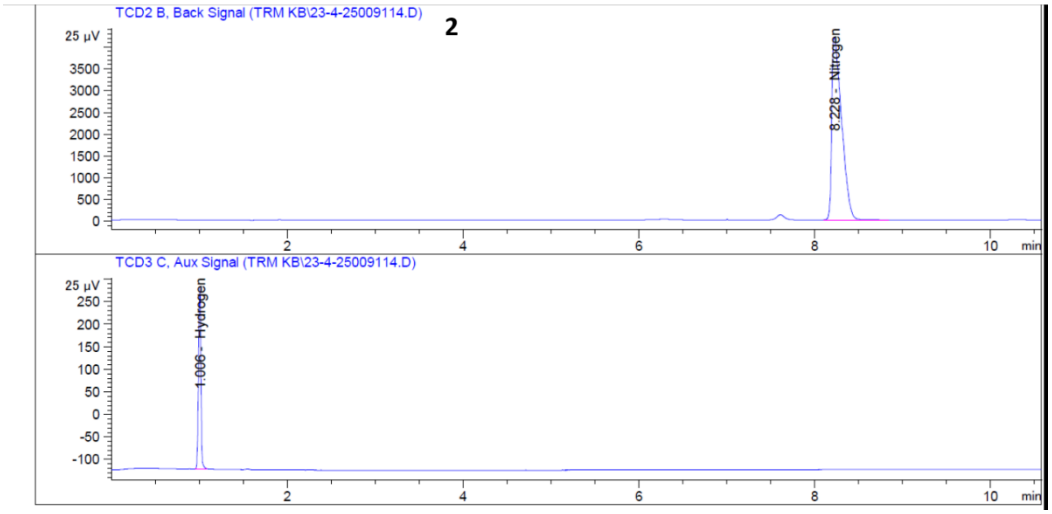


Fig. S14: GC chromatograms for the injected gas collected from the headspace of the Tedlar bag and directly injected into the GC via an airtight syringe. The hydrogen gas is generated during CPE experiments for 2h at potential of -2.3 V in 500 mM AcOH in the presence of 1.0 mM of complex **2** containing 0.1 M $TBAPF_6$ in acetonitrile.

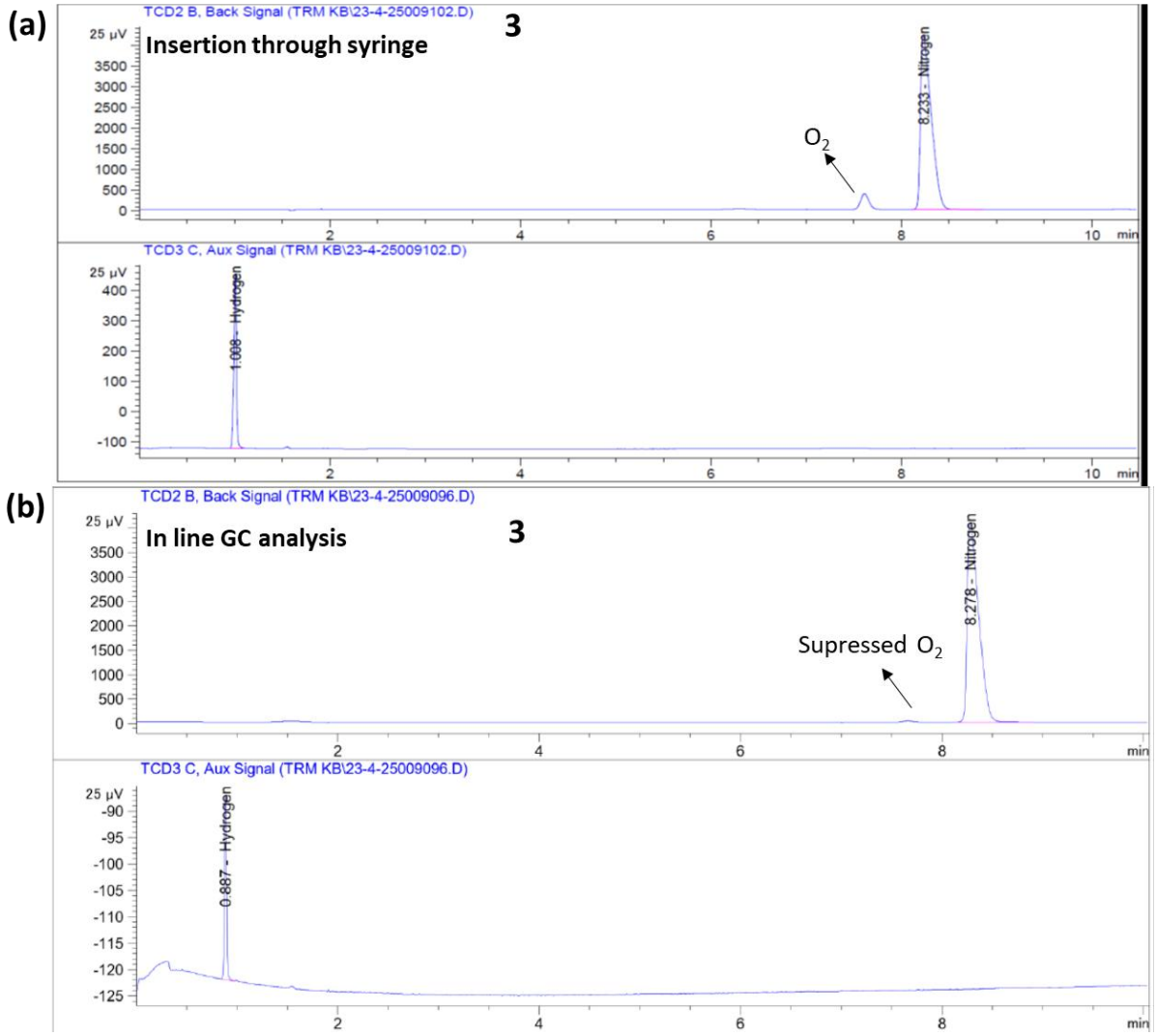


Fig. S15: Gas chromatograms for (a) gas collected from the headspace of the Tedlar bag and directly injected into the GC via an airtight syringe, and (b) gas analyzed in-line with the electrochemical cell directly connected to the GC. H_2 was generated at -2.3 V in 500 mM AcOH with 1.0 mM complex **3** containing 0.1 M $TBAPF_6$ in acetonitrile.

Estimation of Electrochemically Produced H_2 Gas

The charge build-up during bulk electrolysis is shown in **Fig. 5c** and was further used to calculate the theoretical amount of hydrogen generated after 2 h of electrolysis. The

experimentally generated H_2 was estimated by collecting the gas in a Tedlar bag and analyzing it using GC (**Fig. S13–S15**). The GC analysis report is given at the end of this document.

The detailed calculation of the Faradaic efficiency (FE) is provided below:

The FE for catalytic production of H_2 via $2e^-$ reduction process of H^+ was determined using equation S3 as,

$$FE\ (in\ \%) = \frac{2 \times \eta_{product} \times F \times 100}{Q_{total}} \qquad \text{(S3)}$$

where $\eta_{product}$ represents the quantity of H_2 produced in moles and F denotes the Faradaic constant. The Q_{total} is the total charge passed during bulk electrocatalysis experiment and estimated by using following equation,

$$Q_{total}\ (Total\ charge) = Q_{with\ cat} - Q_{blank} \qquad \text{(S4)}$$

Where $Q_{with\ cat}$ is the magnitude of charge generated by catalysts in presence of acid and Q_{blank} is the charge generated only by acid (in absence of catalyst). Further, the net moles of H_2 generated during bulk electrolysis is obtained by subtracting the moles of H_2 generated only by acid (in the absence of catalyst) from moles of H_2 generated in the presence of both catalyst and acid.

For complex 2.

The amount of charge generated by complex **2** in 500 mM AcOH after 2 h of bulk electrolysis is given by $Q_2 = 90.82$ C

Further, the amount of charge generated by 500 mM AcOH (without catalyst) after 2 h of bulk electrolysis is given by $Q_{blank} = 8.76$ C

Therefore, the net charge generated by complex **2** (Q_{total}) = 90.82 – 8.76

= 82.06 C

Theoretically, mole of H_2 generated by complex **2** = $\frac{82.06}{2 \times 96485}$ moles of H_2

= 0.000425 moles of H_2

Volume of H_2 gas collected after 2 h = 160 mL

% of H_2 gas from GC analysis = 5.79 %

Therefore, volume of H_2 gas generated after 2 h = 160 × 0.0579

= 9.264 mL

Further, to eliminate any ambiguity arising from Pt dissolution or side reactions, we subtracted the amount of H_2 generated after 2 hours of bulk electrolysis conducted in the absence of the molecular catalyst, using 10 mL of 500 mM AcOH in 0.1 M $TBAPF_6$ at –2.3 V.

Volume of H_2 gas collected after 2 h in absence of acid = 145 mL

% of H_2 gas from GC analysis = 0.18 %

Therefore, volume of H_2 gas generated after 2 h = 145 × 0.0018

= 0.261 mL

Finally, the net intrinsic volume of H_2 gas generated by complex 2 after 2 h =

= 9.264 - 0.261 mL

= 9.003 mL

The moles of H_2 gas generated after 2 h of bulk electrolysis at 298 K = 0.000367 moles.

Therefore, the Faradic efficiency = $\frac{\text{Experimenta mole of H2}}{\text{Theoretical mole of H2}} \times 100$

= 86.3%

For complex 3. The net charge generated by complex **3** (Q_{total}) = 153.60 – 8.76

= 144.84 C

Theoretically, mole of H_2 generated by complex **3** = $\frac{144.84}{2\times96485}$ moles of H_2

= 0.000750 moles of H_2

Volume of H_2 gas collected after 2 h = 200 mL

% of H_2 gas from GC analysis = 8.25 %

Volume of H_2 gas generated after 2 h = 200 × 0.0825

= 16.5 mL

Finally, the net intrinsic volume of H_2 gas generated by complex **3** after 2 h =

= 16.500 - 0.261 mL

= 16.239 mL

Therefore, the moles of H_2 gas generated after 2 h of bulk electrolysis at 298 K = 0.000663

So, the Faradic efficiency = $\frac{\text{Experimenta mole of H2}}{\text{Theoretical mole of H2}} \times 100$

= 88.4%

Table S5: Comparison of newly synthesized Ni(II) chelate complexes elucidates electronic and geometric factors that influence hydrogen evolution reaction catalysis with acetic acid.

S. No.	Complexes	Solvents	Overpotential η (mV)	TOF (s^{-1})	References
1	$(C_5H_5NiSC_8H_{17})_2$	CH_3CN	610	15	Fan et al.[10]
2	$(C_5H_5NiSC_6H_4CH_3)_2$	CH_3CN	610	28	Fan et al.[10]
3	$[Ni(C_9H_7NOSR_1R_2]_2$ R_1 = H, R_2 = tert-butyl	CH_3CN	610	520	Fan et al.[11]
4	$[Ni(C_9H_7NOSR_1R_2]_2$ R_1 = OMe, R_2 = H	CH_3CN	650	170	Fan et al.[11]
5	$[Ni(C_9H_7NOSR_1R_2]_2$ R_1 = Br, R_2 = H	CH_3CN	610	22000	Fan et al.[11]
6.	Ni(dmbpy)(mp)	CH_3CN	720	0.0036	Mitsopoulou et al.[12]
7	Ni(bpy)(mp)	CH_3CN	580	0.0004	Mitsopoulou et al.[12]
8	$[Ni(L1)_2](ClO_4)$	CH_3CN	580	-	Xiaoming Liu et al.[13]
9	$[Ni(L2)_2](ClO_4)_2$	CH_3CN	620	-	Xiaoming Liu et al.[13]
10	[Ni(bdt)(dppf)]	THF	265	1240	K. Jones et al.[14]
11	Ni(II)(N_2S_2)	CH_3CN +H_2O	730	1250	Mirica et al.[15]
12	$Ni[P_2S_2C_2(C_6H_4R\text{-}P)_2]$, R= CH_3O	DMF	1020	802	Zhang et al.[16]
13	$Ni[P_2S_2C_2(C_6H_4R\text{-}P)_2]$, R= CH3	DMF	1000	894	Zhang et al.[16]
14	$Ni[P_2S_2C_2(C_6H_4R\text{-}P)_2]$, R= Br	DMF	910	557	Zhang et al.[16]

15	$[Ni(PPh_3)_2C_6H_4O_2(CH_3)_2CS_2]$	CH_3CN	450	3283	Anjali et al.[3]
16	$[Ni(dppf)C_6H_4O_2(CH_3)_2CS_2]$	CH_3CN	640	1049	Anjali et al.[3]
17	$[Ni(dppe)C_6H_4O_2(CH_3)_2CS_2]$	CH_3CN	1012	-	Anjali et al.[3]
18	Complex **3**	CH_3CN	600	706	**This Work**
19	Complex **2**	CH_3CN	690	74.5	**This Work**

Calculation of rate-determining step (k_1 and k_2) for mechanistic insight:

The peak current expression for the ECEC mechanism involving both multi-electron and proton transfers can be represented by the following equation,[17]

$$i = \frac{i_{cat}}{1+e^{\left[\frac{RT}{F}\left(E-E_{1/2}\right)\right]}} \quad \text{..... (S5)}$$

where,

$$i_{cat} = 2FS[Cat]\sqrt{D_{cat}}\frac{1}{\frac{1}{\sqrt{k_1+[H^+]}}+\frac{1}{\sqrt{k_2[H^+]}}} \quad \text{..... (S6)}$$

Here, i_{cat} denotes the catalytic plateau current, T stands for temperature, F represents the Faraday constant, R signifies the gas constant, $E_{1/2}$ (or E^0) denotes the half-wave potential for $Ni^{II/I}$, A represents the electrode surface area, D_{cat} refers to the diffusion coefficient of the catalyst, [Cat] denotes the concentration of the catalyst, and $[H^+]$ represents the concentration of acid. The rate constants for the first and second protonation events are designated as k_1 and k_2, respectively.

When equation S5 is divided by the peak current (i_p) corresponding to the reversible one-electron transfer, as described in the Randles-Ševčík equation (eq S1), it results in the simplification of equation S5 to:

$$\frac{i}{i_p} = \frac{i_{cat}}{i_p} \times \frac{1}{1+e^{\left[\frac{F}{RT}\left(E-E_{1/2}\right)\right]}} \quad \text{.....(S7)}$$

When the catalytic enhancement (i/i_p) is plotted against the foot of the wave axis $\frac{1}{1+e^{\left[\frac{F}{RT}\left(E-E_{1/2}\right)\right]}}$, a linear relationship is observed near the base of the catalytic wave. The slope of this linear curve provides an estimation of the relevant rate constants. The protonation step can be classified into two important scenarios:

(i) When $k_2 >> k_1$, indicating that the first protonation step is the rate-determining step,

(ii) When $k_1 >> k_2$, indicating that the rate-determining step is the second protonation step.

The correlation between the $E_{cat/2}$ and formal potential of the $Ni^{II/I}$ redox couple (E^0 or $E_{1/2}$), which initiates the catalytic process, is provided by

$$E_{cat/2} = E^0 + \frac{RT}{F} ln\left(\frac{k_1}{k_2}\right) \text{.....(S8)}$$

Equation S8 illustrates that $E_{cat/2} << E^o$ results in $k_1 < k_2$ and vice versa. Since, $E_{cat/2}$ is more negative than E^0 (table 1 and 2 in the manuscript) results in $k_1 <<< k_2$ which suggests that the initial protonation step, leading to the formation of Ni^{III}-H, is the rate-determining step.

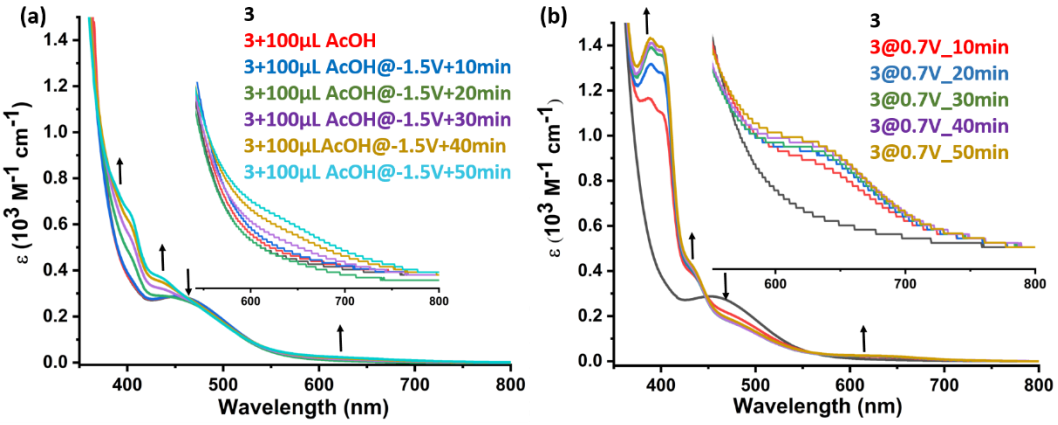


Fig. S16: Spectroelectrochemical profiles of complex **3** recorded at (a) -1.5 V and (b) +0.7 V, in the absence and presence of AcOH, with spectra collected at 10-min intervals.

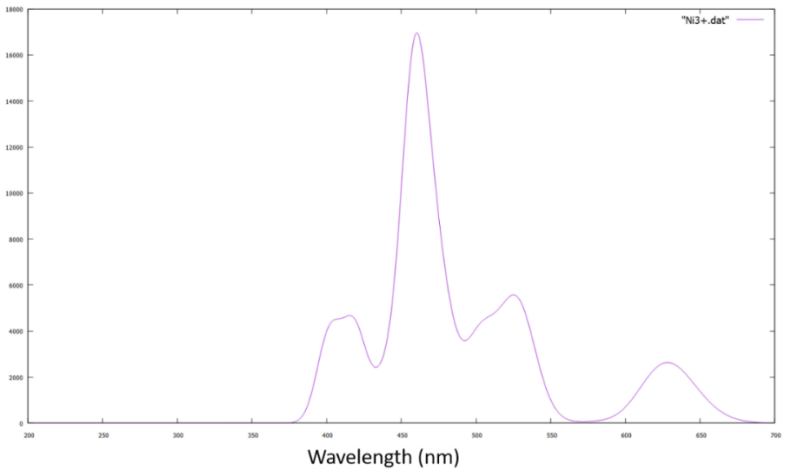


Fig. S17: TD-DFT calculated absorption spectrum of one electron oxidized species (Ni(III) species).

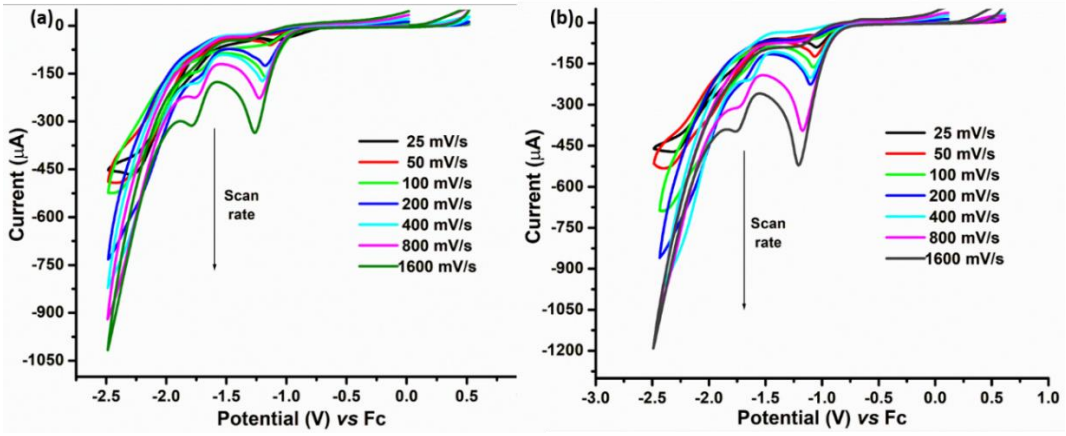


Fig. S18: Variation of scan rate from 25 mV/s to 1600 mV/s of 1 mM complex **2** (a) and **3** (b) in the presence of 4 mM AcOH in CH_3CN containing 0.1 M $TBAPF_6$.

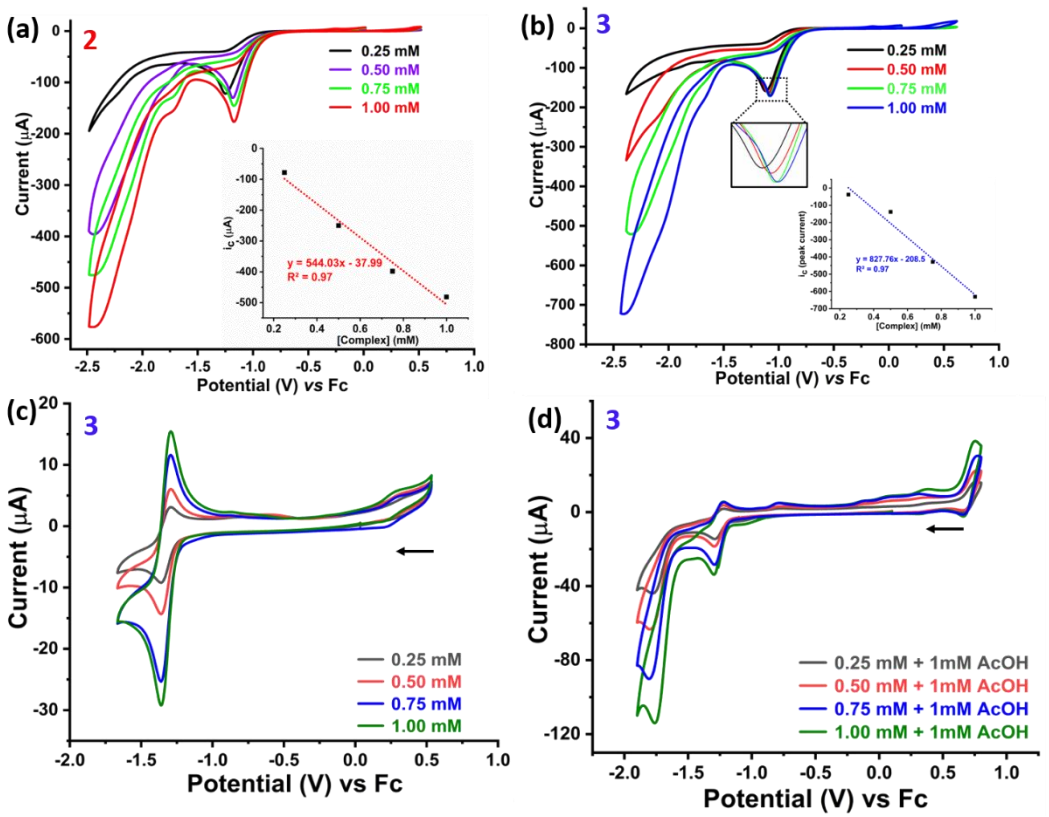


Fig. S19: Concentration variation of complexes (a) **2** and (b) **3** in the presence of 4 mM AcOH in CH_3CN containing 0.1 M $TBAPF_6$ at 100 mV/s scan rate (c) concentration variation of complex **3** in absence of acid (d) concentration variation of complex **3** in presence of 1mM AcOH.

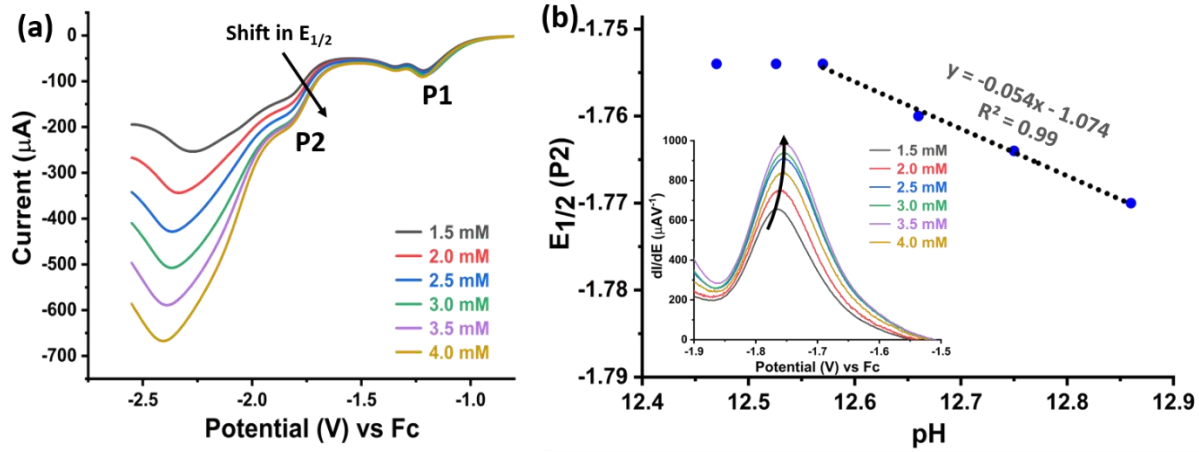


Fig. S20: (a) LSVs of 1.0 mM complex **3** in CH_3CN (0.1 M $TBAPF_6$) recorded at a scan rate of 100 mV s^{-1} with varying AcOH concentrations. P1 and P2 correspond to the first and second reduction peaks, respectively. (b) Pourbaix plot showing the pH-dependent shift of P2. The dashed line represents the linear fit with a slope of −54 mV pH^{-1}. The inset shows the current (I) derivative with respect to potential (E), i.e., the dI/dE vs E plot, used for precise determination of $E_{1/2}$ from the peak potential.

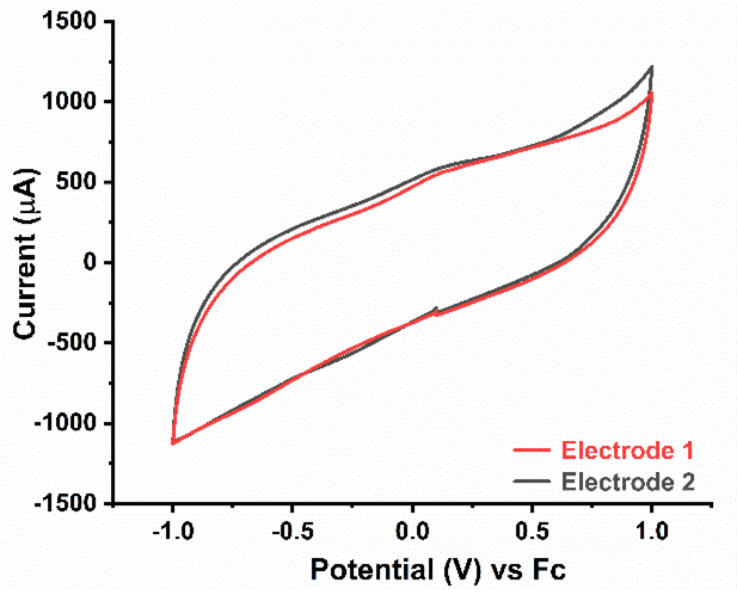
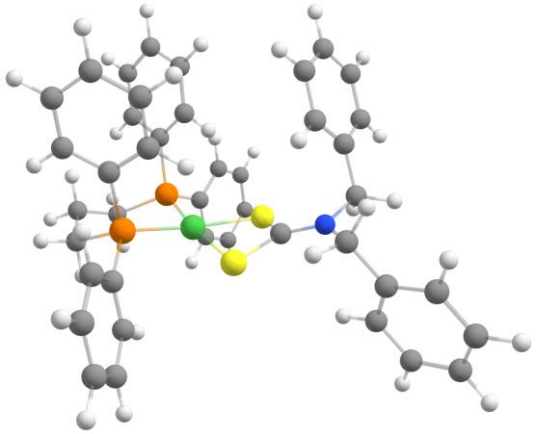


Fig. S21: CV of electrodes 1 and 2 in acetonitrile containing 0.1 $TBAPF_6$ at 100 mV/s scan rate.

XYZ Coordinates for computed structures.



Complex 3. Coordinates from ORCA-job opt E -4664.654624302580

Ni	0.28067130048502	1.78630016932542	-0.02344425217444
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P	0.64643506627325	2.40098479080135	2.04571361805309
P	2.04551541385551	2.87284830644068	-0.73055854348767
N	-1.51708235304805	-1.41892935253226	-1.43137549355149
C	-4.52404831269521	-3.50531898445208	-1.17618247775381
H	-4.07208141629206	-4.37306528758130	-0.70457632629119
C	-5.80943514611567	-3.58884577797871	-1.69606847440923
H	-6.35890420200269	-4.52219737293246	-1.62735398932772
C	-6.38507647797377	-2.48434559232129	-2.31156893112473
H	-7.38665280874764	-2.54981014114228	-2.72388766857833
C	-5.66839127589555	-1.29701677277101	-2.40311510239533
H	-6.10955819309054	-0.43127268365911	-2.88649175767022
C	-4.38586998573881	-1.21199731795610	-1.87760732658964
H	-3.83556743408430	-0.27962115900602	-1.95838363791108
C	-3.80562572399800	-2.31575633044932	-1.25754174474665
C	-2.43187323655331	-2.23628299880275	-0.64083643949022
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C	-0.99122004727442	-2.01829985357204	-2.65419324438906
H	-1.03570672784423	-1.28959459622570	-3.46971498652683
H	-1.66315109158741	-2.83754260677313	-2.92790254694655

C	0.42197108105945	-2.53077899687926	-2.49589225796693
C	1.00282467733172	-2.73846616086069	-1.24884130341511
H	0.44941555913646	-2.52119247236349	-0.34131238259744
C	2.30621950265539	-3.21044530819249	-1.14984094359189
H	2.74690079974094	-3.36178204243749	-0.16953113451421
C	3.04269233696885	-3.48065393994836	-2.29537870270708
H	4.06234427597863	-3.84346338247787	-2.21707804382876
C	2.46507189051832	-3.27839644179329	-3.54373150382118
H	3.03286818596027	-3.48250116797827	-4.44590980472345
C	1.16378838876887	-2.80571882001794	-3.64231690240942
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H	-3.96211395015878	3.63779253412354	3.20775666946276
C	-3.13021787776063	2.30293349763677	4.67584421354602
H	-4.02714577378882	2.28881579890938	5.28636924462860
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H	-2.04402644705353	0.96860725616244	5.96353580264179
C	-0.86856850653248	1.57715950875362	4.27639333608769
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C	1.84693207076026	1.24877272077096	2.78044823630153
C	1.72773361069360	-0.10711129378882	2.47025897250976
H	0.93516944189454	-0.44655259015120	1.81106084982003
C	2.62025189732270	-1.02639306318167	2.99836104368972
H	2.51705389078209	-2.07825559357866	2.75291619652728
C	3.65216704979246	-0.59728123921514	3.82433444255955
H	4.35937132736307	-1.31443639738926	4.22809793353911
C	3.77789465068608	0.75089638111874	4.13218604156203
H	4.58104717041538	1.09013145128507	4.77800243771088
C	2.87514570757051	1.67348427293727	3.61874294224254
H	2.98429449423546	2.71940581932654	3.88032664715710
C	1.25810589036641	4.10851432661114	2.31845574773368

H	0.41692489333397	4.75868969447145	2.04919169863678
H	1.42307794087754	4.23815893489474	3.39346043690640
C	2.49825373901879	4.50723179210436	1.52774581913483
H	2.77072397595995	5.52117359848440	1.83891235763349
H	3.34663280245125	3.86782942725785	1.79021692552619
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H	3.15386094264943	4.99787209116315	-0.47880209991280
H	1.41379513188006	5.12020168643045	-0.24259888133919
C	3.57745366947762	1.93352995910661	-0.45815038451488
C	4.81644467075223	2.56949869213783	-0.37730116704712
H	4.89306612552683	3.64682524833577	-0.47416031441435
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H	6.92758805229757	2.32252109884907	-0.10587573667592
C	5.89037946070569	0.43918354696174	-0.05663161084697
H	6.79243870129493	-0.14212807106475	0.10428588845539
C	4.65990901001808	-0.19779944915326	-0.14569445652909
H	4.59492626830655	-1.27680717429353	-0.05529443811782
C	3.50532629093017	0.54662663030259	-0.34100325858020
H	2.54590249392393	0.04358824938865	-0.39964607912563
C	1.98123248575875	3.21403658159314	-2.51972225057134
C	2.86175404721654	2.60674746189234	-3.41078423687579
H	3.63438774729556	1.93757115120166	-3.04865433361169
C	2.75392525610780	2.85895031968908	-4.77325335934569
H	3.44387707028859	2.38310807158195	-5.46236771141054
C	1.77018176002734	3.71415329065749	-5.24978719484584
H	1.68883086359773	3.91012214000680	-6.31390310438130
C	0.88515951514878	4.31638339927809	-4.36180053195057
H	0.11113962979170	4.98150102583468	-4.73030004768877
C	0.98326677150829	4.06310655114038	-3.00236053738574
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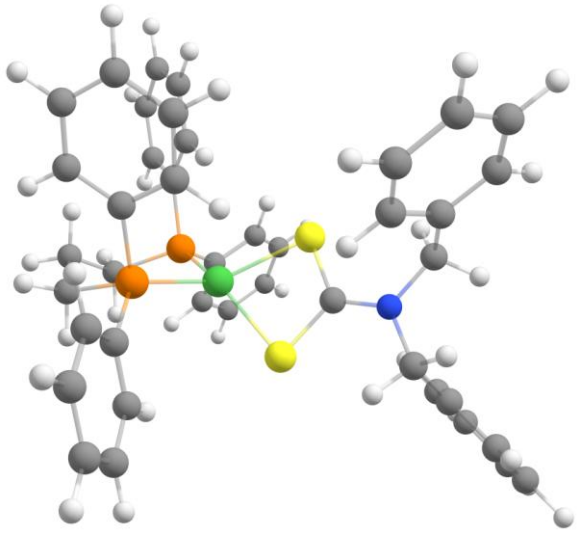

A. Coordinates from ORCA-job opt E -4664.773043380994

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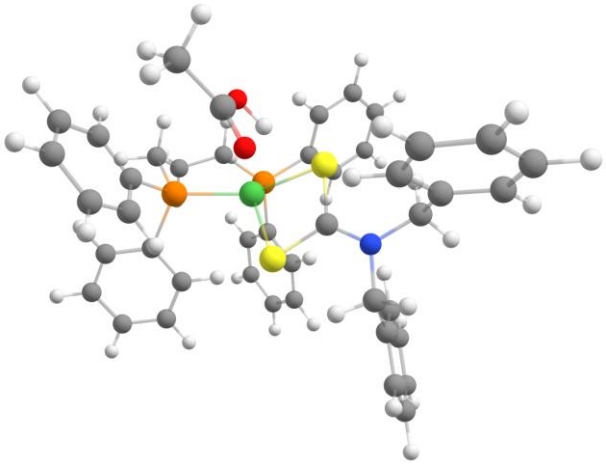
S	0.80693331716543	-0.18111236032856	-1.59022390114548
P	0.88017744757080	2.09825553778099	2.07153113043772
P	1.86642462438319	3.26733275509275	-0.86007708062519
N	-1.39489547835542	-1.71236012458240	-1.44982537326241
C	-4.93867384707983	-2.58222038661455	-2.19163128132118
H	-5.13081017067984	-3.27686868094867	-1.37858003407018
C	-5.88024009059596	-2.42009927237847	-3.19875075885000
H	-6.80539973572448	-2.98688824043095	-3.16785263624757
C	-5.63487383473336	-1.54187532738432	-4.24832859193027
H	-6.36721220094426	-1.41803214571132	-5.03949990776748
C	-4.44314439277594	-0.82930178205023	-4.28038195954042
H	-4.24095050539920	-0.14421683535872	-5.09767259649269
C	-3.50338881463403	-0.98827813857257	-3.26856202523042
H	-2.57527100080443	-0.42726854756651	-3.30643858090318
C	-3.74388494508273	-1.86519996233984	-2.21496447438793
C	-2.76355490030755	-2.03502909256833	-1.07988022000807
H	-3.05738638398168	-1.40154772211204	-0.23766944028184
H	-2.78466178421615	-3.07208345349730	-0.72784842274369
C	-0.67799164517927	-2.77100867203175	-2.14086366973551
H	0.08983380943990	-2.32219325108522	-2.77740959921081
H	-1.38640678153569	-3.28213541137392	-2.80124314147788

C	-0.04033308186375	-3.77325380054518	-1.20788036485327
C	0.16819980664198	-3.50405969687527	0.14095983958774
H	-0.15945684262927	-2.56068145354154	0.56468084877495
C	0.79401382415354	-4.43951039309288	0.95756763607531
H	0.94820738663332	-4.21533248467978	2.00849938102472
C	1.22073583084408	-5.65278146463839	0.43451352150874
H	1.70930876670003	-6.38202785581788	1.07254132542482
C	1.01207118027150	-5.92891220112701	-0.91251735819752
H	1.33614224978043	-6.87663748030763	-1.33079337714575
C	0.38335555571908	-4.99639724351769	-1.72561867611041
H	0.21888762211896	-5.21912949852256	-2.77635485762742
C	-0.82157853544846	-0.54446505521494	-1.14788918930029
C	-0.41143914054729	1.74362304534380	3.32321147354100
C	-1.69469268994361	2.23900760638545	3.08272107229216
H	-1.89443325183121	2.80531798775205	2.17737441993196
C	-2.71903760339445	2.01007301602303	3.98988384036031
H	-3.71128213795790	2.40369002567018	3.79351029382358
C	-2.47735939662575	1.26738097038877	5.14068085074565
H	-3.28043313360006	1.07964703486320	5.84605473275898
C	-1.20550760759376	0.76456740899509	5.38172730175380
H	-1.01056090361942	0.18423240082789	6.27807568030385
C	-0.17506551680868	1.00412136174364	4.47962164238121
H	0.81499690039154	0.60950227889485	4.68209752287529
C	2.30322352873505	1.08793664388084	2.62055470449404
C	2.30608496647514	-0.25582445493761	2.23661066029185
H	1.47135837646109	-0.65325149701015	1.66557480909501
C	3.37083151675356	-1.08152062055946	2.56231983998548
H	3.35792865583630	-2.12389388447476	2.26029837419291
C	4.45998278937344	-0.56861823364568	3.25929215609553
H	5.30150418816205	-1.20923147732542	3.50259559455478
C	4.46717153085730	0.76601066989459	3.64088015526210
H	5.31374726900544	1.17155335089104	4.18572804413840
C	3.39130660359587	1.59047969568407	3.32971750527362
H	3.41652977531937	2.62754507971708	3.64387491514063
C	1.30438476343068	3.84287814029269	2.51207526177588

H	0.35342964317761	4.38695700247022	2.45685764794404
H	1.62227291858738	3.88157618610177	3.56001799990382
C	2.33568260384158	4.52696825350222	1.61568943029391
H	2.56538489753742	5.49617805679608	2.07245161293780
H	3.27708664801276	3.96595994164933	1.61255659361043
C	1.87655573662600	4.79306414015752	0.18127622975298
H	2.52592510781522	5.54045670428714	-0.28740725806830
H	0.85862300488767	5.19907299202581	0.19139234938417
C	3.65018228368064	2.84888651114217	-0.93261078175137
C	4.60134676317297	3.76193886105678	-1.39033971874356
H	4.29079185803060	4.73629250955515	-1.75573249827629
C	5.94805868434236	3.43002935256111	-1.38338796105652
H	6.68242578051045	4.14541216743991	-1.73975303862863
C	6.35820477086322	2.18287303593544	-0.92024623489542
H	7.41296227578453	1.92722337672737	-0.91372763985568
C	5.41685227251257	1.26758290212290	-0.47058073293144
H	5.72898926982925	0.29237754720117	-0.11050374704250
C	4.06705985441629	1.60027389178643	-0.47986452019677
H	3.32961405381102	0.88650582300575	-0.12850228815020
C	1.53835254118334	3.87880965668442	-2.55323217879017
C	1.97746051372398	3.11759414812908	-3.63966450014642
H	2.57132581102842	2.22429387444151	-3.47174742966853
C	1.66774499463379	3.49613406841384	-4.93738475291075
H	2.02134446678813	2.89745541046219	-5.77087088122122
C	0.90828378708577	4.63768117776917	-5.17055658775069
H	0.66677982829104	4.93454289158682	-6.18596995498439
C	0.46246888833967	5.39584390039409	-4.09611118713830
H	-0.12948009772956	6.28919200403624	-4.26841066812234
C	0.77142324246582	5.01862772132223	-2.79424848367104
H	0.40884344771129	5.62523719492994	-1.97161192822407



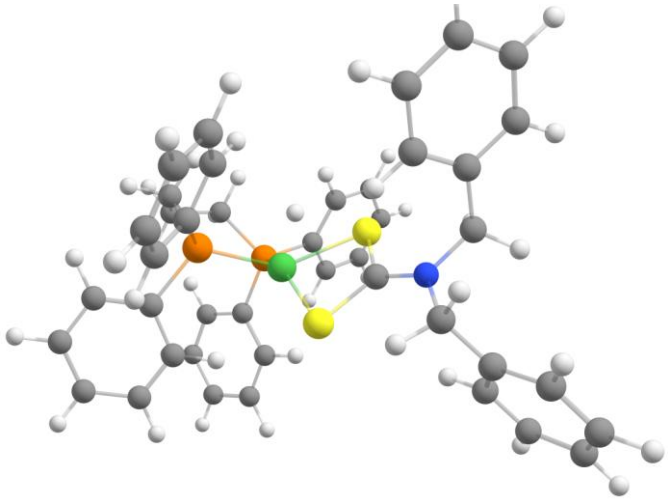
A'. Coordinates from ORCA-job opt E -4893.716695160584

Ni	0.31240468725386	1.72327443826184	-0.08271858698070
S	-1.84255211130086	0.68741656622317	-0.09613163865291
S	0.55467383197348	-0.12403538700034	-1.56213890725011
P	0.76391598297793	2.09614415012704	2.08680257099150
P	1.67102572418477	3.33140229980653	-0.86518873272662
N	-1.58386146617450	-1.71601403102784	-1.28316554235871
C	-4.98377585826477	-2.98850122609112	-1.92279188590265
H	-5.01901718813688	-3.74727387578176	-1.14607892529007
C	-5.96871906599787	-2.95256901100702	-2.90179818747201
H	-6.77141548348670	-3.68303623606349	-2.88588154280495
C	-5.92008861302090	-1.99112644551326	-3.90392655788981
H	-6.68560699516361	-1.96486282527421	-4.67273524684508
C	-4.88083601759115	-1.06820345142888	-3.91938553939073
H	-4.83411312319090	-0.31679989704411	-4.70138744973002
C	-3.89858237654379	-1.10154576738804	-2.93780312199702
H	-3.09337005635855	-0.37454324556055	-2.96533511438593
C	-3.94480584135780	-2.06097443952485	-1.92918946718334
C	-2.91654810423381	-2.08784822537383	-0.82577836135229
H	-3.21203129414378	-1.40796898811710	-0.02193359643811
H	-2.86060004856563	-3.09421576476578	-0.39741526616113
C	-0.85725790086489	-2.76341837447964	-1.98209260548035
H	-0.20987923789104	-2.30957991932676	-2.73742800097572
H	-1.59136835965925	-3.37660105123930	-2.51537037343997
C	-0.03366661091699	-3.64104157897069	-1.06761995628088

C	0.08637839286185	-3.39779253265137	0.29617130110743
H	-0.42876224543146	-2.55656769561214	0.74745851183847
C	0.86645596784067	-4.22752994798484	1.09453584141800
H	0.94828344099495	-4.02458574311183	2.15765374360511
C	1.53773663148295	-5.30724846784507	0.53744321994280
H	2.14755146569702	-5.95341513889120	1.16043340559494
C	1.42098558286534	-5.55579303693585	-0.82621304463718
H	1.94039433223746	-6.39802011616640	-1.27230429985942
C	0.63944265557185	-4.72957956097438	-1.62096208020487
H	0.55115237079806	-4.92903828023041	-2.68546749950473
C	-1.03069528898956	-0.52993980576491	-1.03412918469594
C	-0.51165603093287	1.75346781095786	3.35678436706428
C	-1.77546054018440	2.31770775387626	3.17058851273766
H	-1.97065270984001	2.93034363512215	2.29470363933166
C	-2.78676421963101	2.09861984059296	4.09445101272884
H	-3.76351292577182	2.54629635994242	3.94096862476433
C	-2.55270798212589	1.29690889795857	5.20667941441974
H	-3.34626204567834	1.11725975916985	5.92481637352850
C	-1.30123563269254	0.72438600880587	5.39222939838375
H	-1.11234640036050	0.09735270077557	6.25788165941823
C	-0.28281929221499	0.95404324214340	4.47392549964779
H	0.69190783807186	0.50522693946484	4.63312978446511
C	2.16573944293508	1.02658652676012	2.57510064355536
C	2.13265841924184	-0.29870592905869	2.13322430351127
H	1.28481904706626	-0.65115287357821	1.55247064731166
C	3.18136975084649	-1.16199950065531	2.40972196479767
H	3.14128604420162	-2.18876099160194	2.06018538579293
C	4.28849913363654	-0.70629992170178	3.11763284865390
H	5.11738069213388	-1.37606409684687	3.32285312847119
C	4.33055431520638	0.60929687742855	3.55860686437275
H	5.19128795513514	0.97024843412098	4.11257035838704
C	3.27189645228395	1.47149784733472	3.29502861455259
H	3.32498081682329	2.49302650200108	3.65359719132545
C	1.26070761321141	3.81291433516733	2.55315049211564
H	0.33138276352946	4.39530373875129	2.53268744651702

H	1.60601418566705	3.81861198368831	3.59293767754472
C	2.29749452757843	4.46869233220724	1.64290497730348
H	2.59593046591606	5.40860692555744	2.12051495674727
H	3.20585295848995	3.85760108624633	1.58977779238948
C	1.80953684118807	4.80812125332795	0.23404662316349
H	2.49635284569742	5.52682764053929	-0.22635017216359
H	0.82149930735914	5.28089325768775	0.28608366075117
C	3.43101876063395	2.83467808294419	-1.03120082509522
C	4.38614331304283	3.70020216212385	-1.56607035267522
H	4.08948337794255	4.67751470490929	-1.93555190173554
C	5.71762092049737	3.31706993691112	-1.63186509589511
H	6.45495868122617	3.99561989151058	-2.04901897941724
C	6.10858365859883	2.06527344954545	-1.16473654028355
H	7.15145035660371	1.76908092066131	-1.21579860333040
C	5.16232435718052	1.19662736617755	-0.63897225725064
H	5.45853675384224	0.21728690560313	-0.27654691184970
C	3.82759468557440	1.58030767633500	-0.57631844362814
H	3.08707732548801	0.90118337993782	-0.16798805038587
C	1.33444062774245	4.04012647631446	-2.52039730042409
C	1.39159367974248	3.17711180743240	-3.61783249288141
H	1.64794108402757	2.13188723324632	-3.47165173139836
C	1.12848633672384	3.64306082867758	-4.89656802297818
H	1.18201174081851	2.96128690288123	-5.73941773595865
C	0.79358146612344	4.97817730806280	-5.09779502018585
H	0.58554029761971	5.34345640163357	-6.09825294174815
C	0.72184037922694	5.83879775928821	-4.01144801770931
H	0.45758266336766	6.88117289747066	-4.15910108273218
C	0.98848707352606	5.37404278425673	-2.72795315789171
H	0.92833505549451	6.06604810770815	-1.89575941037757
O	-2.26962973013208	3.08573437280102	-2.26220837674095
H	-2.06511851377034	2.25609281943804	-1.77470801654535
C	-2.38482508783419	2.83353716812345	-3.56716974691451
C	-2.75153352518437	4.05472860993654	-4.34983691582316
H	-3.83009524040178	4.21782374754436	-4.24203021815116
H	-2.24025762412291	4.94046594967971	-3.96826663485992

H	-2.52297748584775	3.90622569892101	-5.40504574430508
O	-2.24067680399286	1.72925288646729	-4.04362104102504



TS-BC. Coordinates from ORCA-job opt E -4665.182995222057

Ni	0.28438595205191	0.52885497383967	0.48199857212464
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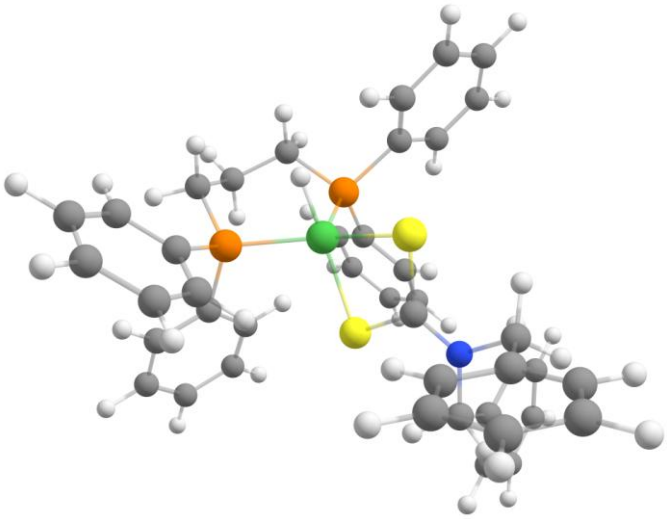
S	0.72800748134142	-1.29132459848054	-0.95441980490914
P	0.45926029922565	1.55687339964418	2.53250272588796
P	1.12207545970114	2.23689145911790	-0.65990315749636
N	-1.60842639190917	-2.58758727924606	-1.32283485123816
C	-5.27191609570843	-2.14993112155330	-2.02887471041595
H	-5.69190971186516	-2.91045921533194	-1.37652923375918
C	-6.10770972048483	-1.39700911230959	-2.83999137950055
H	-7.17866081365143	-1.57157316707340	-2.81850937935617
C	-5.57532394141283	-0.42418606634987	-3.67984517989978
H	-6.22796037977997	0.16380954957673	-4.31678077229646
C	-4.20399588479057	-0.21327335914753	-3.69866538204253
H	-3.77723510283285	0.54141066123477	-4.35132533916539
C	-3.36580452824195	-0.96556600116103	-2.88235651338848
H	-2.29642182730078	-0.78449760456795	-2.91243801679243
C	-3.89377926196874	-1.93871329628039	-2.04169591488359
C	-3.03931525434777	-2.77715457289735	-1.12055566056539
H	-3.29534476848966	-2.57139228628057	-0.07692256705504
H	-3.25200912647441	-3.83853007738042	-1.28292362340117
C	-0.99376417564919	-3.47420599884094	-2.31060673551791

H	-0.01322637101916	-3.07314719523449	-2.57827149173070
H	-1.61474797536048	-3.45225270521737	-3.21170004246992
C	-0.86948176158369	-4.88567788885180	-1.79799520511715
C	-0.36884553774839	-5.14160260105642	-0.52293526307988
H	-0.08460946788378	-4.31828674153637	0.12550359042620
C	-0.23570990610202	-6.44716539270995	-0.07154701056724
H	0.15371719352363	-6.63505084156019	0.92392270946116
C	-0.59838615316474	-7.51087446682179	-0.89071725940908
H	-0.49441828626984	-8.53134414959769	-0.53657331305465
C	-1.09961953400251	-7.26094041538966	-2.16149389973545
H	-1.39185308368523	-8.08530454516444	-2.80396595565870
C	-1.23895279468624	-5.95309799508677	-2.61047634107753
H	-1.64175011934358	-5.75861285603850	-3.60011159284070
C	-0.92857734908987	-1.64969374290680	-0.69030446912720
C	-0.71313885752400	1.01444175180442	3.82142013882931
C	-2.07869143553257	1.17128177475029	3.57292731966033
H	-2.41998671852473	1.63234687309343	2.65030895383181
C	-3.01182989018998	0.74951390003259	4.50804791765995
H	-4.07031426177371	0.88009043394050	4.30802249931206
C	-2.59191719007647	0.15686180540065	5.69383127852013
H	-3.32259917059024	-0.17759694504649	6.42295458668214
C	-1.23557551750761	-0.00622063253351	5.94147753911694
H	-0.90196184304380	-0.46659190031735	6.86583768150126
C	-0.29662630192191	0.42106276286677	5.01017951060602
H	0.76011036102970	0.29038669580039	5.21617897744989
C	2.11865080551392	1.25937824216488	3.21440317508559
C	2.64426847390107	-0.02661175501552	3.07140528932883
H	2.05550567968640	-0.80155872827710	2.58698077275663
C	3.91559461241632	-0.32004804551351	3.54007398162492
H	4.31357142590806	-1.32325097877187	3.42897960809177
C	4.68196038628078	0.67560211935619	4.13483972318932
H	5.68261768469791	0.45159016949773	4.48988411168269
C	4.16686642411475	1.95800720539496	4.27259925376784
H	4.76305150737617	2.73699891842000	4.73644419965226
C	2.88623867217301	2.25082335362632	3.82057530262572

H	2.49899317433228	3.25575076964335	3.94320979102422
C	0.19613472574239	3.37671594970820	2.48285360891764
H	-0.87692240553984	3.50940456259231	2.30105676299939
H	0.39613722182909	3.77986762363193	3.48131427473778
C	0.99408685520840	4.13691097894439	1.42657995752847
H	0.84159069456160	5.20446801657395	1.61749609291808
H	2.06795631188385	3.95835170641321	1.54794715740440
C	0.57552976795997	3.87105861434640	-0.01829964835702
H	0.98519368338959	4.64330923781498	-0.67746715614442
H	-0.51526143318002	3.90669219585306	-0.11564919662252
C	2.94053230338487	2.31778343175324	-0.62863443634010
C	3.62299284203762	3.43774171239577	-1.10706509259780
H	3.07897977117226	4.27142375985471	-1.53864318548293
C	5.00678552547323	3.48929060767861	-1.03567526865075
H	5.53261699110442	4.36246840386811	-1.40775341776818
C	5.71857240429475	2.42697113100273	-0.48786296933215
H	6.80123047890246	2.47283647735325	-0.43060588487130
C	5.04449929440032	1.30966861234327	-0.01512179651521
H	5.59526867648916	0.47854102926947	0.41274207945805
C	3.65853706595420	1.25546348827615	-0.08596927784007
H	3.13706463821772	0.38375150885451	0.29429422883658
C	0.64175662776749	2.23988834742745	-2.41767148855415
C	1.56083509975593	1.98757031192614	-3.43265999333972
H	2.60777454786345	1.83011956576445	-3.19782884470862
C	1.13832514367741	1.93256210084920	-4.75548813418293
H	1.86035100395613	1.73321684557578	-5.54066758686122
C	-0.19849295473176	2.13247629014382	-5.07156967204556
H	-0.52582240294441	2.09144376493562	-6.10528451289450
C	-1.11899280511189	2.38125754337621	-4.05906116322120
H	-2.16580857204587	2.53511333507275	-4.29938190050447
C	-0.70471270178767	2.42401742938942	-2.73664969069756
H	-1.43613464254626	2.59477262548022	-1.95179306618022
H	-0.99183397327192	0.94902889167596	-0.12443791139142

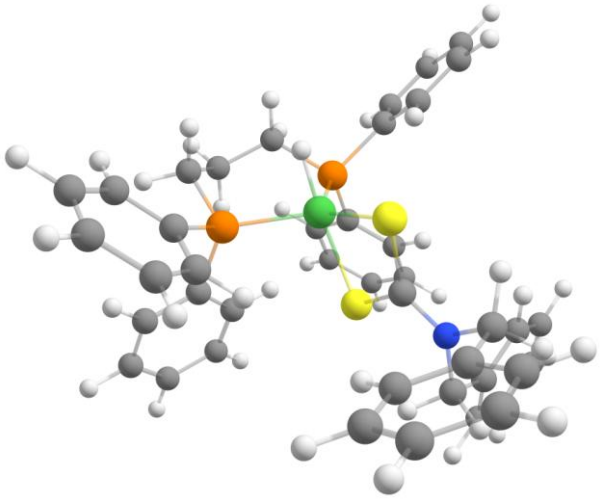


C. Coordinates from ORCA-job opt E -4665.200953328256

Ni	0.25228946203716	1.87752342937187	-0.05662369303381
S	-1.67513626362295	0.69544830962577	-0.15296595098254
S	0.99682569425744	-0.09995114606715	-0.89775379374983
P	0.90089318905973	2.04445161971403	2.12946946996729
P	1.67311090964374	3.34857096874203	-0.90997658954265
N	-1.12572702304412	-1.71384188846303	-1.23743110534477
C	-4.32688172633116	-2.63092765708788	-2.87977635873828
H	-4.69884413029295	-3.35258663474706	-2.15820842554566
C	-4.97875972613567	-2.46770908988070	-4.09436558926163
H	-5.85883333466902	-3.06253990644081	-4.31678606103473
C	-4.50024448585799	-1.55355683097648	-5.02589443749469
H	-5.00549891800486	-1.42932844638201	-5.97805802496740
C	-3.36712986454257	-0.80604895554636	-4.73299724786987
H	-2.98268563277713	-0.09359097524281	-5.45591213704131
C	-2.71746502255974	-0.96565873046012	-3.51498098402980
H	-1.83151910693350	-0.37487572696505	-3.30588078960497
C	-3.19457045185316	-1.87736293025343	-2.57792218727559
C	-2.54494569944023	-2.04811353108684	-1.22577384918220
H	-3.05029710700205	-1.42503074954843	-0.48152829548148
H	-2.64285675841157	-3.08568451481115	-0.89206158648663
C	-0.22379377392672	-2.73628471798650	-1.75063111446734
H	0.58624890817811	-2.25804422640415	-2.30936050779026
H	-0.78814382580078	-3.33714758246018	-2.47077945653469

C	0.34837409627538	-3.62846434392333	-0.67368993348543
C	-0.02728930151964	-3.53237618548329	0.66126650272108
H	-0.75139173548144	-2.78840714299888	0.97593249862004
C	0.52421946030578	-4.38770974894222	1.60975506207977
H	0.22054808453748	-4.30175727905124	2.64815869830037
C	1.45862677954926	-5.34209496916121	1.23403212049345
H	1.89004331579411	-6.00679000122269	1.97532720924382
C	1.84038106510326	-5.43906500376017	-0.10012711820145
H	2.57272077871251	-6.17990275526437	-0.40470108692799
C	1.28775915942179	-4.58913877296451	-1.04654576805361
H	1.58981720367599	-4.66868347896810	-2.08711376203903
C	-0.67149339558876	-0.54910674989143	-0.81952584116811
C	-0.48764964329344	1.88340477901811	3.30130748587164
C	-1.67637165831081	2.55852984967816	3.01923639841550
H	-1.77260886655485	3.13890456260770	2.10679400372168
C	-2.74175716990021	2.49418374769521	3.90440050587053
H	-3.66124083085738	3.02409706857782	3.67821073669130
C	-2.63497341037552	1.74614387259486	5.07149815541704
H	-3.47191617335033	1.69037209511706	5.75986031946867
C	-1.45553779816449	1.06994285579543	5.35338161536397
H	-1.36554746641416	0.48647354872031	6.26380873098358
C	-0.38236227945350	1.13837972771696	4.47379416256571
H	0.53532543474415	0.61061296338991	4.70817142223728
C	2.13084139558743	0.81940039685154	2.66712683325555
C	1.83392943940885	-0.53175029936728	2.47243084609140
H	0.88159023965356	-0.82391325943973	2.04252650810549
C	2.75071834594810	-1.50675509190783	2.83129448895593
H	2.50852470329777	-2.55353679139645	2.68089842869592
C	3.97935832419376	-1.14306370868669	3.37179280411475
H	4.70082588959004	-1.90690556487153	3.64308973437094
C	4.28040507736408	0.19798157012315	3.56519762114376
H	5.23570993493148	0.48727126029170	3.99070357308088
C	3.35927460291935	1.17878430122468	3.21839748582350
H	3.61185245445107	2.21907892522733	3.38554374393000
C	1.57239479633522	3.71015529599268	2.52642717169745

H	0.69807744361884	4.37148497043809	2.54347110015718
H	1.95571358987811	3.67650321926851	3.55231540602922
C	2.62926670788421	4.27300810443042	1.57828205135944
H	3.05605671006184	5.15684191495488	2.06358612145983
H	3.45905639756837	3.57082459161981	1.44979615834061
C	2.09968171170543	4.72585752913151	0.21847759371822
H	2.85495291179200	5.33845859717522	-0.28519446261516
H	1.19469250911094	5.33140232425494	0.34296232396652
C	3.27194606528870	2.64296354099184	-1.43162711575124
C	3.90276865827280	3.08855560148897	-2.59255744813277
H	3.43379163524299	3.84125115858336	-3.21699392004933
C	5.13698076610340	2.56712138526267	-2.95556596648889
H	5.62142775180523	2.91664763950600	-3.86148715968018
C	5.74871129430638	1.60230626703932	-2.16445055372616
H	6.71248588097648	1.19518628378993	-2.45240952485270
C	5.12292700314947	1.15634456439902	-1.00718702365278
H	5.59343103558538	0.40131168596071	-0.38592162570474
C	3.88607598829510	1.66963428609475	-0.64337449912319
H	3.40730868368462	1.30840340132522	0.26022564342876
C	0.94887037846253	4.07536111877694	-2.40909443278739
C	0.33079635857133	3.21023298281251	-3.31458477636361
H	0.29690822072386	2.14289260016877	-3.11525881154795
C	-0.24165832943845	3.70923434333370	-4.47402188544482
H	-0.71869388116963	3.03093651885287	-5.17371833970574
C	-0.20981037398562	5.07486562849707	-4.73332309715611
H	-0.66203407356947	5.46591627602494	-5.63881558404196
C	0.39828113515520	5.93807661571698	-3.83164232876238
H	0.42453107177434	7.00427076979038	-4.03093074512747
C	0.97915832073287	5.44323609137340	-2.67044261379751
H	1.45368018703925	6.13147910985163	-1.98060959423698
H	-0.41811792313275	3.13218511912006	0.21893246832696

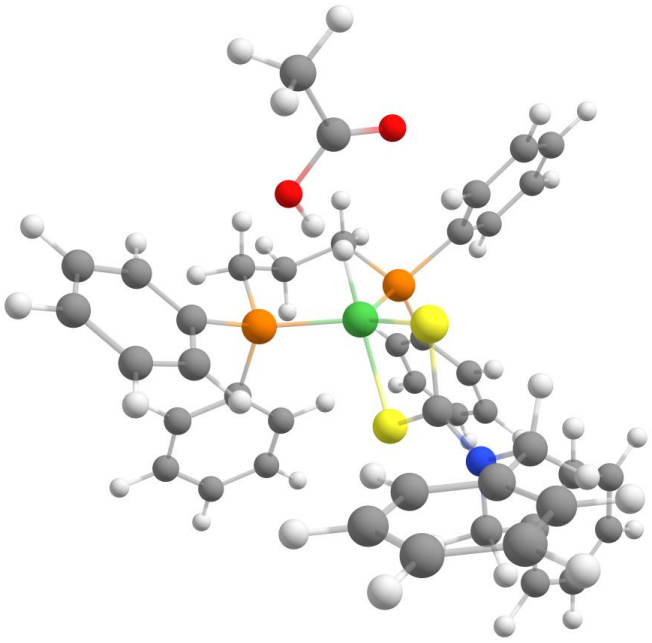


D. Coordinates from ORCA-job opt E -4665.344174554565

Ni	0.15046707075183	1.73620580102993	0.20319580863141
S	-1.82333925562284	0.75070725125488	-0.49059691817806
S	0.83861439691336	-0.30224496015165	-0.54300148083045
P	0.99226432355570	1.90911379007466	2.23491065279891
P	1.38567839569069	3.14085870615166	-0.96444522277087
N	-1.26856093829727	-1.74646425271319	-1.36979368802726
C	-4.25766807817373	-1.99360157483889	-3.62698668667654
H	-4.95330964523287	-2.52016846810910	-2.97929103062287
C	-4.62097373583728	-1.69403366204199	-4.93208714283819
H	-5.59911342687400	-1.98727120928026	-5.29989124086692
C	-3.73372727295437	-1.02420722358568	-5.76822856743890
H	-4.01552406370969	-0.79190490774888	-6.79005757143709
C	-2.48384692958645	-0.65989803561082	-5.28689037731838
H	-1.78189233396604	-0.14164513215749	-5.93250617556786
C	-2.12196167531645	-0.95746293649329	-3.97730891526756
H	-1.14144089823827	-0.66697486616626	-3.61520001233886
C	-3.00586095173265	-1.62466133335653	-3.13612597663375
C	-2.66751175472070	-1.94398087779916	-1.69787418540371
H	-3.27673700166745	-1.32309221969595	-1.03244916147143
H	-2.92482308133051	-2.98625081302129	-1.48310513891364
C	-0.35180546817190	-2.84464308097768	-1.62575423239096
H	0.54584906713084	-2.46638063764179	-2.12655495940756
H	-0.84306861192381	-3.52260771350117	-2.33132436636268
C	0.04828312715776	-3.60511583753595	-0.38203429529000

C	-0.66843378249766	-3.51076164161186	0.80630397694566
H	-1.53259847032385	-2.85751403156083	0.86997690654840
C	-0.27636785431440	-4.23696432066508	1.92499210472673
H	-0.84235488508179	-4.14875599173415	2.84701886467057
C	0.83546214309901	-5.06723844170902	1.86792133189228
H	1.14285208021385	-5.63104638049441	2.74269589002547
C	1.55512576976421	-5.16590176958392	0.68231718141846
H	2.42935862600556	-5.80699463509046	0.62797693587022
C	1.16417348119638	-4.43797427636060	-0.43304649029987
H	1.73750077497231	-4.51014712705060	-1.35319135610737
C	-0.82141006412162	-0.59115588057234	-0.87205002559608
C	-0.13569159751487	1.79965395256808	3.68064643054919
C	-1.50070681137569	1.63677032767888	3.46276219617638
H	-1.87105666995819	1.56055237542879	2.44462732267251
C	-2.38075447451155	1.56526809902418	4.53697386653810
H	-3.44343914455956	1.43671800280567	4.35719144093068
C	-1.89902155017372	1.65309038758134	5.83600154824593
H	-2.58415359291680	1.59528082037757	6.67575625573471
C	-0.53468252268895	1.81114717199231	6.06102906902956
H	-0.15509257701613	1.87657900613809	7.07584275821085
C	0.34324232806538	1.88179317150773	4.98923612106957
H	1.40734687745526	1.99709358212768	5.17307472664881
C	2.29946242195941	0.72352246972171	2.72227526368312
C	1.94026325779769	-0.62607276874109	2.78835244321185
H	0.91398472856379	-0.92104456383427	2.59254317478080
C	2.88137263451365	-1.59360642619866	3.10286234230335
H	2.58482167914629	-2.63657050144759	3.15539450586318
C	4.20349411159223	-1.22955205150408	3.33960159031947
H	4.94336200026296	-1.98701224067691	3.57750305411472
C	4.57027755926617	0.10723248340086	3.27114612376430
H	5.59845790566701	0.40032000791726	3.45869749909153
C	3.62374909230248	1.08045140766478	2.96698695645111
H	3.93313222697234	2.11828120146783	2.92959868893613
C	1.72683726383375	3.58828317318858	2.48921286207202
H	0.86393817370002	4.25369954244720	2.61334264862839

H	2.26791450303387	3.59790860701377	3.44233523701628
C	2.63137873655942	4.12836642963067	1.37703608617130
H	3.13198531330891	5.01550970026701	1.78166780717113
H	3.43232342082780	3.41734937327593	1.14827288789035
C	1.93627815008704	4.56044559457822	0.08362205774676
H	2.62215624953742	5.18754632418764	-0.49680469393476
H	1.04910453425798	5.16154518008189	0.31600332751271
C	2.99329485481376	2.54048288098544	-1.61922354011551
C	3.55916905642564	3.03901311096706	-2.79231084304341
H	3.03397374416046	3.78874896339382	-3.37507465455553
C	4.79730435821531	2.58178990824314	-3.22541587937747
H	5.22487462250911	2.97493072717682	-4.14237936817089
C	5.48850361879103	1.62794999974572	-2.48771035554941
H	6.45611449805811	1.27276413691062	-2.82742835553965
C	4.93354996111754	1.12863088934268	-1.31593375866463
H	5.46478050961341	0.38210817612803	-0.73390073016160
C	3.69002322290799	1.57605315267525	-0.89009476214562
H	3.25972524003891	1.17087840291555	0.01989180568674
C	0.62089692785544	3.91061534429716	-2.43588324071161
C	-0.01940147240677	3.04801815906272	-3.32970492235915
H	-0.03724663011943	1.98098296271630	-3.12553054494452
C	-0.63891788261256	3.54337269286849	-4.46658416867250
H	-1.12801048540253	2.86195556078154	-5.15551230062866
C	-0.64583732637515	4.91247180115194	-4.71462180469257
H	-1.13876279495380	5.30291941372213	-5.59909004425511
C	-0.02485894430560	5.77738980252701	-3.82373253438202
H	-0.02974593722066	6.84655270818371	-4.01088601489762
C	0.61067222484548	5.28035072954042	-2.69073201802623
H	1.09815784223529	5.97201779703569	-2.01292932619974
H	-0.50544251294259	2.96443153030655	0.61578132733552



E. Coordinates from ORCA-job opt E -4894.283556366504

Ni	0.03594265453775	1.64436150580821	0.08409934493057
S	-1.86330208382275	0.42079033300596	-0.39185025685342
S	0.88233332822056	-0.29206941523907	-0.75186814688724
P	0.81196792162628	1.76846767448690	2.19208008133024
P	1.24899128205295	3.14374133684869	-0.94405144226187
N	-1.11217010876118	-1.99690326992929	-1.33910046631492
C	-4.11833274563999	-2.99238482972788	-3.29797061029591
H	-4.55609884938840	-3.70848025223165	-2.60808415217180
C	-4.65042772339902	-2.84549447833779	-4.57177677563948
H	-5.50255894565164	-3.44683282584383	-4.87235129460488
C	-4.08853529980254	-1.93757444312589	-5.46214888517405
H	-4.50052879448425	-1.82435052643971	-6.45963036808340
C	-2.99185431676376	-1.18163502222533	-5.06824679262049
H	-2.54310667226381	-0.47328288269928	-5.75754101341534
C	-2.46206958105720	-1.32683164594903	-3.79149177550036
H	-1.60395392263275	-0.73079486125666	-3.49858574402096
C	-3.02332444849647	-2.23097873016031	-2.89443021299195
C	-2.50481764788273	-2.38295943822706	-1.48430453619352
H	-3.10966370956685	-1.77861353022558	-0.80003400030611
H	-2.60721021976678	-3.42480047363901	-1.16379645515093
C	-0.11286443671136	-2.99166142152003	-1.68494257215135

H	0.72709834683711	-2.50598045618488	-2.19225058941495
H	-0.56527617346296	-3.67394279730292	-2.41261472485021
C	0.39662331799309	-3.77884637760819	-0.49904247532624
C	-0.16928905082568	-3.66870293886161	0.76637507864121
H	-0.99493732362232	-2.98559814469695	0.93570127371343
C	0.32254231010973	-4.42278597294522	1.82617149362673
H	-0.12780436697195	-4.32325660675029	2.80876593705436
C	1.38686531267274	-5.29281123135362	1.63307988234026
H	1.77215172444490	-5.87847631361978	2.46139980453965
C	1.95904181923411	-5.40435216532401	0.37023211799543
H	2.79452303816700	-6.07815583498697	0.20869371355984
C	1.46651793197006	-4.65246158443484	-0.68688852397009
H	1.91968600493386	-4.74099215914486	-1.67051238151285
C	-0.75513036673506	-0.79265541188577	-0.89225044351781
C	-0.37346399678937	1.57807130467811	3.58220443137150
C	-1.73466707464801	1.73706131463241	3.32694190655890
H	-2.07536073757112	1.92780543023588	2.31391449845646
C	-2.65793415131282	1.65088933805066	4.36209756578202
H	-3.71545006323667	1.77717879491691	4.15211160483235
C	-2.23008052557524	1.39383516187802	5.65832147464519
H	-2.95163622163193	1.31926936596981	6.46564937066332
C	-0.87396531247006	1.22880618507757	5.91878198665844
H	-0.53456049433983	1.02751792603421	6.92999464467391
C	0.05012506491748	1.32245412067781	4.88707740369637
H	1.10652545968791	1.19304765124665	5.10077882018325
C	2.16598804556649	0.64589315075939	2.69103887456930
C	1.90207149315005	-0.72639334687618	2.64333466237994
H	0.91398010732593	-1.07580046431279	2.36010176390791
C	2.89013651081852	-1.64713144673767	2.95381313648159
H	2.66697142054943	-2.70877581036138	2.91873736316182
C	4.16657692939537	-1.21184217390324	3.29673287832244
H	4.94356886814407	-1.93245299385896	3.53064645049654
C	4.44062273755598	0.14813007307834	3.33737838660902
H	5.43296405737193	0.49629635830732	3.60615396062319
C	3.44560527049976	1.07353519327017	3.03978128831038

H	3.68165901178049	2.13020643141451	3.08817885631163
C	1.43753190355359	3.47757600971049	2.53358538981975
H	0.53355740644004	4.08877079912783	2.64331948195310
H	1.93502587861052	3.48096519572625	3.51057215799913
C	2.35207388601138	4.10630096133705	1.47952550591217
H	2.78589572287031	5.00555044319549	1.93161008429068
H	3.20004972506687	3.44917269443649	1.25887514061305
C	1.67951634488788	4.54577253499270	0.17669222143322
H	2.34809019824241	5.22877013961316	-0.35895974358433
H	0.75143518868165	5.08677018819392	0.39584620672144
C	2.90636313587599	2.61773807985946	-1.53027751097471
C	3.50246653063763	3.16877021247207	-2.66409312945980
H	2.97264785428044	3.91041213374747	-3.25280258241168
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H	5.22807419803126	3.20680993620365	-3.93709498488448
C	5.47258456560705	1.82924776788010	-2.30469421446556
H	6.46807388955539	1.52172717004208	-2.60827517405487
C	4.88723457759343	1.27858838554123	-1.17149630860023
H	5.42210213273034	0.53961533111545	-0.58330913151996
C	3.60919797061926	1.66543127651628	-0.79133398327655
H	3.15919985946036	1.22161663366279	0.09051215001560
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C	-0.72910457904296	4.94235493158987	-4.70576091995194
H	-1.21700044076644	5.34041064391798	-5.58960776278373
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C	0.39860170140767	5.29715551847505	-2.60527226179145
H	0.78827075960880	5.98697480438793	-1.86534974546020
H	-0.69678034782646	2.83261092072705	0.50498414935271
H	-1.94833614567202	3.25420121927456	-0.64810718085424
O	-2.64193289709781	3.78884294419922	-1.09167759274465

C	-3.73316612758432	3.82883177781637	-0.32235357441726
C	-4.83487918531000	4.61635908918510	-0.95783859888575
H	-5.71007336567282	4.62899390699652	-0.30921730547710
H	-4.49715800676870	5.64021103831932	-1.14545981790122
H	-5.09488219260426	4.17405199211554	-1.92433231623898
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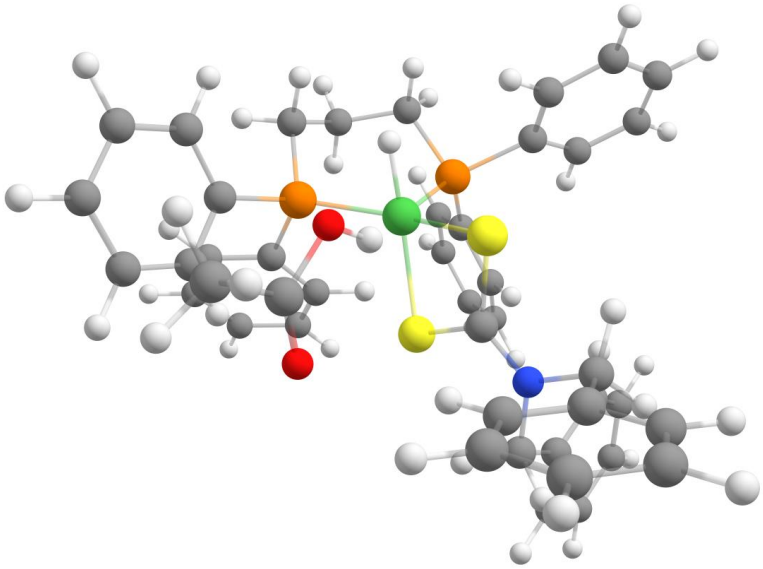

E'. Coordinates from ORCA-job opt E -4894.285519672371

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S	0.65898148112416	0.02582521610308	-1.09925112998723
P	0.88451889954745	1.84842092077356	2.10926911981900
P	1.43130131558198	3.46801567429366	-0.82244682487140
N	-1.47472579593558	-1.61913659058154	-1.17495065710464
C	-4.98372569237825	-2.53418926171164	-2.10057214552293
H	-5.24024570308942	-3.16922644868985	-1.25709671884218
C	-5.86871785778387	-2.40444806701161	-3.16181962857886
H	-6.81311960979360	-2.93917784243457	-3.14417112407249
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H	-6.23525045692584	-1.49566656590142	-5.07759774561680
C	-4.32925608017106	-0.92517506374677	-4.26077720219990
H	-4.06439855797360	-0.29383184566655	-5.10327100071506
C	-3.44363421541737	-1.05504375168671	-3.19692394345433
H	-2.49943797175714	-0.52320056874972	-3.22501368352364

C	-3.76608003257561	-1.85593606372865	-2.10724215381052
C	-2.85825975778455	-1.97873852164256	-0.90752565185356
H	-3.23343661772127	-1.34818350700709	-0.09490876253360
H	-2.87141002969971	-3.00969667530821	-0.53899229966107
C	-0.62661803466230	-2.66018656008673	-1.72713867169849
H	0.11026640975664	-2.20683074403389	-2.39769217606962
H	-1.25839544001464	-3.30659438968087	-2.34556125683586
C	0.07949964964613	-3.49191382190110	-0.68098940832809
C	-0.10065744836678	-3.28965485073609	0.68251827546404
H	-0.76209950664920	-2.50557944524202	1.03565507524338
C	0.57056707242165	-4.08299111570803	1.60701507691237
H	0.42254605265417	-3.90975481637394	2.66825482408605
C	1.43015775066304	-5.08452878789332	1.17790631986604
H	1.95554278245356	-5.70113787110973	1.89988297778398
C	1.61507672598571	-5.29031523242911	-0.18542316672271
H	2.28621808990818	-6.06959817921833	-0.53241892854194
C	0.94323724121769	-4.50025718349122	-1.10675006142815
H	1.09196327391535	-4.66453683073490	-2.17050141892423
C	-0.98504066114747	-0.41670439440696	-0.88284203205256
C	-0.31415886442944	1.44087652812292	3.43761844646299
C	-1.57691989349588	2.03531927801279	3.36998328166104
H	-1.81369925091334	2.70553327948063	2.54899262766998
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H	-3.50745457832278	2.24824411949885	4.27777210639977
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H	-2.99968230422661	0.68572302991194	6.13680319236709
C	-1.00012755818332	0.29409805994808	5.45062646734323
H	-0.76979679364043	-0.39044097579226	6.26100924984426
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H	0.93746037388602	0.09356441112785	4.55827070408530
C	2.30563819363666	0.76159706382930	2.48866092014751
C	2.20128320541033	-0.57790117742622	2.10258566936717
H	1.28355571522824	-0.93631225742494	1.64792632380196
C	3.26330017009628	-1.45147088297602	2.27928244837612
H	3.16265598190593	-2.48913501895270	1.97704102528580

C	4.45674088134750	-0.99491077277879	2.82842173559560
H	5.29403677239387	-1.67370804957640	2.95460871629008
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H	5.49841633626353	0.69777472006823	3.64520442273592
C	3.50170434878813	1.20699882540264	3.04973067630304
H	3.61689479350600	2.23791186266573	3.36337176511013
C	1.41931380100998	3.53498484921732	2.65391445709013
H	0.49160626807777	4.11209642585019	2.74695860700304
H	1.84646491510740	3.47078822291019	3.66108091002002
C	2.38349663761851	4.26746101861379	1.71835104113906
H	2.76517558604362	5.13618674010772	2.26662781525120
H	3.25846874407829	3.64566681567024	1.49821362893500
C	1.77744704256679	4.79244044226545	0.41595541094412
H	2.46351201762635	5.51285996484483	-0.04398926911023
H	0.83693528867558	5.31136009133267	0.62867317326764
C	3.13929337325145	2.92092239912256	-1.21840263449473
C	4.00301387953470	3.73335106478952	-1.95513860891221
H	3.65020354866942	4.67507125601485	-2.36337359043405
C	5.31635630923656	3.34364143867143	-2.17353490037980
H	5.97840868568759	3.98165324837946	-2.75020052054363
C	5.78497613632628	2.14144798901681	-1.65296239513713
H	6.81296974826719	1.83885957312360	-1.82469262177399
C	4.93448005916891	1.33263539917743	-0.91234940217954
H	5.29178656137451	0.39558114499952	-0.49727515083131
C	3.61728818143384	1.72118792204350	-0.69846702232353
H	2.96406487900832	1.08830658717016	-0.10943572514657
C	0.94410169751775	4.37023542183964	-2.33555285735085
C	1.08586198745515	3.73095257917275	-3.56870939306485
H	1.53163810446037	2.74221364768289	-3.61922371317083
C	0.66516547079760	4.35057687102449	-4.73487189295387
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C	0.08223706301753	5.61225660411191	-4.68439550308598
H	-0.25065628816688	6.09602785509467	-5.59692644361306
C	-0.07604411247201	6.24727170415157	-3.45997290450847
H	-0.53234577163073	7.23086318042896	-3.41136317698058

C	0.35260357934884	5.63137282399855	-2.28973954430470
H	0.21957018335447	6.14589942647976	-1.34453625455590
O	-2.42132675440176	2.78405621003880	-2.85999068877576
H	-2.02327720728738	2.17162595151160	-2.20620313828396
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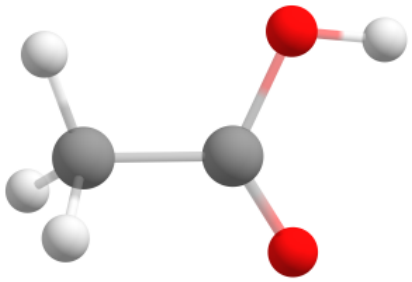
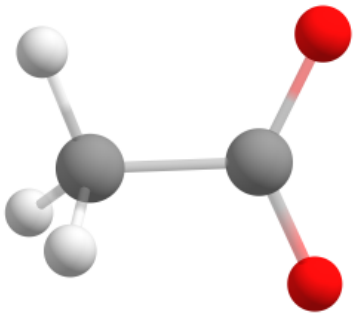
H	-3.85905566196175	2.89892945744466	-5.22700507840413
H	-2.81940229753187	4.27694839017162	-4.84236668162146
H	-2.32352845069313	3.09757133218041	-6.09845661612864
O	-1.47682186986744	1.39733282124027	-4.34417654775400
H	-0.59656894064219	3.21973412081741	0.33326989414066



CH_3COOH. Coordinates from ORCA-job opt E -228.928784219435

C	-0.13392280250455	-0.05168592206920	-0.51898164550441
H	0.23786371423522	-1.08015360707197	-0.53623931078652
H	0.23622885409014	0.44896598304996	-1.41823944667904
H	-1.22368328779050	-0.05456366043214	-0.52186055512181
C	0.43321554367749	0.63976938340501	0.67896981630125
O	1.61338422660447	0.76840447072712	0.90433045278742
O	-0.51331261712591	1.11727818533937	1.50340355984498
H	-0.07107363118636	1.54897516705186	2.25282712915814



CH_3COO^-. Coordinates from ORCA-job opt E -228.446258807168

C	-1.74137653778255	-0.13527952071177	0.05129591529506
H	-1.35669790303992	-1.16090833685389	0.02739203308436
H	-1.36679286604745	0.36607067421617	-0.84819083060429
H	-2.83345893901914	-0.16519730920187	0.01101631992990
C	-1.22264566298928	0.58914571120652	1.30570860889606
O	0.02534754338744	0.64818698872569	1.42440006256986
O	-2.07817563450909	1.05568179261914	2.09448789082905

H_2. Coordinates from ORCA-job opt E -1.166054500538

H	-0.71492068465183	0.40760000000000	-0.24510000000000
H	-1.45967931534817	0.40760000000000	-0.24510000000000

Reference

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Sample Name: H2+N2

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Acq. Instrument : FAST RGA Location : Vial 1
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Inj Volume : Manually
Acq. Method : C:\CHEM32\1\METHODS\TRIAL-HSL-AB-26062024-.M
Last changed : 7/29/2025 11:52:49 AM by KAPIL BHATI
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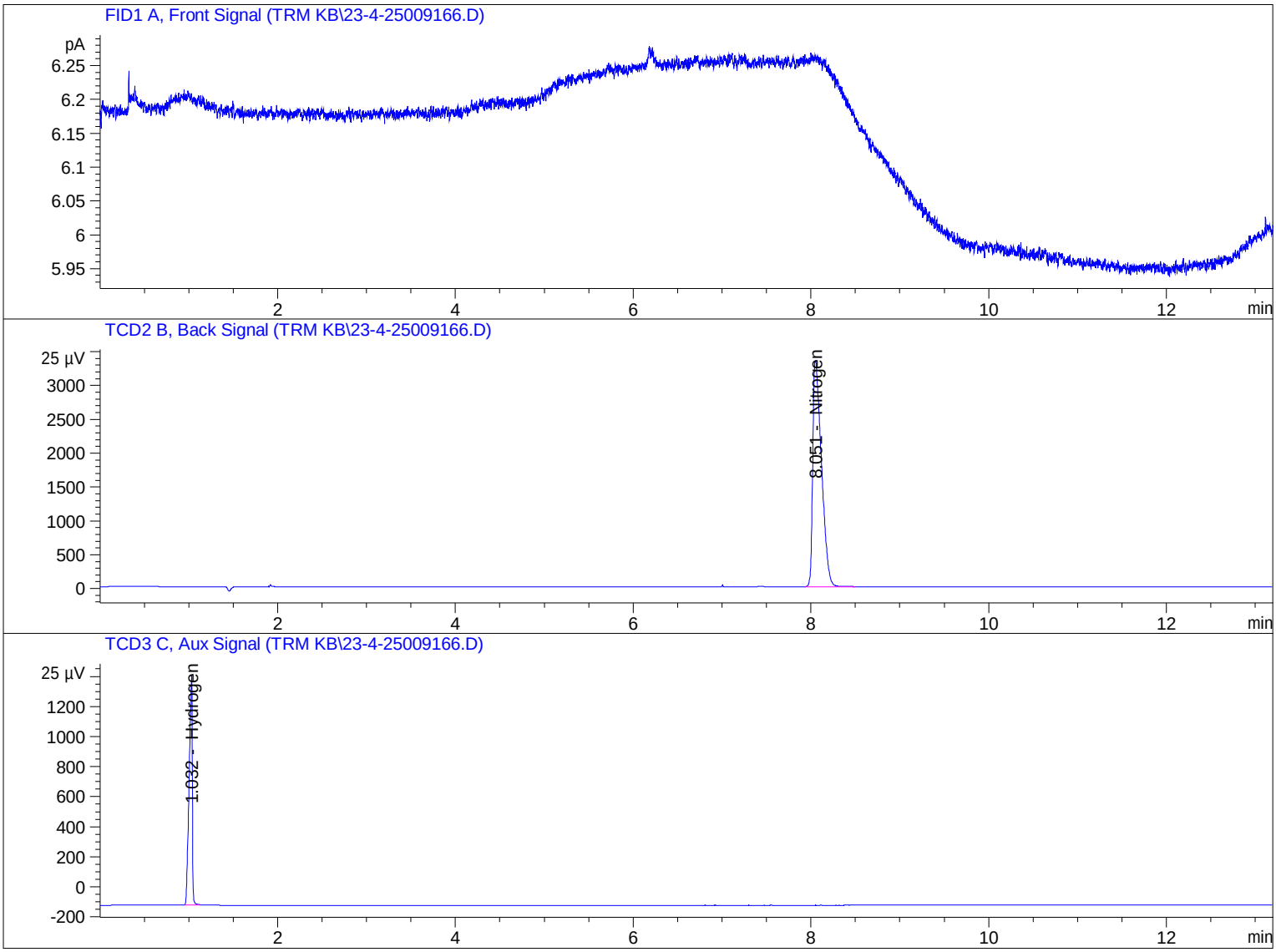
Last changed : 7/29/2025 12:13:43 PM by KAPIL BHATI
Sample Info : H2+N2

Additional Info : Peak(s) manually integrated



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Normalized Percent Report

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Sorted By : Retention Time
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Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009166.D
Sample Name: H2+N2

Signal 1: FID1 A, Front Signal
Signal 2: TCD2 B, Back Signal
Signal 3: TCD3 C, Aux Signal

RetTime [min]	Sig	Type	Area	Amt/Area	Norm %	Grp	Name
0.000	1		-	-	-		Cis-2-Butene
0.000	1		-	-	-		1-pentene
1.032	3	BB	3841.42456	5.06532e-3	30.641878		Hydrogen
1.549	1		-	-	-		Methane
2.241	1		-	-	-		Ethylene
2.357	1		-	-	-		Acetylene
2.578	1		-	-	-		Ethane
5.730	1		-	-	-		Propylene
6.042	2		-	-	-		CO2
6.139	1		-	-	-		Propane
6.338	1		-	-	-		Propadiene
7.457	2		-	-	-		Argon/O2
8.051	2	BB	2.28275e4	1.92940e-3	69.358122		Nitrogen
9.879	2		-	-	-		CO
10.659	1		-	-	-		Iso-Butane
11.113	1		-	-	-		Iso-Butylene
11.201	1		-	-	-		butene-1
11.445	1		-	-	-		1,3-butadiene
11.805	1		-	-	-		n-Butane+c 2 butene
12.049	1		-	-	-		t-2-butane
16.351	1		-	-	-		Iso-Pentane
16.620	1		-	-	-		n- Pentane
17.002	1		-	-	-		T-2-Pentene
17.136	1		-	-	-		cis-2-pentene+1 pentene
21.468	1		-	-	-		n-hexane
21.896	1		-	-	-		1-hexene

Totals : 100.000000

2 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)
Warning : Calibrated compound(s) not found

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Summed Peaks Report
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Final Summed Peaks Report
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*** End of Report ***

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009097.D

Sample Name: Blank(Without catalyst)

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Acq. Instrument : FAST RGA Location : Vial 1
Injection Date : 7/15/2025 12:54:33 PM
Inj Volume : Manually
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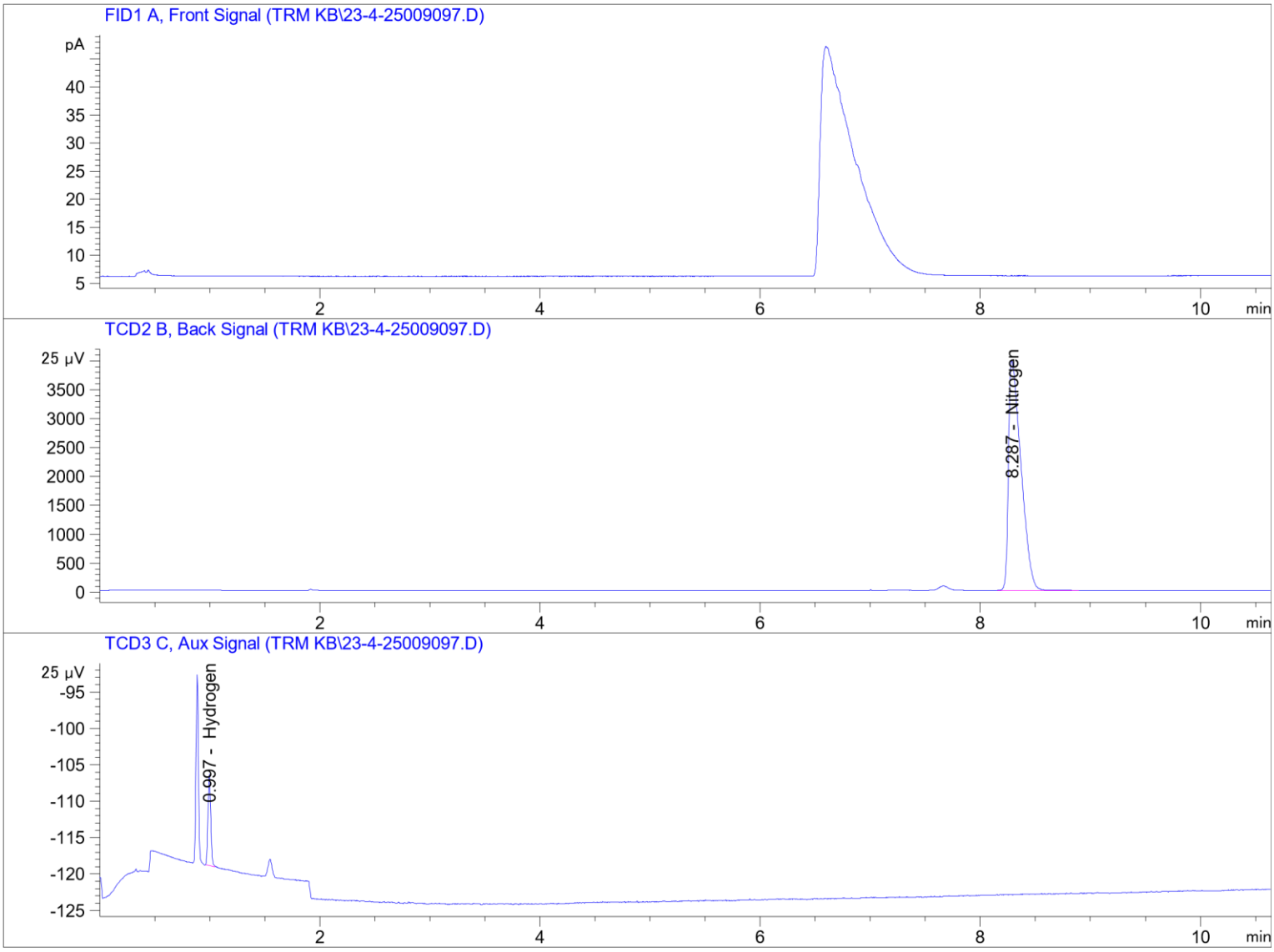

Additional Info : Peak(s) manually integrated

Normalized Percent Report

Sorted By : Retention Time
Calib. Data Modified : 7/15/2025 1:06:33 PM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Sample Name: Blank(Without catalyst)

Signal 1: FID1 A, Front Signal
Signal 2: TCD2 B, Back Signal
Signal 3: TCD3 C, Aux Signal

RetTime [min]	Sig	Type	Area	Amt/Area	Norm %	Grp	Name
0.000	1		-	-	-		Cis-2-Butene
0.000	1		-	-	-		1-pentene
0.997	3	BB	21.94896	5.06532e-3	0.183229		Hydrogen
1.549	1		-	-	-		Methane
2.241	1		-	-	-		Ethylene
2.357	1		-	-	-		Acetylene
2.578	1		-	-	-		Ethane
5.730	1		-	-	-		Propylene
6.042	2		-	-	-		CO2
6.139	1		-	-	-		Propane
6.338	1		-	-	-		Propadiene
7.457	2		-	-	-		Argon/O2
8.287	2	BB	3.13911e4	1.92940e-3	99.816771		Nitrogen
9.879	2		-	-	-		CO
10.659	1		-	-	-		Iso-Butane
11.113	1		-	-	-		Iso-Butylene
11.201	1		-	-	-		butene-1
11.445	1		-	-	-		1,3-butadiene
11.805	1		-	-	-		n-Butane+c 2 butene
12.049	1		-	-	-		t-2-butane
16.351	1		-	-	-		Iso-Pentane
16.620	1		-	-	-		n- Pentane
17.002	1		-	-	-		T-2-Pentene
17.136	1		-	-	-		cis-2-pentene+1 pentene
21.468	1		-	-	-		n-hexane
21.896	1		-	-	-		1-hexene
Totals :					100.000000		

2 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)
Warning : Calibrated compound(s) not found

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Summed Peaks Report

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Final Summed Peaks Report

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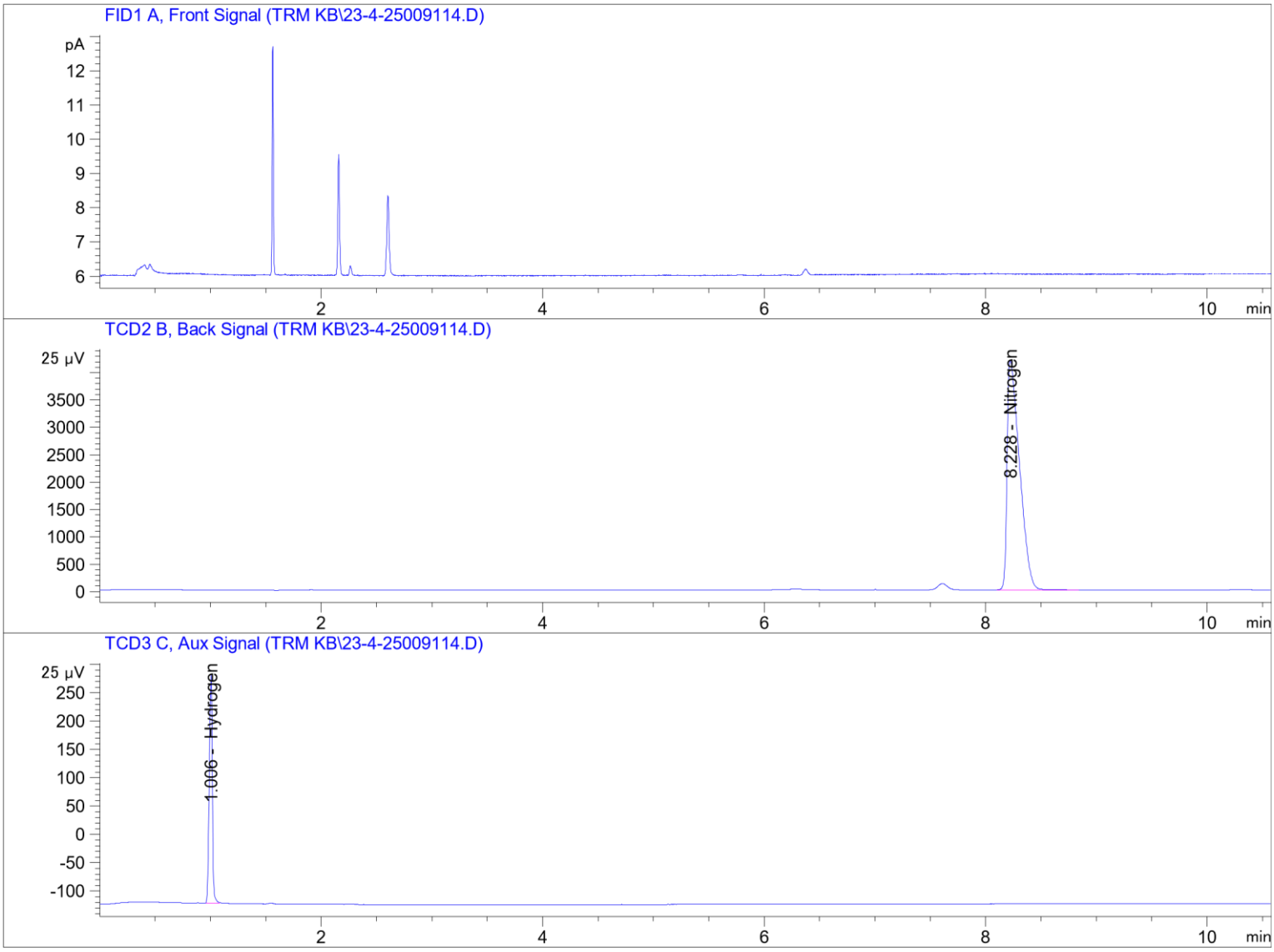
*** End of Report ***

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009114.D

Sample Name: Complex 2

Acq. Operator : KAPIL BHATI
Acq. Instrument : FAST RGA Location : Vial 1
Injection Date : 7/17/2025 11:28:10 AM
Inj Volume : Manually
Acq. Method : C:\CHEM32\1\METHODS\TRIAL-HSL-AB-26062024-.M
Last changed : 7/17/2025 11:21:10 AM by KAPIL BHATI
Analysis Method : C:\CHEM32\1\DATA\TRM KB\23-4-25009114.D\DA.M (TRIAL-HSL-AB-26062024-.M, From Data File)
Last changed : 7/17/2025 11:39:38 AM by KAPIL BHATI (modified after loading)
Sample Info : Complex 2



Additional Info : Peak(s) manually integrated

Normalized Percent Report

Sorted By : Retention Time
Calib. Data Modified : 7/17/2025 11:39:37 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Sample Name: Complex 2

Signal 1: FID1 A, Front Signal
Signal 2: TCD2 B, Back Signal
Signal 3: TCD3 C, Aux Signal

RetTime [min]	Sig	Type	Area	Amt/Area	Norm %	Grp	Name
0.000	1		-	-	-		Cis-2-Butene
0.000	1		-	-	-		1-pentene
1.006	3	BB	765.71039	5.06532e-3	5.789591		Hydrogen
1.549	1		-	-	-		Methane
2.241	1		-	-	-		Ethylene
2.357	1		-	-	-		Acetylene
2.578	1		-	-	-		Ethane
5.730	1		-	-	-		Propylene
6.042	2		-	-	-		CO2
6.139	1		-	-	-		Propane
6.338	1		-	-	-		Propadiene
7.457	2		-	-	-		Argon/O2
8.228	2	BB	3.27114e4	1.92940e-3	94.210409		Nitrogen
9.879	2		-	-	-		CO
10.659	1		-	-	-		Iso-Butane
11.113	1		-	-	-		Iso-Butylene
11.201	1		-	-	-		butene-1
11.445	1		-	-	-		1,3-butadiene
11.805	1		-	-	-		n-Butane+c 2 butene
12.049	1		-	-	-		t-2-butane
16.351	1		-	-	-		Iso-Pentane
16.620	1		-	-	-		n- Pentane
17.002	1		-	-	-		T-2-Pentene
17.136	1		-	-	-		cis-2-pentene+1 pentene
21.468	1		-	-	-		n-hexane
21.896	1		-	-	-		1-hexene
Totals :					100.000000		

2 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)
Warning : Calibrated compound(s) not found

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Summed Peaks Report

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Final Summed Peaks Report

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*** End of Report ***

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009102.D
Sample Name: Complex-3

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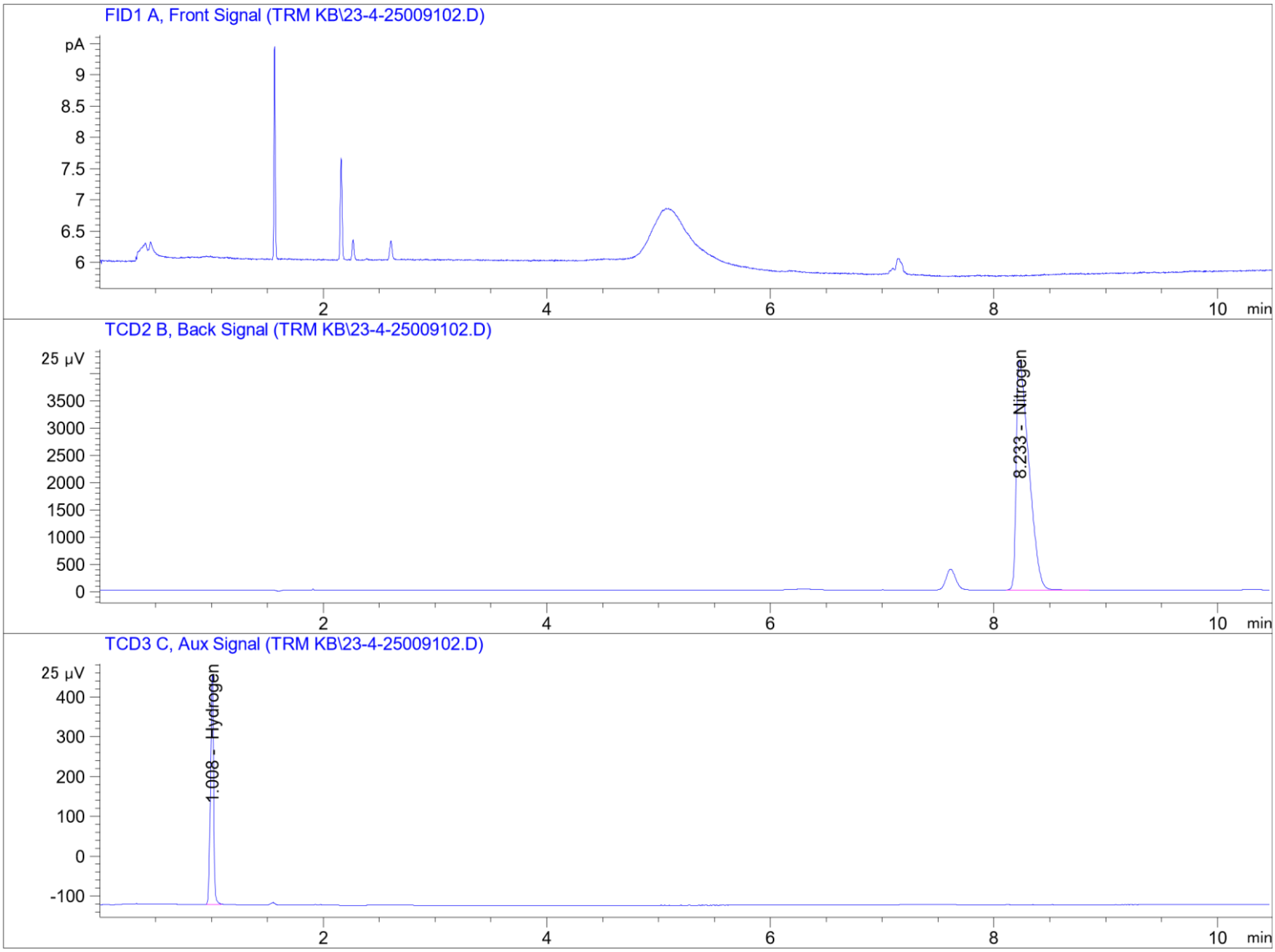
Acq. Operator : KAPIL BHATI
Acq. Instrument : FAST RGA Location : Vial 1
Injection Date : 7/16/2025 3:15:14 PM
Inj Volume : Manually
Acq. Method : C:\CHEM32\1\METHODS\TRIAL-HSL-AB-26062024-.M
Last changed : 7/16/2025 3:10:14 PM by KAPIL BHATI
Analysis Method : C:\CHEM32\1\DATA\TRM KB\23-4-25009102.D\DA.M (TRIAL-HSL-AB-26062024-.M, From Data File)
Last changed : 7/16/2025 3:25:43 PM by KAPIL BHATI
Sample Info : Complex-3

Additional Info : Peak(s) manually integrated



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= Normalized Percent Report

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Sorted By : Retention Time
Calib. Data Modified : 7/1/2024 11:32:18 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009102.D
Sample Name: Complex-3

Signal 1: FID1 A, Front Signal
Signal 2: TCD2 B, Back Signal
Signal 3: TCD3 C, Aux Signal

RetTime [min]	Sig	Type	Area	Amt/Area	Norm %	Grp	Name
0.000	1		-	-	-		Cis-2-Butene
0.000	1		-	-	-		1-pentene
1.008	3	BB	1127.45642	5.06532e-3	8.247827		Hydrogen
1.549	1		-	-	-		Methane
2.241	1		-	-	-		Ethylene
2.357	1		-	-	-		Acetylene
2.578	1		-	-	-		Ethane
5.730	1		-	-	-		Propylene
6.042	2		-	-	-		CO2
6.139	1		-	-	-		Propane
6.338	1		-	-	-		Propadiene
7.457	2		-	-	-		Argon/O2
8.233	2	BB	3.29276e4	1.92940e-3	91.752173		Nitrogen
9.879	2		-	-	-		CO
10.659	1		-	-	-		Iso-Butane
11.113	1		-	-	-		Iso-Butylene
11.201	1		-	-	-		butene-1
11.445	1		-	-	-		1,3-butadiene
11.805	1		-	-	-		n-Butane+c 2 butene
12.049	1		-	-	-		t-2-butane
16.351	1		-	-	-		Iso-Pentane
16.620	1		-	-	-		n- Pentane
17.002	1		-	-	-		T-2-Pentene
17.136	1		-	-	-		cis-2-pentene+1 pentene
21.468	1		-	-	-		n-hexane
21.896	1		-	-	-		1-hexene

Totals : 100.000000

2 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)
Warning : Calibrated compound(s) not found

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Summed Peaks Report

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Final Summed Peaks Report

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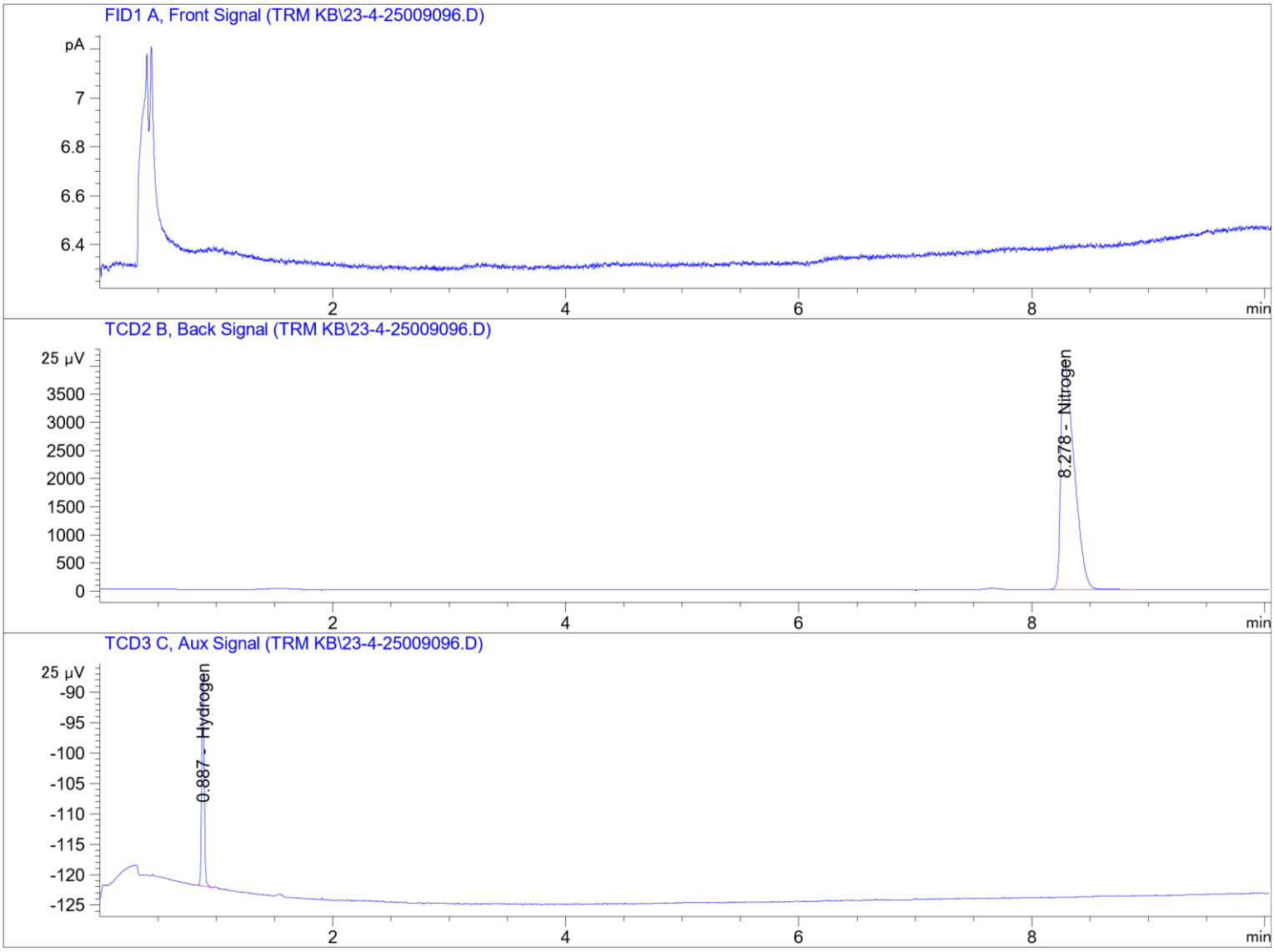
*** End of Report ***

Data File C:\CHEM32\1\DATA\TRM KB\23-4-25009096.D

Sample Name: Complex 3-Online

Acq. Operator : KAPIL BHATI
Acq. Instrument : FAST RGA Location : Vial 1
Injection Date : 7/15/2025 12:08:05 PM
Inj Volume : Manually
Acq. Method : C:\CHEM32\1\METHODS\TRIAL-HSL-AB-26062024-.M
Last changed : 7/15/2025 11:59:27 AM by KAPIL BHATI
Analysis Method : C:\CHEM32\1\DATA\TRM KB\23-4-25009096.D\DA.M (TRIAL-HSL-AB-26062024-.M, From Data File)
Last changed : 7/15/2025 1:02:10 PM by KAPIL BHATI (modified after loading)
Sample Info : Complex 3-Online



Additional Info : Peak(s) manually integrated

Normalized Percent Report

Sorted By : Retention Time
Calib. Data Modified : 7/15/2025 1:02:18 PM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Sample Name: Complex 3-Online

Signal 1: FID1 A, Front Signal
Signal 2: TCD2 B, Back Signal
Signal 3: TCD3 C, Aux Signal

RetTime [min]	Sig	Type	Area	Amt/Area	Norm %	Grp	Name
0.000	1		-	-	-		Cis-2-Butene
0.000	1		-	-	-		1-pentene
0.887	3	BV	52.38462	5.06532e-3	0.425185		Hydrogen
1.549	1		-	-	-		Methane
2.241	1		-	-	-		Ethylene
2.357	1		-	-	-		Acetylene
2.578	1		-	-	-		Ethane
5.730	1		-	-	-		Propylene
6.042	2		-	-	-		CO2
6.139	1		-	-	-		Propane
6.338	1		-	-	-		Propadiene
7.457	2		-	-	-		Argon/O2
8.278	2	BBA	3.22077e4	1.92940e-3	99.574815		Nitrogen
9.879	2		-	-	-		CO
10.659	1		-	-	-		Iso-Butane
11.113	1		-	-	-		Iso-Butylene
11.201	1		-	-	-		butene-1
11.445	1		-	-	-		1,3-butadiene
11.805	1		-	-	-		n-Butane+c 2 butene
12.049	1		-	-	-		t-2-butane
16.351	1		-	-	-		Iso-Pentane
16.620	1		-	-	-		n- Pentane
17.002	1		-	-	-		T-2-Pentene
17.136	1		-	-	-		cis-2-pentene+1 pentene
21.468	1		-	-	-		n-hexane
21.896	1		-	-	-		1-hexene
Totals :					100.000000		

2 Warnings or Errors :

Warning : Calibration warnings (see calibration table listing)
Warning : Calibrated compound(s) not found

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Summed Peaks Report

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Final Summed Peaks Report

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*** End of Report ***