Supplementary information for:

Computational design and molecular modeling of the interaction of nicotinic acid hydrazide nickel-based complexes with H_2S gas

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Spectroscopy

1. Ligand

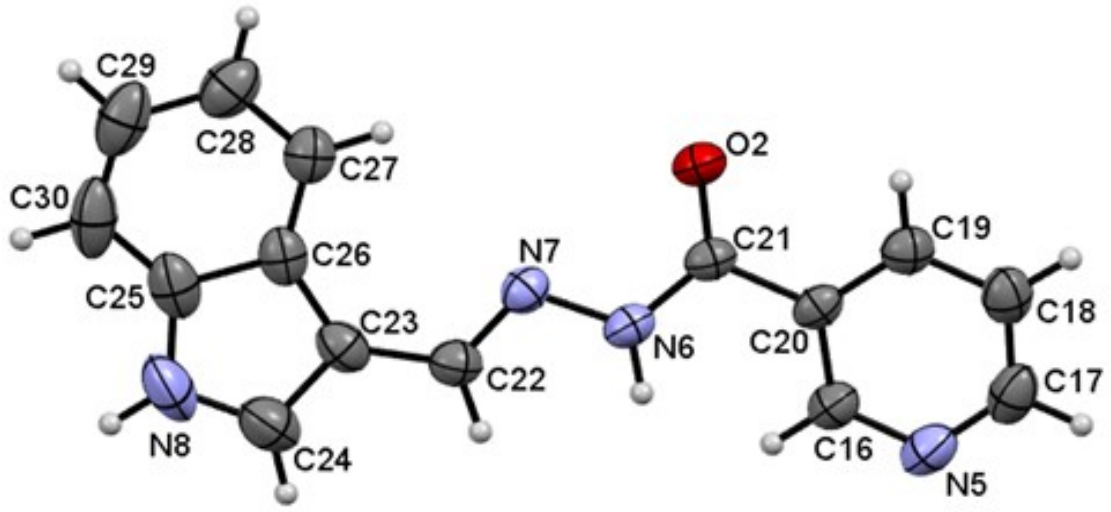
Yield 86 % , Melting point: 209 ◦C, $C_{15}H_{12}N_4O$, m/e 264.10, Elemental Analysis; *Found*; C, 68.17; H, 4.58; N, 21.20; O, 6.05, *Calculated:* C, 68.38; H, 4.69; N, 21.18; O, 6.02, mp 214 °C ;IR (KBr) (υ, cm^{-1}): 3178 (NH), 1657 (CO), 1600 (C=N), 1575 (C=C);^{1}H NMR (400 MHz, DMSO-d6) δ: 7.13–8.76 (m, 7H, Ar-H + [nicotine ring]), 7.87 (s, 1H, indole-H), 8.63 (s,1H, CH=NNH),9.09 (s, 1H, Nicotine [N=CH-CCO]), 11.56 (br.s, 1H,CONHN, exchangeable), 11.64 (br.s, 1H, NH-indole). The X-ray crystal information is presented in table S1 and Figure S1 of the supplementary material.

2. Complex

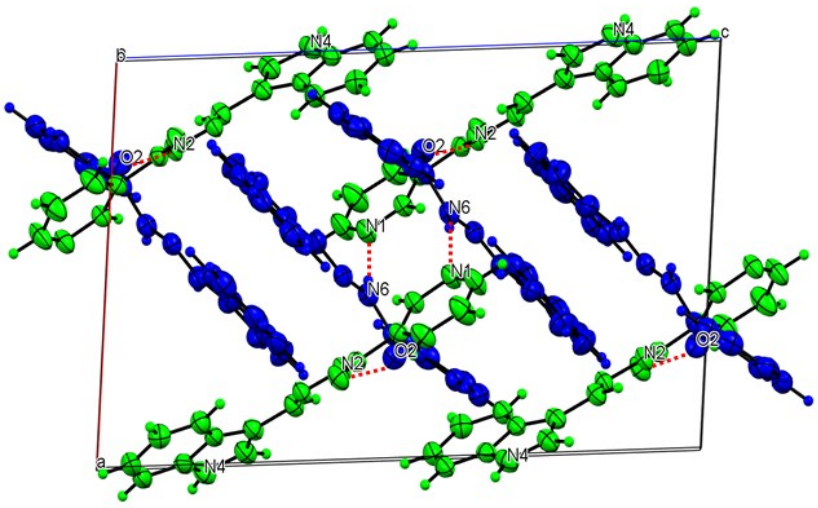
Yield 89%. Melting point: 237 ◦C; IR (KBr)(υ, cm^{-1}): 1590 (C=O), 1540 (C=N), 1332, 1025 ,540 (Zn-O), 481 (Zn-N), *m*/*e* (%) 588.1 (100) ; Elemental analysis for $C_{30}H_{24}ZnN_8O_2$ (%): Calculated C 61.08, H 3.42, N 18.99,O , 5.42; Found: C 61.23, H 3.45, N 19.01,O 5.46. ^{1}H-NMR (400 MHz, DMSO-d_6, δ, ppm): 6.97(m, 3H, Ar-H), 6.99(s, *J* = 8 Hz, 2H, Ar-H), 7.13(d, *J* = 8 Hz, 2H, Ar-H), 7.40(t, *J* = 8 Hz, 2H, Ar-H), 7.44(sbr, 3H, Ar-H), 7.60(d, *J* = 8 Hz, 1H, Ar-H), 7.81(s, 2H, indole-H), 8.29(s, 1H, Ar-H), 8.31(d, 2H, Ar-H), 9.00(s, 2H, Nicotine [N=CH-CCO]), 11.38(s, 2H, N-H) ,11.60 (br.s, 2H, NH-indole).

Crystal structure of the ligand (L1)

The molecular structure of L1 is depicted in **Figure S1a** along with the atomic numbering scheme. The crystal structure refinement data for L1 is given in **Table S1**. The L1 has two independent molecules having different torsion angle in the asymmetric unit of the crystal designated as molecule A (green) with a planar structure, molecule B (blue) with a twisted structure. There are a total of 8 molecules of $C_{15}H_{12}N_4O$ in the unit cell. The Schiff base L1 crystallizes in the monoclinic system in space group $P2_1/c$. In L1, the bond distance C(21)-O(1) is equal to 1.236(3) Å indicating its double bond nature. The bond lengths N(6)-N(7) and C(21)-N(6) are equal to 1.392(3)Å and 1.342(3)Å, respectively while C(21)-N(6)-N(7) equal to 120.63(17). Most of bond distances and angles were within common ranges of normal covalent bonds. The intermolecular hydrogen bond between (indole) N4-H…O1 (carbonyl) was observed for L1 molecule. The 6-membered aromatic rings are stacked *via* weak Π-interaction, and stacked rings of B are perpendicular to C=N bond of A.



(a)



(b)

Figure S1(a) *Molecular structure with atom numbering scheme* (b) *Crystal packing of distinguished Crystallographic independent molecules (A=green, B=blue) and molecular structures of for L1.*

Table S1. Crystal data and structure refinement of **L1**

Empirical formula	$C_{30}H_{24}N_8O_2$
Formula weight	528.57
Temperature (K)	173
Crystal system	monoclinic
Space group	$P2_1/c$ (# 14)
a, (Å)	11.4069(18)
b, (Å)	12.822(2)
c, (Å)	18.149(3)
α (°)	90.0000
β (°)	94.810(4)
γ (°)	90.0000
Volume (Å^3)	2645.1(7)
Z	4
ρ_{calc}(g/cm^3)	1.327
μ (mm^{-1})	0.088
F(000)	1104
Crystal size (mm^3)	0.12 × 0.11 × 0.1

Radiation	Mo Kα (λ = 0.71073)
T_{min}, T_{max}	0.93, 0.98
No. of reflections	5116
No. of parameters	362
Goodness of fit	1.127
$R_1[I>2\sigma(I)]$	0.0367
WR_2	0.1040

Table S2: Second order perturbation theory analysis of fock matrix in NBO basis estimated at DFT/ωB97XD/Gen

Donor Orbital	**Acceptor Orbital**	**E^2 Kcal/mol**	**E(j)-E(i)**	**F(i,j)**
		L_1		
π* N4 - C5	π* C7 - C8	62.43	0.02	0.067
π* C1 - O2	π* C12-C16	37.35	0.04	0.071
		L_2		
π* C1 - O2	π*C12-C16	71.32	0.02	0.071
LP(2) S 11	π*C7 - C8	33.17	0.38	0.101
LP(2) S 13	π*C14-C15	32.15	0.38	0.101
		L_3		
π* C1 - O2	π* C12-C16	44.01	0.03	0.072
LP (2) S 11	π* C7 - C8	33.20	0.38	0.101
		L_4		
π* C9 - C10	π* C7 - C8	121.46	0.01	0.069
LP (2) N 22	π* C12 - C13	67.78	0.26	0.127
π* C1 - O2	π* C11 - C14	66.07	0.04	0.083
		L_1Ni		
π C7 - C13	π* O2 - C6	41.69	0.33	0.108
LP (2) O 2	LP*(6) Ni 45	20.47	1.02	0.131
		L_2Ni		
π*C35-C41	π*C36-C37	66.79	0.02	0.074
π*C7-C13	π*C8-C9	57.27	0.03	0.075
LP (1) N 4	LP*(6) Ni 47	22.78	1.01	0.138
		L_3Ni		
π* C7 - C13	π* C8 - C9	56.34	0.03	0.075
π C7 - C13	π* O2 - C6	41.09	0.33	0.107
		L_4Ni		
π* C17 - C23	π* C18 - C19	51.01	0.03	0.075
π C 18 - C 19	LP*(2) N 46	92.86	0.13	0.123
		L_1Ni-H_2S		
LP (2) O 25	σ*C9 - H12	1227.96	0.07	0.291
π* C18 - C24	σ* C9 - H12	1211.30	0.09	0.654
		L_2Ni-H_2S		
σ C18 - H21	σ* C19 - H22	7484.17	0.29	1.304
σ C36 - C37	π* C25 - C46	15641.30	0.33	2.237
σ C17 - C23	σ* C19 - H22	3289.88	0.93	1.562
		L_3Ni-H_2S		
σ N5 - H14	σ* C36 - H39	5278.79	0.03	0.379

LP (1) S 48	σ* C9 - H12	2093.84	0.57	0.979
L_4Ni-H_2S				
LP (1) S 48	σ* S48 - H50	7726.42	0.07	0.664
σ S48 - H49	σ* S48 - H49	4315.68	0.16	0.735
σ S48 - H49	σ* C33 - C41	8244.44	0.02	0.394

Table S3: Thermodynamic properties for studied adsorptions

Parameters	**L_1Ni**	**H_2S**	**Product(L_1Ni-H_2S)**
E_0	-2266.784910	-399.399992	-2666.243780
E_{zpe}	0.362892	0.015678	0.385088
E_{tot}	0.386786	0.018525	0.411843
H_{corr}	0.387730	0.019470	0.412788
G_{corr}	0.306314	-0.003877	0.325255
$E_o + E_{ZpE}$	-2266.422019	-399.384314	-2665.858692
$E_o + E_{tot}$	-2266.398124	-399.381467	-2665.831937
$E_o + H_{corr}$	-2266.397180	-399.380522	-2665.830993
$E_o + G_{corr}$	-2266.478597	-399.403869	-2665.918526
$\Delta_f H^0$(298k)			35.9821kcal/mol
ΔrG^0 (298k)			24.3477kcal/mol
	L_2Ni	**H_2S**	**Product(L_2Ni-H_2S)**
E_0	-3558.731314	-399.399992	-3958.188657
E_{zpe}	0.346838	0.015678	0.368096
E_{tot}	0.373048	0.018525	0.397139
H_{corr}	0.373992	0.019470	0.398084
G_{corr}	0.286051	-0.003877	0.304812
$E_o + E_{ZpE}$	-3558.384477	-399.384314	-3957.820561
$E_o + E_{tot}$	-3558.358266	-399.381467	-3957.791518
$E_o + H_{corr}$	-3558.357322	-399.380522	-3957.790574
$E_o + G_{corr}$	-3558.445263	-399.403869	-3957.883846
$\Delta_f H^0$(298k)			35.6033 kcal/mol
ΔrG^0 (298k)			23.4389 kcal/mol
	L_3Ni	**H_2S**	**Product(L_3Ni-H_2S)**
E_0	-2912.766458	-399.399992	-3312.225927
E_{zpe}	0.355767	0.015678	0.378181
E_{tot}	0.380530	0.018525	0.405647
H_{corr}	0.381474	0.019470	0.406592
G_{corr}	0.297818	-0.003877	0.317557
$E_o + E_{ZpE}$	-2912.410690	-399.384314	-3311.847746
$E_o + E_{tot}$	-2912.385928	-399.381467	-3311.820279
$E_o + H_{corr}$	-2912.384984	-399.380522	-3311.819335
$E_o + G_{corr}$	-2912.468640	-399.403869	-3311.908370
$\Delta_f H^0$(298k)			36.3453 kcal/mol
ΔrG^0 (298k)			24.2133 kcal/mol
	L_4Ni	**H_2S**	**Product(L_4Ni-H_2S)**
E_0	-2225.730381	-399.399992	-2625.177484
E_{zpe}	0.358415	0.015678	0.377741

E_{tot}	0.382320	0.018525	0.404823
H_{corr}	0.383264	0.019470	0.405767
G_{corr}	0.301689	-0.003877	0.317077
$E_o + E_{ZpE}$	-2225.371966	-399.384314	-2624.799743
$E_o + E_{tot}$	-2225.348061	-399.381467	-2624.772661
$E_o + H_{corr}$	-2225.347117	-399.380522	-2624.771717
$E_o + G_{corr}$	-2225.428693	-399.403869	-2624.860407
$\Delta_f H^0$(298k)			29.7615 kcal/mol
ΔrG^0 (298k)			18.8009 kcal/mol

Table S4- S: Atomic coordinates of the studied compounds

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.256319	1.012120	-0.000481
2	8	0	1.353475	2.220840	-0.000220
3	7	0	-0.005637	0.446900	-0.001169
4	7	0	-0.230677	-0.881142	-0.000620
5	6	0	-1.429203	-1.332699	-0.000259
6	1	0	-1.507333	-2.415584	0.000603
7	6	0	-2.703153	-0.642680	-0.000079
8	6	0	-3.972413	-1.141305	-0.000101
9	6	0	-4.849614	-0.017580	0.000338
10	6	0	-4.055290	1.080268	0.000634
11	8	0	-2.751502	0.719733	0.000512
12	6	0	2.439215	0.129714	-0.000201
13	8	0	3.618190	0.805393	0.000319
14	6	0	4.601263	-0.104249	0.000529
15	6	0	4.096653	-1.365349	0.000481
16	6	0	2.681410	-1.214435	0.000103
17	1	0	-0.766716	1.117616	-0.000878
18	1	0	-4.241395	-2.185817	-0.000422
19	1	0	-5.927524	-0.025366	0.000458
20	1	0	-4.250912	2.139319	0.000954
21	1	0	5.605334	0.287338	0.000712
22	1	0	4.659928	-2.284682	0.000607
23	1	0	1.930383	-1.983693	-0.000183

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.804553	0.034958	-0.995923
2	8	0	0.012454	-1.531687	-0.212355
3	8	0	-1.894360	-0.833600	-1.688415
4	7	0	-0.705652	0.907644	-0.238089
5	7	0	2.125312	-0.902144	-0.044492
6	6	0	1.093872	-1.697328	0.352456
7	6	0	2.255327	-3.117874	2.183358
8	6	0	0.406737	-4.269664	2.576171
9	6	0	1.708786	-4.153242	2.971868
10	1	0	3.272511	-2.757595	2.221360
11	1	0	-0.397567	-4.916327	2.887942
12	1	0	2.207141	-4.739650	3.726961
13	6	0	1.241145	-2.684750	1.368162
14	8	0	0.111750	-3.391290	1.615028
15	1	0	3.053495	-0.958354	0.336874
16	6	0	2.782268	0.772647	-1.412086
17	1	0	2.523977	1.494043	-2.182132
18	6	0	5.036141	0.167314	-0.210831
19	6	0	6.132763	1.640283	-1.439112
20	6	0	6.308020	0.718463	-0.445343
21	1	0	4.839802	-0.593292	0.530279
22	1	0	6.817444	2.297417	-1.952008
23	1	0	7.234802	0.466680	0.043952
24	6	0	4.158459	0.794037	-1.076313
25	8	0	4.859372	1.702232	-1.818004
26	6	0	-2.618549	-0.138194	-0.953358
27	6	0	-4.663027	-1.292956	-1.703503
28	6	0	-5.070697	0.312391	-0.194985
29	1	0	-4.295849	-2.027476	-2.401185
30	6	0	-6.221076	-0.278222	-0.574535
31	1	0	-4.987791	1.114561	0.520383
32	1	0	-7.254953	-0.136290	-0.309279
33	7	0	-2.068939	0.841077	-0.208708
34	1	0	-2.604556	1.434767	0.412358
35	6	0	-0.158396	1.821680	0.480972
36	1	0	0.919109	1.881095	0.407664
37	6	0	-0.066107	3.712751	2.140813
38	6	0	-2.243996	3.823563	2.509910
39	6	0	-1.063550	4.393658	2.872360
40	1	0	0.998242	3.888874	2.164508
41	1	0	-3.265962	4.005681	2.800186
42	1	0	-0.932783	5.201964	3.573768
43	6	0	-0.702971	2.766331	1.380900
44	8	0	-2.050818	2.839707	1.610706
45	28	0	-0.088561	-0.347017	-1.638012
46	6	0	-4.031506	-0.350990	-0.934622
47	8	0	-5.967916	-1.254081	-1.489526

Rotational constants (GHZ): 0.1601282 0.0889583 0.0762542

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.754088	0.007487	-0.744125
2	8	0	-0.097893	-1.574795	-0.351279
3	8	0	-1.913965	-0.566324	-1.651966
4	7	0	-0.689654	0.779059	0.124963
5	7	0	2.044640	-1.148472	-0.078001
6	6	0	0.970939	-1.967283	0.115848
7	6	0	2.249615	-3.844482	1.332888
8	6	0	0.424678	-5.047433	1.676322
9	6	0	1.773596	-5.053502	1.883929
10	1	0	3.278192	-3.515590	1.312521
11	1	0	-0.356082	-5.749202	1.922871
12	1	0	2.345559	-5.825482	2.372984
13	6	0	1.150931	-3.196285	0.825935
14	8	0	0.037855	-3.937238	1.040502
15	1	0	2.969599	-1.340817	0.264164
16	6	0	2.729480	0.830959	-0.922539
17	1	0	2.492370	1.725456	-1.486303
18	6	0	4.962094	-0.109039	0.096035
19	6	0	6.064976	1.677714	-0.585061
20	6	0	6.232949	0.496740	0.077927
21	1	0	4.762558	-1.065487	0.554360
22	1	0	6.750692	2.467136	-0.847511
23	1	0	7.151000	0.114651	0.493835
24	6	0	4.097049	0.740093	-0.565572
25	8	0	4.801576	1.839699	-0.968498
26	6	0	-2.597256	-0.148675	-0.705119
27	6	0	-4.717420	-0.907021	-1.737836
28	6	0	-4.978606	-0.116775	0.339241
29	1	0	-4.420930	-1.251494	-2.715091
30	6	0	-6.165469	-0.508450	-0.165339
31	1	0	-4.826909	0.289592	1.326535
32	1	0	-7.171081	-0.524122	0.219082
33	7	0	-2.034025	0.618537	0.245879
34	1	0	-2.544919	1.049817	1.005003
35	6	0	-0.146596	1.649442	0.896658
36	1	0	0.905578	1.822389	0.718964
37	6	0	-0.020694	3.256280	2.838663
38	6	0	-2.134446	3.051525	3.452510
39	6	0	-0.982845	3.698329	3.774128
40	1	0	1.016773	3.546307	2.779743
41	1	0	-3.124065	3.064758	3.879040
42	1	0	-0.845858	4.397309	4.582995
43	6	0	-0.649304	2.370792	2.003838
44	8	0	-1.958969	2.249504	2.385822
45	28	0	-0.113409	-0.101627	-1.503933
46	6	0	-4.011542	-0.370688	-0.693730
47	8	0	-6.002591	-0.985668	-1.428899
48	16	0	0.226573	2.576639	-2.535107
49	1	0	-1.097190	2.818254	-2.511161
50	1	0	0.298773	2.584696	-3.878987

Rotational constants (GHZ): 0.1383769 0.0875953 0.0736604

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.241597	0.898831	0.219101
2	8	0	1.341998	2.099141	0.391208
3	7	0	-0.029395	0.352797	0.182516
4	7	0	-0.281174	-0.974432	0.210754
5	6	0	-1.488250	-1.396927	0.182756
6	1	0	-1.576983	-2.478192	0.249773
7	6	0	-2.764951	-0.693770	0.094005
8	6	0	-3.968057	-1.263138	0.428241
9	6	0	-5.077747	-0.407178	0.217719
10	6	0	-4.711813	0.803943	-0.287840
11	16	0	-3.014848	0.915606	-0.518559
12	6	0	2.430076	0.048116	0.019907
13	16	0	3.954939	0.867708	0.141146
14	6	0	4.804914	-0.577495	-0.194589
15	6	0	3.969653	-1.638803	-0.396806
16	6	0	2.604247	-1.281118	-0.273473
17	1	0	-0.751745	1.035763	0.392781
18	1	0	-4.045033	-2.270288	0.817957
19	1	0	-6.102805	-0.679310	0.428665
20	1	0	-5.343506	1.639623	-0.548833
21	1	0	5.884657	-0.572467	-0.226981
22	1	0	4.314384	-2.638544	-0.624095
23	1	0	1.779572	-1.966045	-0.387336

Rotational constants (GHZ): 1.6328077 0.2016621 0.1824498

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.799740	-0.108995	-0.790825
2	8	0	-0.131737	-1.577873	-0.396691
3	8	0	-1.840461	-0.550228	-1.819432
4	7	0	-0.631630	0.823446	-0.077482
5	7	0	2.019845	-1.250997	-0.074893
6	6	0	0.910484	-2.021188	0.100270
7	6	0	2.080338	-3.886756	1.369864
8	6	0	0.398996	-5.347734	1.943605
9	6	0	1.744703	-5.088357	2.015608
10	1	0	3.100249	-3.525963	1.302842
11	1	0	-0.129581	-6.195420	2.356321
12	1	0	2.454431	-5.740208	2.504641
13	6	0	0.983350	-3.254072	0.820666
14	1	0	2.939731	-1.501381	0.252396
15	6	0	2.810616	0.673599	-0.960283
16	1	0	2.627141	1.509558	-1.625652
17	6	0	4.700291	-0.033947	0.652960
18	6	0	6.567900	0.981770	-0.233653
19	6	0	6.079933	0.198053	0.779990
20	1	0	4.136500	-0.570643	1.405790
21	1	0	7.590765	1.292531	-0.391704
22	1	0	6.691755	-0.186375	1.583570
23	6	0	4.144043	0.576615	-0.461735
24	6	0	-2.553049	-0.066611	-0.930364
25	6	0	-4.658233	-0.838315	-1.997754
26	6	0	-6.388070	-0.408815	-0.530395
27	6	0	-6.043555	-0.907099	-1.756996
28	1	0	-4.170926	-1.174257	-2.903340
29	1	0	-7.373398	-0.348219	-0.090978
30	1	0	-6.767345	-1.307763	-2.452061

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.944116	0.307500	-1.057998
2	8	0	0.172392	-1.362490	-0.472241
3	8	0	-1.730590	-0.515242	-1.843288
4	7	0	-0.567171	1.044678	-0.211718
5	7	0	2.271514	-0.726382	-0.216990
6	6	0	1.254020	-1.581092	0.085128
7	6	0	2.538413	-3.032492	1.722629
8	6	0	1.057832	-4.680595	2.330616
9	6	0	2.327786	-4.186050	2.494552
10	1	0	3.484303	-2.503952	1.715719
11	1	0	0.630445	-5.553607	2.803583
12	1	0	3.067414	-4.637178	3.140427
13	6	0	1.428687	-2.672332	0.986877
14	1	0	3.195058	-0.804621	0.171856
15	6	0	2.914921	1.098008	-1.383406
16	1	0	2.647868	1.901862	-2.064044
17	6	0	5.183064	0.369930	-0.280564
18	6	0	6.244437	2.033820	-1.275413
19	6	0	6.442882	0.975588	-0.433603
20	1	0	5.007604	-0.508107	0.322894
21	1	0	6.912933	2.775413	-1.683671
22	1	0	7.377207	0.671473	0.009528
23	6	0	4.290254	1.099639	-1.043462
24	6	0	-2.469734	0.053011	-1.018612
25	6	0	-4.490071	-1.027427	-1.946321
26	6	0	-6.291578	-0.405148	-0.643820
27	6	0	-5.876812	-1.125071	-1.731460
28	1	0	-3.957932	-1.510349	-2.754263
29	1	0	-7.295284	-0.308093	-0.255181
30	1	0	-6.554525	-1.700860	-2.345200
31	7	0	-1.928255	0.954305	-0.172088
32	1	0	-2.460613	1.471052	0.518529
33	6	0	-0.025788	1.884449	0.597731
34	1	0	1.049786	1.969931	0.524154
35	6	0	0.044738	3.586302	2.455185
36	6	0	-2.133305	3.612899	2.843315
37	6	0	-0.961941	4.165816	3.258432
38	1	0	1.105401	3.781421	2.492052
39	1	0	-3.157432	3.740981	3.153942
40	1	0	-0.842597	4.896656	4.042077
41	6	0	-0.578310	2.714326	1.600724
42	16	0	0.114439	-3.768557	1.247636
43	16	0	-5.006209	0.397328	0.143291
44	6	0	-3.871099	-0.230228	-1.008643
45	8	0	-1.925061	2.735369	1.843639
46	8	0	4.968767	2.123791	-1.640885
47	28	0	0.070102	-0.020522	-1.756886

Rotational constants (GHZ): 0.1446323 0.0813105 0.0684826

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.926273	-0.191418	-0.770548
2	8	0	-0.057637	1.393361	-0.510634
3	8	0	1.728614	0.280909	-1.753454
4	7	0	0.533770	-0.931799	0.091062
5	7	0	-2.192801	1.003355	-0.163985
6	6	0	-1.114332	1.828743	-0.042124
7	6	0	-2.366586	3.704969	1.126878
8	6	0	-0.786476	5.343373	1.462143
9	6	0	-2.102499	4.990369	1.627652
10	1	0	-3.351471	3.254620	1.161907
11	1	0	-0.313372	6.268843	1.758749
12	1	0	-2.840094	5.632244	2.088131
13	6	0	-1.244602	3.103262	0.593286
14	1	0	-3.107507	1.218081	0.191481
15	6	0	-2.915900	-1.009306	-0.884723
16	1	0	-2.700655	-1.941260	-1.393810
17	6	0	-5.130076	0.040968	0.067693
18	6	0	-6.247776	-1.801669	-0.411424
19	6	0	-6.403117	-0.557741	0.127691
20	1	0	-4.924157	1.044134	0.408483
21	1	0	-6.939624	-2.610995	-0.580847
22	1	0	-7.314566	-0.129658	0.511929
23	6	0	-4.276648	-0.875634	-0.514158
24	6	0	2.441655	-0.075488	-0.804361
25	6	0	4.543396	0.657459	-1.909375
26	6	0	6.249668	0.467329	-0.366095
27	6	0	5.918530	0.810596	-1.648331
28	1	0	4.066387	0.868908	-2.857126
29	1	0	7.224932	0.497904	0.098205
30	1	0	6.643477	1.162171	-2.368340
31	7	0	1.884042	-0.801103	0.185941
32	1	0	2.389050	-1.204498	0.964976
33	6	0	-0.012152	-1.738363	0.928882
34	1	0	-1.071805	-1.896722	0.785707
35	6	0	-0.135681	-3.217147	2.972037
36	6	0	1.998352	-3.035963	3.521657
37	6	0	0.837417	-3.626636	3.911150
38	1	0	-1.181644	-3.480649	2.955041
39	1	0	2.998282	-3.051187	3.923267
40	1	0	0.702013	-4.271365	4.764111
41	6	0	0.495069	-2.401580	2.070020
42	16	0	0.141284	4.132709	0.706634
43	16	0	4.900025	-0.046227	0.545945
44	6	0	3.850930	0.188182	-0.816030
45	8	0	1.816083	-2.295701	2.413075
46	8	0	-4.990652	-2.006949	-0.794517
47	28	0	-0.080708	-0.141267	-1.574719
48	16	0	-0.422132	-2.881343	-2.408517
49	1	0	-0.502935	-2.989439	-3.747721
50	1	0	0.919228	-2.998405	-2.384832

Rotational constants (GHZ): 0.1253792 0.0808957 0.0658211

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.348193	1.024430	0.034184
2	8	0	1.271702	2.245389	0.072376
3	7	0	0.053754	0.400115	-0.009344
4	7	0	-0.210125	-0.881718	0.144661
5	6	0	-1.415809	-1.335523	0.173655
6	1	0	-1.500012	-2.410224	0.303362
7	6	0	-2.686958	-0.647482	0.062059
8	6	0	-3.964149	-1.136023	0.085469
9	6	0	-4.832977	-0.013117	-0.063209
10	6	0	-4.031373	1.074473	-0.166056
11	6	0	2.545924	0.226542	0.004530
12	6	0	4.672324	-0.105388	0.028586
13	6	0	4.094928	-1.379444	-0.181702
14	6	0	2.720617	-1.166762	-0.194962
15	1	0	-0.688569	1.091324	-0.032245
16	1	0	-4.238843	-2.173090	0.195788
17	1	0	-5.911401	-0.014286	-0.090354
18	1	0	-4.214416	2.128330	-0.289724
19	1	0	5.731101	0.127560	0.103968
20	1	0	4.613422	-2.322922	-0.305279
21	1	0	1.944714	-1.903736	-0.325142
22	7	0	3.760096	0.856704	0.136175
23	8	0	-2.730000	0.704749	-0.091895

Rotational constants (GHZ): 2.0335666 0.2652676 0.2353042

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.533439	1.200448	-0.509986
2	8	0	1.910609	-0.644316	-1.471294
3	8	0	-1.556054	0.577832	-1.782153
4	7	0	-0.377240	-1.192044	-0.496188
5	7	0	1.815929	1.107571	-0.101887
6	6	0	2.528277	0.127094	-0.713978
7	6	0	4.890705	0.596810	0.224097
8	6	0	5.759970	-1.123919	-0.856707
9	6	0	6.087312	-0.111546	0.002542
10	1	0	4.772050	1.465136	0.855152
11	1	0	6.342694	-1.908445	-1.313276
12	1	0	7.063681	0.098008	0.408444
13	6	0	3.921617	-0.042875	-0.511889
14	1	0	2.203025	1.742930	0.580632
15	6	0	-0.200492	2.151260	0.068369
16	1	0	-1.152809	2.338202	-0.407364
17	6	0	1.117560	3.042068	2.150775
18	6	0	-0.433217	4.666939	2.363180
19	6	0	0.805761	4.093320	2.932265
20	1	0	1.924593	2.347556	2.337286
21	1	0	-0.955870	5.538560	2.737991
22	1	0	1.324712	4.446317	3.812121
23	6	0	0.073629	2.987538	1.127599
24	6	0	-2.278479	-0.096978	-1.017412
25	6	0	-4.479610	1.004971	-1.611131
26	6	0	-5.657987	-0.150320	-0.128904
27	6	0	-5.774799	0.811571	-1.094970
28	1	0	-4.164663	1.680034	-2.391421
29	1	0	-6.375828	-0.614470	0.529014
30	1	0	-6.684867	1.309108	-1.388294

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.833795	-0.037187	-1.055982
2	8	0	-0.025436	-1.555331	-0.341638
3	8	0	-1.847398	-0.809864	-1.872612
4	7	0	-0.675676	0.892647	-0.393574
5	7	0	2.100908	-0.998779	-0.114447
6	6	0	1.042767	-1.775834	0.242098
7	6	0	2.235501	-3.140258	2.014119
8	6	0	0.665835	-4.639387	2.762202
9	6	0	1.959162	-4.199132	2.892801
10	1	0	3.208114	-2.664571	1.969348
11	1	0	0.186953	-5.437906	3.311308
12	1	0	2.670303	-4.626679	3.584883
13	6	0	1.150266	-2.789963	1.237773
14	1	0	3.035005	-1.128513	0.241039
15	6	0	2.842752	0.685978	-1.421366
16	1	0	2.624324	1.375107	-2.232553
17	6	0	4.799438	0.344274	0.237224
18	6	0	6.614814	1.183268	-0.908224
19	6	0	6.176475	0.612442	0.260875
20	1	0	4.279474	-0.034337	1.108874
21	1	0	7.626508	1.468738	-1.161125
22	1	0	6.824354	0.400751	1.099591
23	6	0	4.191463	0.720994	-0.954469
24	6	0	-2.589242	-0.129857	-1.143355
25	6	0	-4.623336	-1.228855	-2.018726
26	6	0	-6.432090	-0.428849	-0.827979
27	6	0	-6.017497	-1.257272	-1.835711
28	1	0	-4.090527	-1.796401	-2.769492
29	1	0	-7.440297	-0.264420	-0.475347
30	1	0	-6.700482	-1.864220	-2.412398
31	7	0	-2.038722	0.849743	-0.389831
32	1	0	-2.598195	1.470206	0.176738
33	6	0	-0.103467	1.801163	0.314609
34	1	0	0.973866	1.831679	0.210302
35	6	0	0.254372	3.727269	1.782533
36	6	0	-1.721522	4.331206	2.788420
37	6	0	-0.388585	4.610890	2.664819
38	1	0	1.309619	3.776011	1.544934
39	1	0	-2.456292	4.834993	3.399873
40	1	0	0.099604	5.419290	3.190243
41	6	0	-0.586779	2.781152	1.227088
42	16	0	-2.199653	2.991990	1.847333
43	16	0	-0.222130	-3.785502	1.587759
44	16	0	5.364062	1.431781	-2.026165
45	16	0	-5.138121	0.397940	-0.081731
46	6	0	-3.998874	-0.367189	-1.143184
47	28	0	-0.028823	-0.371955	-1.773564

Rotational constants (GHZ): 0.1278738 0.0724412 0.0610746