Supporting Information for

A Density Functional Study of Neutral Salicylaldiminato Ni(II) Complexes as Olefin Polymerization Catalysts

Mary S.W. Chan, Liqun Deng, Tom Ziegler

Department of Chemistry, The University of Calgary, Calgary, Alberta, T2N 1N4, Canada

Contents

Force field parameters used:

BONDS Ebond = 0.5*K(r-ro)**2

Atoms i	- j	K (kcal/molA^2)	ro (Ang)	Source
CA	CA	1 938.0	1.400	amber95
CT	CT	1 620.0	1.526	amber95
CT	HC	1 680.0	1.090	amber95
CA	HA	1 734.0	1.080	amber95
CA	CT	1 634.0	1.510	amber95
CM	CT	1 634.0	1.510	amber95
CM	HA	1 868.0	1.010	amber95
CT	F	1 734.0	1.380	amber95

BENDS Ebend = 0.5*k(a-ao)^2

Atoms i - j - k			k (kcal/mol)	ao (deg)	Source
CA	CA	HA 1	70.00	120.00	amber95
CA	CA	CA 1	126.00	120.00	amber95
CT	CT	HC 1	100.00	109.50	amber95
HC	CT	HC 1	70.00	109.50	amber95
CT	CT	CT 1	80.00	109.50	amber95
N2	CA	CA 1	140.00	120.10	amber95 N2-CA-CM
P	CA	CA 1	140.00	120.10	amber95 N2-CA-CM
CA	CA	CT 1	140.00	120.0	amber95
CM	CT	HC 1	100.00	109.50	amber95
Cr	N2	CA 1	70.00	120.0	amber95 H-N2-CA
Fe	N2	CA 1	70.00	120.0	amber95 H-N2-CA
Co	N2	CA 1	70.00	120.0	amber95 H-N2-CA
Ni	N2	CA 1	70.00	120.0	amber95 H-N2-CA
Pd	N2	CA 1	70.00	120.0	amber95 H-N2-CA
CM	N2	CA 1	140.00	120.0	amber95 CM-N*-CT
N2	CM	CT 1	140.00	119.70	amber95 CM-CM-CT
CM	CM	CT 1	140.00	119.70	amber95
N2	CM	HA 1	70.00	119.10	amber95 H4-CM-N*
CM	CM	HA 1	70.00	119.70	amber95
CT	CT	CA 1	126.00	114.0	amber95
CA	CT	HC 1	100.00	109.5	amber95
CT	CT	F 1	77.00	109.1	amber95 F-CT-F
CA	CT	F 1	77.00	109.1	amber95 F-CT-F

TORSIONS Etors=K(1+cos(nt-to))

Atoms i - j - k - l				no. paths	K	per. n	shift to	Source
*	CA	CA	* 1	3.625	2	180.0	amber95	
*	N2	CA	* 1	1.80	2	180.0	amber95 = 2.4	
*	P	CA	* 1	0.01	2	180.0	amber95 = 2.4	
*	CT	CT	* 1	0.156	3	0.0	amber95	
*	CA	CT	* 1	0.00	2	0.0	amber95	
*	CT	CM	* 1	0.00	3	0.0	amber95	
*	N2	Ni	* 1	0.00	2	0.0		
*	N2	Pd	* 1	0.00	2	0.0		
*	N2	CM	* 1	2.40	2	180.0	amber95	X-N2-CA-X
*	CM	CM	* 1	6.65	2	180.0	amber95	
*	CM	CT	* 1	0.00	3	0.0	amber95	

IMPROPER TORSIONS Eimp=K(1-cos(nt-to)) (i is central atom)

Atoms i - j - k - l				K	shift to	per n	Source
CA	CA	N2	CA	1 0.00	0.0		
CA	CA	P	CA	1 0.00	0.0		
N2	Fe	CM	CA	1 0.0	0.0		
N2	Co	CM	CA	1 0.0	0.0		
N2	Ni	CM	CA	1 0.0	0.0		
N2	Pd	CM	CA	1 0.0	0.0		
CM	N2	CM	CT	1 0.0	0.0		
CA	CA	CA	CA	1 1.10	180.0	amber95	
CA	CA	CA	HA	1 1.10	180.0	amber95	
CA	CA	CA	CT	1 1.10	180.0	amber95	
CM	N2	CM	HA	1 1.10	180.0	amber95	

VAN DER WAALS

1-4 scale type				
0.5 atom(s)	LJ emin	rmin	Source	
CA	.0860	3.81600	12.00	amber95
HA	.0150	2.91800	12.00	amber95
CT	.1094	3.81600	12.00	amber95
CM	.0860	3.81600	12.00	amber95
HC	.0157	2.91400	12.00	amber95
Ti	.0170	3.17500	12.00	UFF I rappe
Zr	.0690	3.12400	12.00	UFF I rappe
Cr	.0150	3.02300	12.00	UFF I rappe
Fe	.013	2.912	12.00	UFF I rappe
Co	.014	2.834	12.00	UFF I rappe
Col	.0860	3.81600	12.00	as CA and C in amber95
Pd	.0480	2.89900	12.00	
Ni	.0480	2.7	12.00	
N2	.17	3.648	12.00	amber95
F	.061	3.50	12.00	amber95
Cl	.227	3.947	12.00	UFF I rappe
O2	.060	3.50	12.00	UFF I rappe
N	.1700	3.648	12.00	amber95
O	.2100	3.3224	12.00	amber95
P	.2000	4.200	12.00	amber95

Geometries (Å)

Structure **1a**

E_{total} = -8.07059265 a.u.

Atom	X	Y	Z
Ni	-0.1029	0.1057	-0.1116
N	1.6605	0.2518	-0.7501
C	2.4494	1.2948	-0.7034
C	2.1291	2.5472	-0.1138
C	0.8703	2.7677	0.5362
C	0.6543	4.0527	1.1152
C	1.6094	5.0428	1.0530
C	2.8471	4.8206	0.4118
C	3.0894	3.5888	-0.1557
O	-0.0683	1.8773	0.6337
C	-0.2322	-1.6514	-0.9799
C	-0.4285	-1.4748	-2.4847
C	-0.5037	-2.8059	-3.2447
H	0.7263	-2.1627	-0.7610
H	-1.0212	-2.3154	-0.5822
H	-1.3521	-0.9018	-2.6792
H	0.3877	-0.8619	-2.9044
H	-1.3486	-3.4160	-2.8866
H	-0.6370	-2.6440	-4.3262
H	0.4154	-3.3956	-3.0980
H	4.0421	3.3942	-0.6532
H	3.5963	5.6098	0.3700
H	1.4044	6.0139	1.5082
H	3.4500	1.2111	-1.1470
H	-0.3021	4.2213	1.6115
P	-2.1148	-0.1855	0.6489
C	-3.4535	-0.5884	-0.5739
C	-2.3317	-1.5338	1.9078
C	-2.8328	1.2788	1.5271
H	-3.8416	1.0510	1.9006
H	-2.1699	1.5528	2.3573
H	-2.8671	2.1269	0.8314
H	-4.4182	-0.7124	-0.0589
H	-3.5325	0.2302	-1.3027
H	-3.2060	-1.5146	-1.1088
H	-3.3843	-1.6067	2.2204
H	-2.0080	-2.4931	1.4826
H	-1.7039	-1.3081	2.7808
H	2.0919	-0.5537	-1.2173

Structure **1b-O**

E_{total} = -5.66455336 a.u.

Atom	X	Y	Z
Ni	-0.0008	-0.0002	-0.0001
N	1.8191	0.0002	0.0018
C	2.5692	1.0775	0.0012
C	2.1050	2.4193	0.0063
C	0.7040	2.7513	0.0143
C	0.3620	4.1325	0.0242
C	1.3271	5.1148	0.0223
C	2.6999	4.7876	0.0108
C	3.0676	3.4613	0.0035
C	-0.3478	-1.8783	-0.0154
C	-1.7242	-1.3139	-0.0056
O	-0.2542	1.8716	0.0117
H	-1.6793	-0.1299	-0.0397
H	-2.2640	-1.4958	-0.9496
C	-2.5925	-1.6113	1.2178
H	-0.0281	-2.3799	-0.9385
H	-0.0403	-2.4077	0.8976
H	-2.0417	-1.3936	2.1439
H	-3.5161	-1.0146	1.2170
H	-2.8684	-2.6764	1.2208
H	4.1247	3.1869	-0.0053
H	3.4542	5.5731	0.0070
H	1.0230	6.1631	0.0288
H	3.6570	0.9382	-0.0037
H	2.3486	-0.8756	-0.0008
H	-0.7005	4.3795	0.0321

Structure **1b-N**

E_{total} = -5.65801290 a.u.

Atom	X	Y	Z
Ni	-0.0307	0.0536	-0.0529
O	1.8222	-0.0471	0.0065
C	2.6247	0.9843	0.0130
C	2.2196	2.3611	-0.0364
C	0.8551	2.7573	-0.0976
C	3.2065	3.3792	-0.0237
C	4.5505	3.0880	0.0355
C	4.9504	1.7362	0.0850
C	4.0214	0.7196	0.0746
C	-0.2906	-1.8624	0.0095
C	-1.6546	-1.3328	0.0049
N	-0.1668	1.9391	-0.1144
H	-1.6231	-0.1090	-0.1202
H	-2.2106	-1.5504	-0.9222
C	-2.5073	-1.5351	1.2563
H	0.0893	-2.3360	-0.9024
H	0.0876	-2.2919	0.9448
H	-1.9325	-1.2865	2.1596
H	-3.4167	-0.9170	1.2406
H	-2.8103	-2.5912	1.3194
H	2.8721	4.4181	-0.0625
H	5.2923	3.8852	0.0433
H	6.0122	1.4884	0.1323
H	0.6669	3.8381	-0.1326
H	-1.0613	2.4357	-0.1593
H	4.3234	-0.3279	0.1126

Structure **1c-O**

E_{total} = -6.84801996 a.u.

Atom	X	Y	Z
Ni	-0.0038	0.0017	-0.0053
N	1.8714	-0.0087	0.0096
C	2.6586	1.0361	0.0216
C	2.2598	2.3945	0.0019
C	0.8781	2.7865	-0.0216
C	0.6044	4.1852	-0.0608
C	1.6174	5.1176	-0.0899
C	2.9745	4.7265	-0.0786
C	3.2762	3.3853	-0.0311
O	-0.1092	1.9482	-0.0127
C	0.0635	-1.9497	0.1099
C	0.4387	-2.3969	1.5168
H	1.4242	-1.9916	1.8045
H	-0.2784	-1.9822	2.2467
C	0.4624	-3.9257	1.6593
H	-0.9104	-2.3774	-0.1811
H	0.8082	-2.2840	-0.6373
H	1.1878	-4.3757	0.9630
H	0.7376	-4.2256	2.6826
H	-0.5267	-4.3538	1.4331
H	4.3181	3.0582	-0.0267
H	3.7656	5.4746	-0.1107
H	1.3661	6.1794	-0.1254
H	3.7421	0.8586	0.0298
C	-2.0011	0.0024	0.4769
C	-1.8452	-0.0116	-0.9003
H	-2.1391	0.9503	1.0031
H	-2.2424	-0.9090	1.0285
H	-1.8558	0.9254	-1.4630
H	-1.9530	-0.9324	-1.4774
H	2.3821	-0.8978	0.0103
H	-0.4435	4.4877	-0.0736

Strucutre **4a**

E_{total} = -5.757577 a.u.

Atom	X	Y	Z
Ti	0.0037	-0.0011	0.0198
N	1.8678	0.0031	-0.0458
C	2.6239	1.2647	-0.2095
C	1.9304	2.4584	0.4425
C	0.5713	2.8595	-0.1269
N	-0.4608	1.8119	0.0364
H	2.4901	-0.8180	-0.0092
H	2.8023	1.4598	-1.2832
H	3.6112	1.1413	0.2639
H	1.8208	2.2605	1.5229
H	2.6001	3.3285	0.3414
H	0.6642	3.1237	-1.1969
H	0.2311	3.7654	0.4002
H	-1.4067	2.2183	0.0959
C	-1.1653	-1.5950	0.7063
C	-0.7472	-1.0942	2.0743
H	-2.2404	-1.4642	0.5013
H	-0.8434	-2.6201	0.4754
H	-0.0818	-0.1550	2.0146
H	-0.0575	-1.8021	2.5602
C	-1.8906	-0.6867	3.0050
H	-1.5138	-0.2589	3.9444
H	-2.5477	0.0536	2.5259
H	-2.4956	-1.5735	3.2422
C	-0.5783	0.0549	-2.4409
C	-0.6711	-1.2526	-2.1103
H	0.3852	0.5048	-2.7014
H	-1.4682	0.6716	-2.5855
H	0.2184	-1.8905	-2.0876
H	-1.6349	-1.7487	-1.9930

Structure **1c-N**

E_{total} = -6.84326440 a.u.

Atom	X	Y	Z
Ni	0.0409	0.0926	0.2498
N	1.8721	0.1880	0.9136
C	2.6885	1.2016	0.8277
C	2.3603	2.4658	0.2649
C	1.0641	2.7450	-0.2816
C	0.8519	4.0524	-0.8009
C	1.8452	5.0077	-0.7853
C	3.1194	4.7266	-0.2521
C	3.3582	3.4713	0.2612
O	0.0698	1.9014	-0.3403
C	-1.7286	0.0333	-0.5911
C	-1.5436	0.0096	-2.0979
H	-0.9439	0.8815	-2.4052
H	-0.9798	-0.8902	-2.4031
C	-2.8864	0.0230	-2.8463
H	-2.3242	-0.8278	-0.2440
H	-2.1937	0.9722	-0.2473
H	-3.4655	0.9240	-2.5910
H	-2.7295	0.0128	-3.9364
H	-3.4957	-0.8554	-2.5804
H	2.3111	-0.6262	1.3605
H	3.7112	1.0990	1.2139
H	-0.1352	4.2673	-1.2121
H	1.6393	5.9986	-1.1935
H	3.8974	5.4887	-0.2457
H	4.3361	3.2280	0.6832
C	0.0204	-1.9313	0.3848
C	-0.4773	-1.3564	1.5549
H	1.0529	-2.2885	0.3258
H	-0.6559	-2.3428	-0.3679
H	0.1572	-1.2351	2.4378
H	-1.5520	-1.2995	1.7405

Structure **1d-O**

E_{total} = -6.80822886 a.u.

Atom	X	Y	Z
Ni	0.0023	-0.0019	-0.0056
N	1.9139	0.0024	-0.0099
C	2.6989	1.0477	-0.0050
C	2.2499	2.3957	0.0072
C	0.8552	2.7270	0.0369
C	0.5194	4.1109	0.0505
C	1.4883	5.0901	0.0259
C	2.8592	4.7594	-0.0080
C	3.2185	3.4301	-0.0148
O	-0.1299	1.8711	0.0472
C	-1.9303	-0.0283	-0.0019
C	-1.6922	-1.4289	-0.1630
H	-2.2345	0.5625	-0.8717
H	-2.2735	0.3501	0.9674
H	-1.8728	-1.8323	-1.1649
H	-2.0663	-2.0823	0.6337
C	0.0926	-2.2048	0.0691
C	0.5189	-2.4731	1.5066
H	1.1125	-1.6353	1.9048
H	-0.3794	-2.5376	2.1457
C	1.3129	-3.7793	1.6321
H	-0.3842	-3.1067	-0.3375
H	0.9231	-2.0165	-0.6309
H	2.2285	-3.7514	1.0206
H	1.6097	-3.9600	2.6763
H	0.7143	-4.6405	1.2951
H	4.2730	3.1468	-0.0415
H	3.6168	5.5414	-0.0303
H	1.1867	6.1391	0.0304
H	3.7860	0.8963	-0.0118
H	2.4435	-0.8796	-0.0127
H	-0.5417	4.3627	0.0752

Structure **1d-N**

E = -6.81886317 a.u.

Atom	X	Y	Z
Ni	-0.0277	0.0067	-0.0146
N	1.8301	0.0022	-0.0110
C	2.6397	1.0332	0.0022
C	2.2518	2.3982	0.0165
C	0.8686	2.7827	0.0038

C	0.5836	4.1771	0.0171
C	1.5902	5.1180	0.0455
C	2.9481	4.7354	0.0596
C	3.2597	3.3938	0.0448
O	-0.1189	1.9392	-0.0202
C	-0.0288	-1.9273	0.0212
C	-1.4213	-1.6340	0.1312
C	-2.1865	0.2448	-0.1776
C	-2.3743	0.6125	-1.6389
H	-1.5050	1.1847	-1.9975
H	-2.4425	-0.3010	-2.2565
C	-3.6455	1.4493	-1.8414
H	-3.0894	-0.2373	0.2180
H	-1.9774	1.1153	0.4625
H	-3.5937	2.3824	-1.2603
H	-3.7741	1.7150	-2.9018
H	-4.5419	0.8966	-1.5173
H	3.7187	0.8333	0.0037
H	2.3323	-0.8899	-0.0180
H	-0.4664	4.4720	0.0064
H	1.3297	6.1779	0.0577
H	3.7340	5.4891	0.0836
H	4.3038	3.0730	0.0557
H	0.5053	-2.2527	0.9219
H	0.3523	-2.3274	-0.9262
H	-1.8742	-1.7584	1.1193
H	-2.0646	-1.9649	-0.6898

Structure **1e-O**

E_{total} = -6.85186850 a.u.

Atom	X	Y	Z
Ni	0.1046	-0.0302	-0.0384
N	1.9950	-0.0226	0.0161
C	2.7306	1.0605	0.0456
C	2.2316	2.3922	0.0335
C	0.8287	2.6925	-0.0106
C	0.4573	4.0660	-0.0172
C	1.3993	5.0702	0.0157
C	2.7775	4.7735	0.0594
C	3.1710	3.4544	0.0679
O	-0.1369	1.8129	-0.0423
C	-1.7894	-0.4100	-0.0805
C	-1.1766	-1.7377	-0.0801
H	-2.2431	-0.0554	-1.0144
H	-2.2767	-0.0524	0.8330
H	0.0496	-1.6317	-0.0302
H	-1.3222	-2.2932	0.8620
C	-1.3862	-2.6288	-1.3087
C	-2.8027	-3.2078	-1.3460
H	-2.9875	-3.7736	-0.4153
H	-3.5281	-2.3765	-1.3530
C	-3.0388	-4.1142	-2.5526
H	-0.6527	-3.4540	-1.3092
H	-1.1998	-2.0321	-2.2179
H	-2.3473	-4.9713	-2.5477
H	-4.0652	-4.5098	-2.5564
H	-2.8861	-3.5652	-3.4951
H	4.2325	3.1998	0.1019
H	3.5154	5.5740	0.0867
H	1.0707	6.1108	0.0093
H	3.8225	0.9555	0.0823
H	2.5617	-0.8754	0.0308
H	-0.6100	4.2884	-0.0502

Structure **1e-N**

E = -6.85790100 a.u.

Atom	X	Y	Z
Ni	-0.0178	0.0371	-0.0542
N	1.8033	0.0095	-0.0252
C	2.5733	1.0724	0.0042
C	2.1347	2.4225	0.0188
C	0.7400	2.7734	0.0372
C	0.4143	4.1587	0.0389
C	1.3915	5.1282	0.0157
C	2.7600	4.7820	-0.0019
C	3.1113	3.4509	0.0026
O	-0.2277	1.9063	0.0468
C	-0.3905	-1.8335	-0.1716
C	-1.7593	-1.2520	-0.1682
C	-2.6304	-1.4873	-1.4098
C	-3.1638	-2.9203	-1.4693
H	-2.3139	-3.6242	-1.4572
H	-3.7500	-3.1251	-0.5555
C	-4.0318	-3.1775	-2.7000
H	-3.4789	-0.7812	-1.4121
H	-2.0328	-1.2695	-2.3119
H	-4.9036	-2.5048	-2.7185
H	-4.4054	-4.2122	-2.7137
H	-3.4620	-3.0126	-3.6279
H	3.6584	0.9124	0.0110
H	2.3182	-0.8749	-0.0378
H	-0.6452	4.4183	0.0492
H	1.1012	6.1802	0.0081
H	3.5240	5.5577	-0.0217
H	4.1645	3.1628	-0.0129
H	-0.0679	-2.2953	-1.1160
H	-0.0915	-2.4062	0.7163
H	-1.7006	-0.0707	-0.0889
H	-2.3147	-1.4718	0.7595

Structure **1h**

E_{total} = -6.80710717 a.u.

Atom	X	Y	Z
Ni	-0.0005	-0.0011	-0.0009
N	1.9386	-0.0001	-0.0013
C	2.7184	1.0429	-0.0011
C	2.3104	2.4069	-0.0254
C	0.9237	2.8116	-0.0642
C	0.6797	4.2186	-0.1415
C	1.7031	5.1397	-0.1533
C	3.0543	4.7349	-0.1011
C	3.3343	3.3881	-0.0424
O	-0.0879	2.0118	-0.0283
C	0.0557	-0.2504	2.1501
C	-1.2860	-0.1777	1.8358
H	-1.4536	-0.0110	-0.0091
H	-1.8327	-1.1220	1.7404
C	-2.1147	1.0504	2.1030
H	0.5474	-1.2163	2.2753
H	0.5898	0.6354	2.5032
H	-1.5359	1.9590	1.8910
H	-3.0273	1.0687	1.4920
H	-2.4152	1.0535	3.1642
H	4.3724	3.0479	-0.0108
H	3.8557	5.4722	-0.1141
H	1.4629	6.2033	-0.2071
H	3.8049	0.8756	0.0050
C	-0.1412	-1.7800	-0.9599
C	-0.2067	-0.7293	-1.8917
H	-1.0470	-2.3255	-0.6815
H	0.7919	-2.3340	-0.8142
H	-1.1620	-0.4395	-2.3326
H	0.6836	-0.4168	-2.4423
H	2.4534	-0.8865	0.0122
H	-0.3641	4.5332	-0.1872

Structure **1i**

E_{total} = -6.80782280 a.u.

Ni	-0.0325	0.0078	-0.0629
N	1.9260	0.0014	-0.0181
C	2.7116	1.0393	-0.0011
C	2.3039	2.4038	-0.0131
C	0.9183	2.8049	-0.0746
C	0.6713	4.2121	-0.1345
C	1.6917	5.1362	-0.1140
C	3.0428	4.7343	-0.0429
C	3.3255	3.3876	0.0019
O	-0.0960	2.0049	-0.0745
C	0.0954	-0.2272	2.1721
C	-1.2450	-0.1411	1.9313
H	-1.4687	0.0326	-0.2149
H	-1.8056	-1.0726	1.8035
C	-2.0498	1.1059	2.1488
H	0.5917	-1.1958	2.2481
H	0.6686	0.6552	2.4677
H	-1.4397	2.0009	1.9725
H	-2.9252	1.1468	1.4870
H	-2.4146	1.1192	3.1905
H	4.3639	3.0499	0.0477
H	3.8421	5.4739	-0.0311
H	1.4493	6.1998	-0.1574
H	3.7979	0.8712	0.0129
C	-0.1451	-1.8170	-0.9078
C	-0.1452	-0.8181	-1.9016
H	-1.0723	-2.3380	-0.6555
H	0.7713	-2.3733	-0.6830
H	-1.0694	-0.5516	-2.4170
H	0.7777	-0.5489	-2.4215
H	2.4391	-0.8868	-0.0170
H	-0.3724	4.5242	-0.1967

Structure **2a**

E_{total} = -8.88910252 a.u.

Atom	X	Y	Z
Ni	-0.0619	0.0728	-0.1326
N	1.7010	0.3179	-0.7171
C	2.4174	1.4134	-0.6548
C	1.9850	2.6600	-0.1297
C	0.6613	2.8457	0.3805
C	0.3425	4.1445	0.8759
C	1.2573	5.1682	0.8787
C	2.5652	4.9726	0.3810
C	2.9164	3.7379	-0.1169
O	-0.2547	1.9201	0.4227
C	0.0543	-1.7989	-0.7022
C	-0.2646	-1.9490	-2.1877
C	-0.1123	-3.3912	-2.6915
H	1.0970	-2.1127	-0.4970
H	-0.5870	-2.4718	-0.1085
H	-1.2954	-1.6071	-2.3895
H	0.3870	-1.2857	-2.7834
H	-0.7865	-4.0710	-2.1460
H	-0.3443	-3.4703	-3.7657
H	0.9168	-3.7535	-2.5377
H	3.9144	3.5502	-0.5098
O	3.3890	6.0749	0.4491
H	0.9952	6.1539	1.2671
H	3.4475	1.3798	-1.0314
H	-0.6647	4.3007	1.2636
P	-2.1067	-0.1406	0.5903
C	-3.2520	1.0646	-0.2318
C	-3.0612	-1.7258	0.5095
C	-2.2595	0.3326	2.3773
H	-3.3138	0.3899	2.6866
H	-1.7317	-0.4063	2.9957
H	-1.7708	1.3084	2.4998
H	-4.2320	1.0884	0.2676
H	-2.7740	2.0520	-0.1848
H	-3.3806	0.7841	-1.2862
H	-4.0857	-1.5690	0.8785
H	-3.0995	-2.0849	-0.5280
H	-2.5684	-2.4889	1.1269
H	2.2128	-0.4732	-1.1239
C	4.7172	5.8950	-0.0373
H	5.2458	5.1166	0.5363
H	5.2208	6.8580	0.0995
H	4.7145	5.6278	-1.1064

Structure **2b-O**

E_{total} = -6.48282698 a.u.

Atom	X	Y	Z
Ni	-0.0034	0.0019	-0.0042
N	1.8156	-0.0020	0.0001
C	2.5659	1.0784	0.0170
C	2.1017	2.4165	0.0201
C	0.7079	2.7384	-0.0249
C	0.3583	4.1200	-0.0015
C	1.3074	5.1063	0.0738
C	2.6844	4.7846	0.1201
C	3.0702	3.4643	0.0888
O	-0.2515	1.8607	-0.0704
C	-0.3713	-1.8694	0.0942
C	-1.7360	-1.2793	0.1570
H	-1.6819	-0.1072	-0.0082
H	-2.3540	-1.5381	-0.7192
C	-2.5026	-1.4399	1.4702
H	-0.1148	-2.4203	-0.8207
H	-0.0187	-2.3595	1.0123
H	-1.8689	-1.1544	2.3223
H	-3.4089	-0.8174	1.4924
H	-2.8010	-2.4914	1.5964
H	4.1214	3.1836	0.1235
O	3.5284	5.8693	0.1989
H	1.0229	6.1594	0.1047
H	3.6534	0.9388	0.0339
H	2.3477	-0.8756	0.0063
H	-0.7039	4.3653	-0.0308
C	4.9225	5.5775	0.2581
H	5.1617	4.9730	1.1478
H	5.4292	6.5460	0.3248
H	5.2536	5.0480	-0.6496

Structure **2b-N**

E_{total} = -6.47673828 a.u.

Atom	X	Y	Z
Ni	-0.0014	-0.0092	0.0016
O	1.8510	0.0173	0.0144
C	2.5748	1.1084	0.0119
C	2.0811	2.4506	-0.0054
C	0.6940	2.7508	-0.0187
C	2.9942	3.5462	-0.0121
C	4.3538	3.3379	-0.0014
C	4.8483	2.0135	0.0193
C	3.9904	0.9426	0.0255
C	-0.1221	-1.9383	0.0305
C	-1.5187	-1.5049	0.0719
N	-0.2705	1.8616	-0.0165

H	-1.5778	-0.2792	-0.0303
H	-2.0837	-1.7454	-0.8439
C	-2.3187	-1.7853	1.3425
H	0.2659	-2.3668	-0.9002
H	0.3112	-2.3561	0.9469
H	-1.7363	-1.5079	2.2324
H	-3.2692	-1.2325	1.3616
H	-2.5441	-2.8610	1.3980
H	2.5762	4.5512	-0.0265
O	5.3160	4.3226	-0.0092
H	5.9291	1.8653	0.0296
H	0.4286	3.8155	-0.0314
H	-1.1974	2.2960	-0.0284
H	4.3688	-0.0800	0.0398
C	4.8363	5.6650	-0.0392
H	5.7265	6.3025	-0.0462
H	4.2408	5.8508	-0.9476
H	4.2291	5.8877	0.8529

Structure **2c-O**

E_{total} = -7.66675035 a.u.

Atom	X	Y	Z
Ni	-0.0237	-0.0045	-0.0460
N	1.8467	-0.0041	-0.1838
C	2.6458	1.0359	-0.1668
C	2.2543	2.3917	-0.0641
C	0.8750	2.7706	-0.0076
C	0.5993	4.1675	0.0932
C	1.6033	5.1002	0.1624
C	2.9643	4.7132	0.1266
C	3.2781	3.3806	0.0031
O	-0.1181	1.9359	-0.0369
C	0.0426	-1.9399	0.2277
C	0.3813	-2.2141	1.6888
H	1.3727	-1.7976	1.9368
H	-0.3363	-1.6922	2.3461
C	0.3602	-3.7112	2.0333
H	-0.9261	-2.3962	-0.0379
H	0.8048	-2.3611	-0.4545
H	1.0834	-4.2696	1.4184
H	0.6119	-3.8766	3.0927
H	-0.6373	-4.1406	1.8499
H	4.3126	3.0436	-0.0311
O	3.8698	5.7431	0.2270
H	1.3754	6.1633	0.2526
H	3.7254	0.8489	-0.2304
C	-2.0326	0.0156	0.4239
C	-1.8528	-0.0737	-0.9485
H	-2.1845	0.9892	0.8957
H	-2.2847	-0.8660	1.0176
H	-1.8587	0.8304	-1.5632
H	-1.9529	-1.0251	-1.4754
H	2.3492	-0.8955	-0.2484
H	-0.4479	4.4695	0.1264
C	5.2458	5.3647	0.2605
H	5.8114	6.2955	0.3711
H	5.4500	4.7017	1.1167
H	5.5410	4.8627	-0.6747

Structure **2c-N**

E_{total} = -7.66215984 a.u.

Atom	X	Y	Z
Ni	0.0045	-0.0020	-0.0098
N	1.9464	-0.0328	-0.0183
C	2.7506	0.9965	-0.0194
C	2.3297	2.3522	0.0238
C	0.9488	2.7147	0.0516
C	0.6512	4.1063	0.1166
C	1.6380	5.0595	0.1561
C	3.0029	4.6921	0.1241
C	3.3366	3.3581	0.0568
O	-0.0621	1.8865	0.0301
C	-1.9545	0.1285	-0.1503
C	-2.3200	0.6149	-1.5416
H	-1.7972	1.5631	-1.7442
H	-1.9802	-0.1088	-2.3042
C	-3.8344	0.8238	-1.7051
H	-2.4492	-0.8295	0.0835
H	-2.2034	0.8738	0.6235
H	-4.2059	1.5666	-0.9820
H	-4.0759	1.1811	-2.7187
H	-4.3842	-0.1155	-1.5346
H	3.8346	0.8265	-0.0512
H	2.4561	-0.9239	-0.0458
H	-0.4017	4.3884	0.1419
H	1.3904	6.1207	0.2112
O	3.8946	5.7377	0.1670
H	4.3758	3.0349	0.0343
C	-0.1104	-1.9596	-0.5285
C	-0.1436	-1.8168	0.8596
H	0.8134	-2.2366	-1.0451
H	-1.0283	-2.1338	-1.0948
H	0.7571	-1.9627	1.4630
H	-1.0865	-1.8690	1.4082
C	5.2766	5.3829	0.1507
H	5.5339	4.7618	1.0237
H	5.8297	6.3267	0.1947
H	5.5349	4.8453	-0.7757

Structure **2d-O**

E_{total} = -7.62686167 a.u.

Atom	X	Y	Z
Ni	0.0228	-0.0023	-0.0522
N	1.9274	0.0188	0.0647
C	2.7013	1.0734	0.1295
C	2.2390	2.4147	0.1288
C	0.8465	2.7266	0.0659
C	0.4978	4.1082	0.0881
C	1.4478	5.0967	0.1604
C	2.8242	4.7787	0.2169
C	3.2075	3.4574	0.2023
O	-0.1351	1.8650	-0.0088
C	-1.9056	-0.0554	-0.1733
C	-1.6454	-1.4564	-0.3051
H	-2.1557	0.5238	-1.0679
H	-2.3213	0.3258	0.7658
H	-1.7451	-1.8705	-1.3141
H	-2.0758	-2.1058	0.4660
C	0.1217	-2.2103	0.0830
C	0.4308	-2.4327	1.5579
H	0.9766	-1.5730	1.9779
H	-0.5172	-2.4942	2.1211
C	1.2308	-3.7204	1.7893
H	-0.3083	-3.1289	-0.3391
H	1.0040	-2.0249	-0.5506
H	2.1964	-3.6923	1.2606
H	1.4368	-3.8680	2.8603
H	0.6776	-4.6010	1.4258
H	4.2568	3.1707	0.2472
O	3.6751	5.8598	0.2848
H	1.1611	6.1492	0.1747
H	3.7875	0.9301	0.1939
H	2.4659	-0.8574	0.0917
H	-0.5638	4.3545	0.0437
C	5.0673	5.5550	0.3412
H	5.5851	6.5186	0.3877
H	5.3061	4.9633	1.2397
H	5.3884	5.0055	-0.5585

Structure **2d-N**

E_{total} = -7.63750869 a.u.

Atom	X	Y	Z
Ni	-0.02770	0.00670	-0.01460
N	1.83010	0.00220	-0.01100
C	2.63970	1.03320	0.00220
C	2.25180	2.39820	0.01650
C	0.86860	2.78270	0.00380
C	0.58360	4.17710	0.01710
C	1.59020	5.11800	0.04550
C	2.94810	4.73540	0.05960
C	3.25970	3.39380	0.04480
O	-0.11890	1.93920	-0.02020
C	-0.02880	-1.92730	0.02120
C	-1.42130	-1.63400	0.13120
C	-2.18650	0.24480	-0.17760
C	-2.37430	0.61250	-1.63890
H	-1.50500	1.18470	-1.99750
H	-2.44250	-0.30100	-2.25650
C	-3.64550	1.44930	-1.84140
H	-3.08940	-0.23730	0.21800
H	-1.97740	1.11530	0.46250
H	-3.59370	2.38240	-1.26030
H	-3.77410	1.71500	-2.90180
H	-4.54190	0.89660	-1.51730
H	3.71870	0.83330	0.00370
H	2.33230	-0.88990	-0.01800
H	-0.46640	4.47200	0.00640
H	1.32970	6.17790	0.05770
O	4.02106	5.76440	0.09237
H	4.30380	3.07300	0.05570
H	0.50530	-2.25270	0.92190
H	0.35230	-2.32740	-0.92620
H	-1.87420	-1.75840	1.11930
H	-2.06460	-1.96490	-0.68980
C	5.34911	5.09559	0.10137
H	5.45619	4.48622	-0.79941
H	6.13764	5.85181	0.12545
H	5.42950	4.45724	0.98469

Structure **2e**

E_{total} = -7.67040930 a.u.

Atom	X	Y	Z
Ni	-0.0030	-0.0295	0.1469
N	1.8855	-0.0211	0.0734
C	2.6231	1.0622	0.0187
C	2.1236	2.3905	0.0123
C	0.7246	2.6840	0.0602
C	0.3548	4.0598	0.0500
C	1.2889	5.0637	-0.0019
C	2.6706	4.7669	-0.0496
C	3.0741	3.4520	-0.0433
O	-0.2473	1.8083	0.1121
C	-1.8906	-0.4451	0.2122
C	-1.2444	-1.7574	0.2144
H	-2.3977	-0.1259	-0.7066
H	-2.3445	-0.0796	1.1398
H	-0.0207	-1.6239	0.2205
H	-1.3386	-2.2965	1.1726
C	-1.4681	-2.6808	-0.9873
C	-2.8541	-3.3278	-0.9533
H	-2.9685	-3.8884	-0.0083
H	-3.6204	-2.5342	-0.9385
C	-3.0944	-4.2629	-2.1367
H	-1.3485	-2.0937	-1.9140
H	-0.6970	-3.4710	-1.0066
H	-2.3570	-5.0808	-2.1522
H	-4.0966	-4.7141	-2.0896
H	-3.0132	-3.7202	-3.0915
H	4.1284	3.1837	-0.0791
O	3.5053	5.8609	-0.0991
H	0.9851	6.1115	-0.0073
H	3.7144	0.9540	-0.0252
H	2.4507	-0.8747	0.0688
H	-0.7109	4.2871	0.0871
C	4.9022	5.5784	-0.1455
H	5.4051	6.5505	-0.1784
H	5.2235	5.0258	0.7522
H	5.1581	4.9987	-1.0471

Structure **2h**

E_{total} = -7.62506762 a.u.

Atom	X	Y	Z
Ni	-0.0004	-0.0002	-0.0001
N	1.9398	-0.0004	-0.0004
C	2.7202	1.0453	-0.0019
C	2.3131	2.4068	-0.0265
C	0.9309	2.8058	-0.0287
C	0.6861	4.2147	-0.1078
C	1.7015	5.1354	-0.1572
C	3.0565	4.7294	-0.1405
C	3.3489	3.3872	-0.0775
O	-0.0849	2.0105	0.0435
C	0.0565	-0.3262	2.1410
C	-1.2843	-0.2291	1.8321
H	-1.4528	-0.0032	-0.0216
H	-1.8413	-1.1634	1.7031
C	-2.0998	0.9985	2.1391
H	0.5386	-1.3008	2.2311
H	0.6006	0.5418	2.5215
H	-1.5103	1.9071	1.9587
H	-3.0107	1.0481	1.5274
H	-2.4028	0.9695	3.1993
H	4.3793	3.0348	-0.0721
O	3.9774	5.7537	-0.1971
H	1.4862	6.2042	-0.2130
H	3.8060	0.8762	0.0006
C	-0.1409	-1.7361	-1.0353
C	-0.1989	-0.6448	-1.9202
H	-1.0498	-2.2911	-0.7872
H	0.7905	-2.2973	-0.9096
H	-1.1511	-0.3333	-2.3530
H	0.6951	-0.3096	-2.4510
H	2.4559	-0.8856	0.0145
H	-0.3569	4.5333	-0.1248
C	5.3479	5.3619	-0.2002
H	5.9270	6.2899	-0.2529
H	5.6066	4.8174	0.7225
H	5.5777	4.7329	-1.0757

Structure **2i**

E_{total} = -7.63061004 a.u.

Atom	X	Y	Z
Ni	-0.0087	0.0055	0.0057
N	1.9666	-0.0335	0.0494
C	2.7486	1.0094	0.0384
C	2.3379	2.3707	0.0772

C	0.9627	2.7718	0.2004
C	0.7250	4.1817	0.2853
C	1.7396	5.1023	0.2311
C	3.0873	4.6962	0.0904
C	3.3728	3.3529	0.0207
O	-0.0636	1.9859	0.2622
C	-0.2631	-1.5289	1.4356
C	-0.3785	-0.3156	2.0919
H	-1.4453	0.0413	-0.0704
H	-1.3811	0.1043	2.2224
C	0.6906	0.2999	2.9407
H	-1.1507	-2.0842	1.1294
H	0.6682	-2.1001	1.4968
H	1.6745	-0.1490	2.7477
H	0.7568	1.3850	2.7710
H	0.4443	0.1471	4.0069
H	4.3982	2.9998	-0.0785
O	4.0069	5.7215	0.0390
H	1.5291	6.1716	0.2938
H	3.8358	0.8482	0.0019
C	-0.1384	-1.2608	-1.6640
C	-0.0953	0.0637	-2.0760
H	-1.0847	-1.8043	-1.6354
H	0.7651	-1.8756	-1.6655
H	-1.0090	0.5919	-2.3529
H	0.8440	0.5287	-2.3832
H	2.4862	-0.9170	0.0246
H	-0.3132	4.4994	0.3907
C	5.3721	5.3322	-0.0854
H	5.9501	6.2623	-0.0982
H	5.6877	4.7132	0.7702
H	5.5434	4.7789	-1.0233

Structure **3a**

E_{total} = -8.63031447 a.u.

Atom	X	Y	Z
Ni	-0.0560	0.0476	-0.1358
N	1.6954	0.2312	-0.7938
C	2.4399	1.3019	-0.8125
C	2.0516	2.5885	-0.3277
C	0.7598	2.8279	0.2666
C	0.4866	4.1574	0.7150
C	1.3985	5.1733	0.5812
C	2.6518	4.9114	-0.0071
C	2.9717	3.6419	-0.4466
O	-0.1480	1.9213	0.4124
C	-0.0263	-1.8215	-0.7070
C	-0.3693	-1.9414	-2.1896
C	-0.2234	-3.3746	-2.7208
H	1.0069	-2.1722	-0.5147
H	-0.6852	-2.4721	-0.1089
H	-1.4035	-1.5979	-2.3690
H	0.2724	-1.2688	-2.7854
H	-0.8817	-4.0664	-2.1716
H	-0.4814	-3.4340	-3.7899
H	0.8106	-3.7347	-2.5992
H	3.9518	3.4745	-0.8929
N	3.6135	5.9845	-0.1608
O	4.7214	5.7136	-0.6570
O	3.2695	7.1194	0.2122
H	1.1805	6.1847	0.9202
H	3.4516	1.2316	-1.2308
H	-0.4870	4.3397	1.1706
P	-2.0768	-0.1009	0.6813
C	-3.2186	1.1333	-0.0992
C	-3.0762	-1.6578	0.6531
C	-2.1271	0.3830	2.4700
H	-3.1642	0.4680	2.8268
H	-1.5915	-0.3684	3.0661
H	-1.6111	1.3469	2.5708
H	-4.1762	1.1821	0.4399
H	-2.7189	2.1106	-0.0763
H	-3.3985	0.8533	-1.1462
H	-4.0767	-1.4689	1.0695
H	-3.1756	-2.0183	-0.3798
H	-2.5773	-2.4331	1.2499
H	2.1695	-0.5908	-1.1872

Structure **3b-O**

E_{total} = -6.22287902 a.u.

Atom	X	Y	Z
Ni	0.0079	0.0175	-0.0624
N	1.8330	0.0215	-0.0641
C	2.5860	1.0910	-0.0513
C	2.1190	2.4374	-0.0459
C	0.7166	2.7762	-0.0775
C	0.3775	4.1626	-0.0626
C	1.3348	5.1429	-0.0092
C	2.6979	4.7851	0.0242
C	3.0800	3.4610	0.0020
C	-0.3159	-1.8579	0.0645
C	-1.6909	-1.3000	0.1088
O	-0.2343	1.9020	-0.1154
H	-1.6592	-0.1263	-0.0880
H	-2.2958	-1.5879	-0.7671
C	-2.4609	-1.4444	1.4209
H	-0.0330	-2.4171	-0.8371
H	0.0539	-2.3081	0.9963
H	-1.8413	-1.1229	2.2702
H	-3.3824	-0.8450	1.4202
H	-2.7334	-2.4995	1.5709
H	2.3633	-0.8550	-0.0570
H	3.6738	0.9539	-0.0379
H	-0.6830	4.4134	-0.0891
H	1.0710	6.1992	0.0099
H	4.1433	3.2229	0.0307
N	3.7153	5.8172	0.0927
O	4.9058	5.4613	0.1151
O	3.3322	6.9982	0.1283

Structure **3b-N**

E_{total} = -6.21668656 a.u.

Atom	X	Y	Z
Ni	0.0210	0.0228	-0.0167
O	1.8829	0.0317	-0.0416
C	2.6251	1.0963	-0.0313
C	2.1378	2.4517	-0.0374
C	0.7476	2.7759	-0.0606
C	3.0529	3.5177	-0.0208
C	4.4111	3.2814	0.0021
C	4.9124	1.9643	0.0035
C	4.0391	0.9076	-0.0141
C	-0.1192	-1.9039	0.0609
C	-1.5092	-1.4587	0.1307
N	-0.2213	1.9015	-0.0609
H	-1.5558	-0.2325	-0.0080
H	-2.1008	-1.7135	-0.7642
C	-2.2754	-1.6935	1.4307
H	0.2420	-2.3538	-0.8704
H	0.3393	-2.3006	0.9746
H	-1.6664	-1.4020	2.2979
H	-3.2186	-1.1295	1.4606
H	-2.5121	-2.7644	1.5198
H	2.6999	4.5486	-0.0228
N	5.3297	4.4033	0.0295
H	5.9906	1.8129	0.0200
H	0.5026	3.8450	-0.0775
H	-1.1438	2.3474	-0.0792
H	4.3989	-0.1216	-0.0124
O	6.5448	4.1475	0.0528
O	4.8498	5.5497	0.0305

Structure **3c-O**

E_{total} = -7.40568259 a.u.

Atom	X	Y	Z
Ni	0.0235	0.0238	0.0090
N	1.9098	0.0288	0.0500
C	2.7010	1.0666	0.0503
C	2.2912	2.4294	0.0104
C	0.9026	2.8143	-0.0111
C	0.6130	4.2127	-0.0627
C	1.6056	5.1554	-0.1201
C	2.9557	4.7494	-0.1132
C	3.2913	3.4150	-0.0409
O	-0.0736	1.9755	0.0068
C	0.0873	-1.9269	0.1059
C	0.4494	-2.3916	1.5099
H	1.4321	-1.9919	1.8144
H	-0.2756	-1.9906	2.2393
C	0.4724	-3.9232	1.6255
H	-0.8848	-2.3485	-0.1984
H	0.8370	-2.2479	-0.6416
H	1.1993	-4.3613	0.9237
H	0.7459	-4.2389	2.6442
H	-0.5162	-4.3477	1.3911
H	4.3453	3.1377	-0.0409
N	4.0075	5.7451	-0.2091
H	1.3804	6.2192	-0.1777
H	3.7841	0.8926	0.0694
C	-1.9850	0.0136	0.4681
C	-1.8150	0.0097	-0.9061
H	-2.1324	0.9566	1.0011
H	-2.2302	-0.9023	1.0105
H	-1.8233	0.9496	-1.4641
H	-1.9155	-0.9075	-1.4902
H	2.4179	-0.8625	0.0693
H	-0.4382	4.5017	-0.0713
O	5.1848	5.3496	-0.2029
O	3.6623	6.9345	-0.2979

Structure **3c-N**

E_{total} = -7.40020586 a.u.

Atom	X	Y	Z
Ni	0.0076	0.0095	-0.0152
N	1.9595	-0.0041	-0.0210
C	2.7570	1.0233	-0.0143
C	2.3214	2.3833	-0.0330
C	0.9331	2.7433	-0.1441
C	0.6209	4.1344	-0.1856
C	1.5905	5.0991	-0.0822
C	2.9399	4.7194	0.0480
C	3.2982	3.3875	0.0606
O	-0.0544	1.9064	-0.2038
C	-1.9559	0.1076	-0.0772
C	-2.4267	0.4689	-1.4739
H	-1.9582	1.4140	-1.7896
H	-2.1169	-0.3047	-2.1990
C	-3.9571	0.6102	-1.5357
H	-2.4194	-0.8312	0.2687
H	-2.1663	0.9110	0.6497
H	-4.3067	1.3920	-0.8438
H	-4.2872	0.8772	-2.5517
H	-4.4525	-0.3324	-1.2535
H	3.8428	0.8651	0.0079
H	2.4739	-0.8939	-0.0065
H	-0.4322	4.4011	-0.2786
H	1.3418	6.1592	-0.0938
N	3.9667	5.7394	0.1728
H	4.3523	3.1277	0.1535
C	-0.1172	-1.9789	-0.4013
C	-0.0961	-1.7553	0.9742
H	0.7882	-2.2729	-0.9407
H	-1.0555	-2.1912	-0.9191
H	0.8283	-1.8577	1.5497
H	-1.0159	-1.7796	1.5627
O	5.1463	5.3654	0.2847
O	3.5990	6.9254	0.1605

Structure **3d-O**

E_{total} = -7.36734306 a.u.

Atom	X	Y	Z
Ni	-0.0102	0.0062	-0.0061
N	1.9041	-0.0023	-0.0225
C	2.6962	1.0327	-0.0228
C	2.2483	2.3872	0.0064
C	0.8526	2.7294	0.0740
C	0.5208	4.1169	0.1269
C	1.4829	5.0935	0.0994
C	2.8429	4.7321	0.0203
C	3.2163	3.4037	-0.0241
O	-0.1271	1.8814	0.0921
C	-1.9437	0.0084	0.0118
C	-1.7324	-1.3927	-0.1711
H	-2.2418	0.6178	-0.8474
H	-2.2706	0.3793	0.9895
H	-1.9228	-1.7802	-1.1772
H	-2.1080	-2.0500	0.6211
C	0.0489	-2.1903	0.0483
C	0.4682	-2.4721	1.4855
H	1.0553	-1.6368	1.8992
H	-0.4348	-2.5477	2.1165
C	1.2659	-3.7765	1.6004
H	-0.4419	-3.0814	-0.3651
H	0.8818	-2.0126	-0.6520
H	2.1901	-3.7358	1.0031
H	1.5477	-3.9729	2.6457
H	0.6749	-4.6337	1.2414
H	4.2765	3.1577	-0.0791
N	3.8608	5.7646	-0.0106
H	1.2224	6.1501	0.1361
H	3.7822	0.8800	-0.0439
H	2.4269	-0.8891	-0.0359
H	-0.5380	4.3707	0.1858
O	5.0502	5.4090	-0.0801
O	3.4808	6.9473	0.0353

Structure **3c-N**

E_{total} = -7.37777956 a.u.

Atom	X	Y	Z
Ni	0.0101	0.0341	0.0161
N	1.8706	0.0263	-0.0102
C	2.6838	1.0483	-0.0368
C	2.2914	2.4169	-0.0277
C	0.9057	2.8071	-0.0087
C	0.6209	4.2054	0.0135
C	1.6183	5.1469	0.0276

C	2.9669	4.7378	0.0099
C	3.2961	3.3978	-0.0213
O	-0.0767	1.9703	-0.0062
C	0.0240	-1.9010	0.0831
C	-1.3685	-1.6196	0.1898
C	-2.1371	0.2601	-0.1686
C	-2.3014	0.5914	-1.6414
H	-1.4350	1.1681	-2.0003
H	-2.3435	-0.3371	-2.2380
C	-3.5815	1.4024	-1.8866
H	-3.0395	-0.2258	0.2226
H	-1.9516	1.1442	0.4603
H	-3.5571	2.3490	-1.3261
H	-3.6915	1.6418	-2.9550
H	-4.4745	0.8413	-1.5687
H	3.7622	0.8508	-0.0619
H	2.3697	-0.8684	-0.0178
H	-0.4288	4.4993	0.0274
H	1.3959	6.2126	0.0534
N	4.0224	5.7320	0.0307
H	4.3487	3.1160	-0.0335
H	0.5667	-2.2012	0.9873
H	0.4089	-2.3090	-0.8595
H	-1.8206	-1.7231	1.1804
H	-2.0093	-1.9636	-0.6270
O	5.1988	5.3325	-0.0155
O	3.6844	6.9263	0.0953

Structure **3e**

E_{total} = -7.41058074 a.u.

Atom	X	Y	Z
Ni	-0.0008	0.0389	-0.0193
N	1.8950	0.0287	-0.0519
C	2.6480	1.0951	-0.0620
C	2.1601	2.4367	-0.0471
C	0.7556	2.7557	-0.0462
C	0.3962	4.1365	-0.0289
C	1.3385	5.1318	-0.0060
C	2.7068	4.7949	-0.0053
C	3.1067	3.4751	-0.0282
O	-0.2111	1.8903	-0.0580
C	-1.8979	-0.3323	0.0123
C	-1.2887	-1.6599	0.0260
H	-2.3777	0.0041	-0.9150
H	-2.3514	0.0514	0.9329
H	-0.0593	-1.5536	0.0489
H	-1.4049	-2.1912	0.9860
C	-1.5193	-2.5809	-1.1758
C	-2.9221	-3.1923	-1.1515
H	-3.0584	-3.7473	-0.2061
H	-3.6686	-2.3798	-1.1455
C	-3.1762	-4.1243	-2.3343
H	-0.7680	-3.3896	-1.1834
H	-1.3766	-2.0007	-2.1036
H	-2.4598	-4.9606	-2.3420
H	-4.1895	-4.5498	-2.2920
H	-3.0756	-3.5866	-3.2900
H	4.1731	3.2506	-0.0274
N	3.7079	5.8443	0.0227
H	1.0568	6.1834	0.0135
H	3.7389	0.9792	-0.0800
H	2.4477	-0.8343	-0.0649
H	-0.6691	4.3687	-0.0283
O	4.9046	5.5091	0.0201
O	3.3058	7.0192	0.0487

Structure **3h-O**

E_{total} = -7.36754638 a.u.

Atom	X	Y	Z
Ni	0.0042	0.0020	0.0028
N	1.9423	-0.0003	0.0008
C	2.7314	1.0310	-0.0005
C	2.3290	2.4034	0.0043
C	0.9399	2.8205	0.0178
C	0.6960	4.2334	-0.0069
C	1.7119	5.1518	-0.0226
C	3.0532	4.7149	-0.0243
C	3.3504	3.3661	-0.0151
O	-0.0627	2.0249	0.0575
C	0.0269	-0.3297	2.1250
C	-1.3150	-0.2524	1.7935
H	-1.4513	-0.0039	0.0159
H	-1.8527	-1.1978	1.6612
C	-2.1600	0.9504	2.1234
H	0.5185	-1.2987	2.2257
H	0.5431	0.5408	2.5377
H	-1.5870	1.8769	1.9892
H	-3.0616	1.0026	1.4986
H	-2.4804	0.8774	3.1760
H	4.3980	3.0646	-0.0218
N	4.1257	5.6841	-0.0393
H	1.5124	6.2225	-0.0362
H	3.8160	0.8596	-0.0157
C	-0.1593	-1.7043	-1.0841
C	-0.2241	-0.5939	-1.9398
H	-1.0671	-2.2586	-0.8310
H	0.7708	-2.2721	-0.9810
H	-1.1814	-0.2635	-2.3464
H	0.6634	-0.2497	-2.4758
H	2.4516	-0.8908	-0.0062
H	-0.3476	4.5503	-0.0097
O	5.2962	5.2613	-0.0400
O	3.8133	6.8880	-0.0491

Structure **3h-N**

E_{total} = -7.36196347 a.u.

Atom	X	Y	Z
Ni	0.2143	-0.1788	-0.1767
N	2.0770	0.0555	-0.6138
C	2.7453	1.1695	-0.5733
C	2.2351	2.4410	-0.1552
C	0.9158	2.6082	0.4111
C	0.5756	3.9196	0.8715
C	1.4329	4.9828	0.7502
C	2.7040	4.7956	0.1714
C	3.0967	3.5436	-0.2606
O	0.0457	1.6689	0.5355
C	-0.4823	-1.4338	1.3682
C	-1.4943	-0.6341	0.7866
H	0.4615	-1.6094	-0.0590
H	-2.2641	-1.1187	0.1767
C	-0.5863	-2.9459	1.4035
H	0.0768	-0.9998	2.2052
H	-1.7531	0.3315	1.2263
H	0.3939	-3.4284	1.5175
H	-1.2060	-3.2349	2.2690
H	-1.0702	-3.3389	0.4977
H	-0.4133	4.0450	1.3138
H	1.1552	5.9795	1.0901
N	3.6108	5.9157	0.0388
O	3.2219	7.0229	0.4512
O	4.7233	5.7084	-0.4794
H	4.0938	3.4277	-0.6854
H	3.8016	1.1603	-0.8732
C	-0.4876	-0.7312	-2.2673
C	-0.6731	0.6080	-2.1076
H	-1.3063	-1.4388	-2.1231
H	0.4108	-1.1232	-2.7475
H	-1.6350	1.0163	-1.7934
H	0.0850	1.3284	-2.4213
H	2.6512	-0.7370	-0.9160

Structure **3i**

E_{total} = -7.35427115 a.u.

Atom	X	Y	Z
Ni	0.0132	0.0402	0.0097
N	1.9932	0.0296	0.0090
C	2.7678	1.0707	-0.0069
C	2.3387	2.4344	0.0732
C	0.9548	2.8216	0.2652
C	0.6907	4.2233	0.4049
C	1.6824	5.1655	0.3193
C	3.0152	4.7590	0.1170
C	3.3367	3.4212	-0.0011
O	-0.0402	2.0119	0.3362
C	-0.2145	-1.5624	1.3633
C	-0.2999	-0.3888	2.0917
H	-1.4226	0.0549	-0.0364
H	-1.2952	0.0320	2.2683
C	0.7954	0.1647	2.9483
H	-1.1151	-2.0925	1.0505
H	0.7117	-2.1454	1.3676
H	1.7671	-0.2953	2.7233
H	0.8825	1.2558	2.8362
H	0.5596	-0.0350	4.0088
H	4.3843	3.1454	-0.1322
N	4.0654	5.7452	-0.0111
H	1.4638	6.2307	0.4038
H	3.8549	0.9261	-0.0800
C	-0.1374	-1.1572	-1.7128
C	-0.1194	0.1809	-2.0743
H	-1.0757	-1.7139	-1.6832
H	0.7736	-1.7594	-1.7586
H	-1.0446	0.7090	-2.3109
H	0.8077	0.6668	-2.3866
H	2.5177	-0.8511	-0.0503
H	-0.3469	4.5115	0.5770
O	5.1648	5.5246	0.6368
N	3.8795	6.7168	-0.7533

Structure **4a**

E_{total} = -8.61199907 a.u.

Atom	X	Y	Z
Ni	0.0597	-0.0134	0.0486
N	1.9662	0.0019	0.0293
C	2.7163	1.0694	0.0049
C	2.2429	2.4154	-0.1029
C	0.8645	2.7615	0.1301
C	0.5208	4.1447	0.0783
C	1.4425	5.1135	-0.2233
C	2.7815	4.7454	-0.4702
C	3.1752	3.4229	-0.3855
O	-0.0577	1.9003	0.4017
C	-0.0349	-1.8018	-0.7619
C	-0.0480	-1.5958	-2.2751
C	-0.0478	-2.9240	-3.0459
H	0.8475	-2.4016	-0.4772
H	-0.9092	-2.3926	-0.4483
H	-0.9346	-1.0110	-2.5777
H	0.8274	-0.9985	-2.5819
H	-0.9387	-3.5229	-2.7978
H	-0.0415	-2.7547	-4.1344
H	0.8388	-3.5248	-2.7888
H	4.2215	3.1759	-0.5649
N	3.7547	5.7571	-0.8243
O	4.9328	5.3987	-1.0026
O	3.3515	6.9284	-0.9364
H	1.1690	6.1658	-0.2854
H	3.8055	0.9686	0.0945
H	-0.5182	4.4080	0.2768
P	-2.0849	0.0044	0.4174
C	-3.0046	1.1267	-0.7367
C	-3.1417	-1.5139	0.4270
C	-2.4345	0.7513	2.0766
H	-3.5121	0.9287	2.2079
H	-2.0722	0.0743	2.8622
H	-1.8811	1.6972	2.1408
H	-4.0473	1.2621	-0.4127
H	-2.4835	2.0934	-0.7513
H	-2.9872	0.7018	-1.7498
H	-4.1693	-1.2486	0.7169
H	-3.1571	-1.9688	-0.5725
H	-2.7377	-2.2437	1.1416
C	2.7193	-1.2140	0.2920
C	3.7546	-1.6452	-0.5697
C	4.4720	-2.8114	-0.2580
C	4.1706	-3.5478	0.8923
C	2.4049	-1.9701	1.4421
C	3.1389	-3.1291	1.7382
C	4.0683	-0.9303	-1.8782
H	5.2604	-3.1562	-0.9105
H	4.7309	-4.4415	1.1243
C	1.3206	-1.5135	2.4093
H	2.9209	-3.7022	2.6270
H	3.3548	-0.1208	-2.0179
C	5.4706	-0.3159	-1.9043
C	3.9261	-1.8409	-3.1006
H	5.6117	0.2361	-2.8338
H	5.5890	0.3669	-1.0633
H	6.2223	-1.1024	-1.8349
H	4.0732	-1.2584	-4.0103
H	4.6671	-2.6394	-3.0624
H	2.9279	-2.2774	-3.1145
H	0.7506	-0.7137	1.9424
C	0.3155	-2.6124	2.7658
C	1.8969	-0.9441	3.7066
H	-0.4833	-2.1921	3.3772
H	-0.1151	-3.0247	1.8536
H	0.8107	-3.4083	3.3219
H	1.0876	-0.5760	4.3376
H	2.4476	-1.7194	4.2397
H	2.5709	-0.1198	3.4723

Structure **4b-O**

E_{total} = -6.20508429 a.u.

Atom	X	Y	Z
Ni	0.0056	0.0239	-0.0904
N	1.8352	0.0345	-0.1798
C	2.5722	1.1172	-0.1808
C	2.0900	2.4566	-0.1258
C	0.6954	2.7750	0.0577
C	0.3411	4.1551	0.1304
C	1.2790	5.1498	0.0245
C	2.6367	4.8129	-0.1534
C	3.0328	3.4939	-0.2227
C	-0.3924	-1.8044	-0.5048
C	-1.7422	-1.2463	-0.2425
O	-0.2365	1.8866	0.1643
H	-1.6685	-0.0791	-0.0417

H	-2.3749	-1.2142	-1.1453
C	-2.4925	-1.7926	0.9717
H	-0.1439	-2.0352	-1.5492
H	-0.0479	-2.5716	0.2006
H	-1.8476	-1.7840	1.8619
H	-3.3945	-1.2044	1.1923
H	-2.7973	-2.8311	0.7747
H	4.0908	3.2708	-0.3577
N	3.6340	5.8620	-0.2579
O	4.8174	5.5254	-0.4357
O	3.2425	7.0371	-0.1611
H	1.0021	6.2016	0.0740
H	3.6629	1.0074	-0.2060
H	-0.7150	4.3884	0.2689
C	2.5939	-1.1999	-0.1373
C	3.4148	-1.5868	-1.2188
C	4.1577	-2.7750	-1.1323
C	4.0928	-3.5709	0.0164
C	2.5196	-2.0087	1.0157
C	3.2787	-3.1879	1.0876
C	3.4733	-0.7779	-2.5073
H	4.7850	-3.0865	-1.9543
H	4.6731	-4.4797	0.0771
C	1.6894	-1.5701	2.2155
H	3.2547	-3.8057	1.9724
H	2.7740	0.0526	-2.4326
C	4.8575	-0.1815	-2.7741
C	3.0492	-1.5873	-3.7352
H	4.8237	0.4374	-3.6709
H	5.1593	0.4345	-1.9270
H	5.5859	-0.9803	-2.9146
H	3.0328	-0.9404	-4.6126
H	3.7493	-2.4052	-3.9053
H	2.0509	-1.9947	-3.5735
H	0.8801	-0.9366	1.8557
C	1.0300	-2.7226	2.9796
C	2.5023	-0.7420	3.2126
H	0.3576	-2.3192	3.7370
H	0.4564	-3.3411	2.2893
H	1.7888	-3.3335	3.4684
H	1.8565	-0.4043	4.0233
H	3.3114	-1.3476	3.6216
H	2.9243	0.1266	2.7068

Structure **4b-N**

E_{total} = -6.19994462 a.u.

Atom	X	Y	Z
Ni	-0.0044	-0.0016	0.0418
N	1.8921	-0.0077	-0.1228
C	2.6274	1.0724	-0.1088
C	2.1259	2.4077	-0.0748
C	0.7237	2.7178	0.0140
C	0.3540	4.0955	0.0291
C	1.2888	5.0968	-0.0204
C	2.6577	4.7686	-0.0851
C	3.0658	3.4517	-0.1123
O	-0.2318	1.8442	0.0934
C	-1.8889	-0.3629	0.2615
C	-1.3196	-1.6924	0.0542
H	-0.0972	-1.6012	-0.0480
H	-1.3482	-2.3286	0.9532
C	-1.7006	-2.4525	-1.2139
H	-2.2076	-0.0797	1.2708
H	-2.4804	0.0756	-0.5509
H	-1.6279	-1.7990	-2.0944
H	-1.0578	-3.3296	-1.3750
H	-2.7410	-2.7991	-1.1246
H	4.1320	3.2331	-0.1672
N	3.6498	5.8252	-0.1201
O	4.8486	5.4999	-0.1447
O	3.2380	6.9972	-0.1224
H	1.0017	6.1469	-0.0060
H	3.7212	0.9857	-0.1061
H	-0.7111	4.3207	0.0882
C	2.6765	-1.2286	-0.1011
C	3.5656	-1.5444	-1.1540
C	4.3256	-2.7231	-1.0884
C	4.2103	-3.5837	0.0078
C	2.5476	-2.1080	0.9944
C	3.3252	-3.2761	1.0458
C	3.6764	-0.6785	-2.4026
H	5.0040	-2.9792	-1.8887
H	4.8042	-4.4847	0.0527
C	1.6501	-1.7578	2.1731
H	3.2610	-3.9428	1.8924
H	2.9579	0.1355	-2.3329
C	5.0617	-0.0494	-2.5726
C	3.3337	-1.4412	-3.6848
H	5.0618	0.6077	-3.4425
H	5.3109	0.5333	-1.6859
H	5.8103	-0.8298	-2.7106
H	3.3501	-0.7571	-4.5335
H	4.0581	-2.2382	-3.8525
H	2.3368	-1.8732	-3.5942
H	0.8863	-1.0634	1.8295
C	0.9117	-2.9602	2.7689
C	2.4154	-1.0590	3.2983
H	0.1871	-2.6141	3.5062
H	0.3879	-3.4964	1.9776
H	1.6183	-3.6334	3.2542
H	1.7251	-0.7796	4.0945
H	3.1779	-1.7282	3.6975
H	2.8942	-0.1603	2.9086

Structure **4c-O**

E_{total} = -7.38692631 a.u.

Atom	X	Y	Z
Ni	0.0163	0.0346	0.0982
N	1.9426	0.0593	0.1761
C	2.6817	1.1376	0.1649
C	2.2236	2.4865	0.1520
C	0.8468	2.8271	-0.0953
C	0.5162	4.2164	-0.1447
C	1.4564	5.1905	0.0680
C	2.7968	4.8270	0.3137
C	3.1762	3.5017	0.3371
O	-0.0786	1.9537	-0.2853
C	-0.0735	-1.7645	0.8625
C	0.0587	-1.6041	2.3698
H	0.9729	-1.0398	2.6162
H	-0.7829	-1.0112	2.7673
C	0.0964	-2.9615	3.0892
H	-1.0297	-2.2443	0.5970
H	0.7290	-2.4043	0.4595
H	0.9476	-3.5662	2.7395
H	0.1953	-2.8270	4.1773
H	-0.8244	-3.5339	2.8969
H	4.2229	3.2584	0.5185
N	3.7899	5.8578	0.5469
O	4.9678	5.5035	0.7221
O	3.3978	7.0359	0.5604
H	-0.5249	4.4733	-0.3433
H	1.1968	6.2481	0.0508
H	3.7733	1.0316	0.1362
C	-2.0434	0.1412	0.2233
C	-1.6458	-0.2686	-1.0405
H	-2.2448	1.1965	0.4210
H	-2.4155	-0.5763	0.9575
H	-1.5274	0.4649	-1.8432
H	-1.6936	-1.3178	-1.3395
C	2.7440	-1.1492	0.0497
C	2.5754	-1.9619	-1.0922
C	3.3684	-3.1078	-1.2599
C	4.3208	-3.4553	-0.2974
C	3.7119	-1.5003	1.0211
C	4.4897	-2.6548	0.8366
C	1.5951	-1.5735	-2.1895
H	3.2616	-3.7238	-2.1402
H	4.9289	-4.3376	-0.4321
C	3.9070	-0.6954	2.3007
H	5.2283	-2.9372	1.5720
H	0.9247	-0.8118	-1.7986
C	2.2943	-0.9665	-3.4069
C	0.7124	-2.7316	-2.6636
H	1.5503	-0.6498	-4.1381
H	2.8796	-0.1014	-3.0946
H	2.9564	-1.7047	-3.8600
H	-0.0296	-2.3590	-3.3701
H	1.3203	-3.4923	-3.1530
H	0.1995	-3.1739	-1.8096
H	3.1322	0.0669	2.3578
C	3.7757	-1.5437	3.5692
C	5.2616	0.0168	2.3598
H	3.8189	-0.8984	4.4468
H	2.8224	-2.0702	3.5610
H	4.5858	-2.2710	3.6203
H	5.3176	0.6237	3.2637
H	6.0667	-0.7182	2.3694
H	5.3792	0.6626	1.4904

Strcuture **4b'**

E_{total} = -5.785458 a.u.

Atom	X	Y	Z
Zr	0.0003	-0.0058	-0.0156
N	2.0156	0.0042	0.0042
C	2.6940	1.3246	0.0211
C	1.8753	2.4349	0.6947
C	0.5945	2.9442	0.0187
N	-0.5060	1.9492	-0.0238
H	2.6953	-0.7652	-0.0201
H	2.9750	1.6262	-1.0049
H	3.6299	1.2214	0.5927
H	1.6353	2.1238	1.7285
H	2.5452	3.3064	0.7846
H	0.8194	3.3041	-1.0025
H	0.2469	3.8153	0.5969
H	-1.4206	2.4128	-0.0837
C	-1.3371	-1.7380	0.5759
C	-0.9540	-1.3602	1.9936
H	-2.4050	-1.5575	0.3711
H	-1.0799	-2.7734	0.3193
H	-0.3501	-0.3760	2.0631
H	-0.2332	-2.0784	2.4125
C	-2.1200	-1.1238	2.9564
H	-1.7692	-0.7821	3.9396
H	-2.8198	-0.3771	2.5554
H	-2.6685	-2.0673	3.0871
C	-0.4054	-0.1842	-2.6044
C	-0.8311	-1.4060	-2.2032
H	0.6433	-0.0107	-2.8643
H	-1.1138	0.6159	-2.8317
H	-0.1402	-2.2473	-2.1119
H	-1.8900	-1.6390	-2.0987

Structure **5b'**

E_{total} = -5.783931 a.u.

Atom	X	Y	Z
Zr	-0.0122	0.0215	0.0193
N	1.9937	-0.0193	-0.0007
C	2.7388	1.2673	-0.0375
C	2.2609	2.2137	-1.1403
C	0.8730	2.8261	-0.9542
N	-0.2144	1.8225	-0.8894
H	2.6007	-0.8234	-0.2028
H	3.8043	1.0483	-0.1979
H	2.6708	1.7674	0.9452
H	2.9774	3.0501	-1.1990
H	2.2975	1.6826	-2.1063
H	0.6785	3.5040	-1.7989
H	0.8622	3.4491	-0.0399
H	-1.0586	2.1564	-1.3722
C	-1.0925	-1.6840	-0.8925
C	-1.1372	-2.4323	0.4385
H	-2.0975	-1.4290	-1.2702
H	-0.5454	-2.2256	-1.6798
H	-0.5795	-1.8699	1.2614
H	-0.5558	-3.3661	0.3853
C	-2.5316	-2.6987	0.9999
H	-2.4877	-3.1691	1.9926
H	-3.1196	-1.7718	1.0812
H	-3.0765	-3.3746	0.3249
C	-0.7869	1.5077	2.1542
C	-0.4797	0.3036	2.6837
H	-0.0381	2.2959	2.0522
H	-1.8201	1.7869	1.9340
H	0.5338	0.0743	3.0230
H	-1.2612	-0.4214	2.9232

Structure **4c-N**

E_{total} = -7.38179670 a.u.

Atom	X	Y	Z
Ni	0.0891	-0.0502	-0.2851
N	2.0670	-0.0070	-0.1499
C	2.8015	1.0681	-0.0756
C	2.3082	2.4022	0.0411
C	0.9180	2.7281	-0.1312
C	0.5577	4.1079	-0.0600
C	1.4858	5.0877	0.1854
C	2.8403	4.7395	0.3536
C	3.2442	3.4236	0.2697
O	-0.0187	1.8673	-0.3603
C	-1.7849	0.0114	-0.8383
C	-1.7227	0.1630	-2.3461
H	-1.1376	1.0600	-2.6073
H	-1.2148	-0.7050	-2.8020
C	-3.1274	0.2813	-2.9662
H	-2.3524	-0.8833	-0.5370
H	-2.1871	0.9066	-0.3396
H	-3.6628	1.1502	-2.5547
H	-3.0604	0.4021	-4.0584
H	-3.7266	-0.6180	-2.7560
H	4.3017	3.1893	0.3914
N	3.8249	5.7751	0.6083
O	5.0086	5.4285	0.7562
O	3.4207	6.9478	0.6627
H	-0.4957	4.3519	-0.1971
H	1.2027	6.1370	0.2531
H	3.8961	0.9870	-0.1255
C	-0.0875	-2.0761	-0.0329
C	-0.3653	-1.3713	1.1411
H	0.8707	-2.5878	-0.1510
H	-0.8960	-2.4650	-0.6563
H	0.4061	-1.2504	1.9077
H	-1.3919	-1.1957	1.4700
C	2.8827	-1.1872	-0.3832

C	2.7954	-1.8478	-1.6261
C	3.6132	-2.9597	-1.8828
C	4.5005	-3.4248	-0.9063
C	3.7768	-1.6582	0.6031
C	4.5781	-2.7788	0.3322
C	1.8743	-1.3242	-2.7188
H	3.5755	-3.4608	-2.8382
H	5.1255	-4.2819	-1.1086
C	3.8525	-1.0195	1.9832
H	5.2610	-3.1539	1.0800
H	1.1080	-0.7092	-2.2513
C	2.6086	-0.4370	-3.7252
C	1.1381	-2.4241	-3.4894
H	1.8990	-0.0391	-4.4509
H	3.0846	0.3912	-3.1998
H	3.3704	-1.0193	-4.2441
H	0.4221	-1.9718	-4.1759
H	1.8470	-3.0233	-4.0605
H	0.6032	-3.0655	-2.7890
H	3.1089	-0.2272	2.0447
C	3.5264	-2.0031	3.1097
C	5.2150	-0.3850	2.2733
H	3.5147	-1.4764	4.0641
H	2.5450	-2.4440	2.9333
H	4.2756	-2.7941	3.1453
H	5.1900	0.1094	3.2446
H	5.9890	-1.1527	2.2796
H	5.4465	0.3517	1.5041

Structure **4d-O**

E_{total} = -7.34825953 a.u.

Atom	X	Y	Z
Ni	-0.0005	0.0029	0.0120
N	1.9586	0.0039	0.0283
C	2.6931	1.0850	0.0315
C	2.2157	2.4208	0.1857
C	0.8208	2.7495	0.1037
C	0.4635	4.1299	0.1981
C	1.4053	5.1070	0.3943
C	2.7680	4.7551	0.4834
C	3.1649	3.4387	0.3627
O	-0.1278	1.8886	-0.0747
C	-1.8979	0.0446	-0.3664
C	-1.7615	-1.3475	-0.1030
H	-1.9298	0.3978	-1.4031
H	-2.4006	0.6834	0.3661
H	-1.7601	-2.0237	-0.9637
H	-2.3322	-1.7306	0.7489
C	-0.1122	-2.0692	0.7451
C	0.1062	-1.8018	2.2263
H	0.8544	-1.0067	2.3694
H	-0.8282	-1.4354	2.6851
C	0.5563	-3.0788	2.9488
H	-0.6605	-3.0124	0.6240
H	0.8154	-2.2477	0.1900
H	1.4629	-3.4966	2.4843
H	0.7788	-2.8753	4.0068
H	-0.2268	-3.8519	2.9071
H	-0.5958	4.3754	0.1204
H	3.7766	1.0084	-0.1244
H	1.1294	6.1566	0.4843
N	3.7657	5.7818	0.7037
O	4.9599	5.4373	0.7425
O	3.3649	6.9496	0.8448
H	4.2274	3.2031	0.4216
C	2.7783	-1.1628	-0.2784
C	2.5091	-1.8965	-1.4542
C	3.3136	-2.9959	-1.7924
C	4.3739	-3.3774	-0.9647
C	3.8530	-1.5497	0.5581
C	4.6394	-2.6580	0.2047
C	1.3995	-1.4674	-2.4044
H	3.1317	-3.5501	-2.7008
H	4.9894	-4.2241	-1.2302
C	4.1618	-0.8335	1.8687
H	5.4599	-2.9668	0.8351
H	0.7165	-0.8155	-1.8645
C	1.9302	-0.6691	-3.5962
C	0.5576	-2.6313	-2.9352
H	1.0974	-0.3363	-4.2161
H	2.4773	0.2019	-3.2345
H	2.5984	-1.2925	-4.1908
H	-0.2855	-2.2407	-3.5056
H	1.1606	-3.2683	-3.5821
H	0.1797	-3.2199	-2.0992
H	3.3859	-0.0942	2.0579
C	4.1684	-1.7688	3.0806
C	5.5057	-0.0988	1.8470
H	5.6405	0.4466	2.7813
H	6.3184	-0.8158	1.7285
H	5.5294	0.6067	1.0173
H	4.3157	-1.1871	3.9908
H	3.2151	-2.2900	3.1437
H	4.9725	-2.4988	2.9884

Structure **4d-N**

E_{total}= -7.35956452 a.u.

Ni	-0.0215	0.0162	0.0225
N	1.8586	0.0118	-0.0087
C	2.6451	1.0557	-0.0512
C	2.2277	2.4169	-0.0401
C	0.8460	2.7842	-0.1967
C	0.5428	4.1782	-0.2374
C	1.5158	5.1346	-0.0981
C	2.8612	4.7453	0.0599
C	3.2112	3.4107	0.0741
O	-0.1118	1.9284	-0.3116
C	-0.0809	-1.7817	0.7753
C	-1.4600	-1.4526	0.6522
H	0.3992	-1.6983	1.7570
H	0.3166	-2.5682	0.1245
H	-1.9982	-1.1647	1.5602
H	-2.0461	-2.0728	-0.0316
C	-2.1245	0.1662	-0.4537
C	-2.0499	0.0139	-1.9626
H	-1.1420	0.5006	-2.3528
H	-1.9902	-1.0544	-2.2349
C	-3.2804	0.6358	-2.6393
H	-3.0832	-0.2119	-0.0786
H	-2.0255	1.2053	-0.1088
H	-3.3553	1.7079	-2.4040
H	-3.2174	0.5295	-3.7327
H	-4.2076	0.1470	-2.3011
H	-0.5035	4.4570	-0.3642
H	3.7281	0.8978	-0.1281
H	1.2762	6.1969	-0.1070
N	3.8924	5.7518	0.2107
O	5.0713	5.3668	0.3000
O	3.5333	6.9411	0.2433
H	4.2612	3.1430	0.1896
C	2.5905	-1.2333	-0.1581
C	2.3724	-2.0199	-1.3085
C	3.1070	-3.2015	-1.4952
C	4.0407	-3.6114	-0.5379
C	3.5308	-1.6500	0.8106
C	4.2472	-2.8410	0.6113
C	1.3980	-1.5639	-2.3855
H	2.9683	-3.8001	-2.3829
H	4.6014	-4.5225	-0.6855
C	3.7443	-0.8773	2.1054
H	4.9635	-3.1751	1.3472
H	0.7110	-0.8480	-1.9400
C	2.0993	-0.8513	-3.5428
C	0.5344	-2.6901	-2.9611
H	1.3577	-0.4907	-4.2560
H	2.6660	-0.0035	-3.1572
H	2.7792	-1.5409	-4.0437
H	-0.2034	-2.2700	-3.6450
H	1.1560	-3.4023	-3.5033
H	0.0161	-3.2038	-2.1515
H	3.0504	-0.0395	2.1335
C	3.4531	-1.7172	3.3516
C	5.1572	-0.3016	2.2316
H	5.2313	0.2918	3.1431
H	5.8866	-1.1109	2.2684
H	5.3712	0.3352	1.3734
H	3.5423	-1.0946	4.2420
H	2.4392	-2.1135	3.2934
H	4.1599	-2.5443	3.4198

Structure **4e-O**

E_{total} = -7.39389627 a.u.

Atom	X	Y	Z
Ni	-0.0578	0.0198	0.1337
N	1.8419	-0.0222	0.0540
C	2.5994	1.0419	0.0828
C	2.1261	2.3793	0.2295
C	0.7282	2.7164	0.2825
C	0.3899	4.0970	0.4052
C	1.3482	5.0750	0.4731
C	2.7107	4.7196	0.4154
C	3.0892	3.3999	0.2928
O	-0.2507	1.8682	0.2163
C	-1.9580	-0.3299	0.2202
C	-1.3720	-1.6689	0.2528
H	-2.4608	-0.0140	-0.7028
H	-2.3813	0.0844	1.1413
H	-1.4325	-2.1529	1.2419
H	-0.1498	-1.5836	0.1692
C	-1.7027	-2.6440	-0.8823
C	-3.1062	-3.2351	-0.7332
H	-3.8438	-2.4147	-0.7233
H	-3.1860	-3.7385	0.2467
C	-3.4419	-4.2255	-1.8469
H	-0.9645	-3.4642	-0.9009
H	-1.6237	-2.1125	-1.8456
H	-2.7354	-5.0702	-1.8539
H	-4.4547	-4.6355	-1.7204
H	-3.3954	-3.7409	-2.8347
H	-0.6716	4.3431	0.4431
H	3.6857	0.9399	-0.0331
H	1.0835	6.1268	0.5691
N	3.7289	5.7499	0.4789
O	4.9192	5.3989	0.4108
O	3.3460	6.9253	0.5976
H	4.1512	3.1603	0.2470
C	2.5918	-1.2412	-0.1849
C	2.3719	-1.9593	-1.3790
C	3.1161	-3.1225	-1.6373
C	4.0588	-3.5802	-0.7110
C	3.5417	-1.7061	0.7522
C	4.2676	-2.8763	0.4793
C	1.4027	-1.4316	-2.4292
H	2.9834	-3.6724	-2.5564
H	4.6263	-4.4760	-0.9155
C	3.7598	-1.0083	2.0884
H	4.9924	-3.2462	1.1893
H	0.5616	-0.9751	-1.9101
C	2.0300	-0.3560	-3.3195
C	0.8215	-2.5081	-3.3519
H	1.2855	0.0207	-4.0211
H	2.3883	0.4693	-2.7048
H	2.8680	-0.7798	-3.8735
H	0.0302	-2.0747	-3.9639
H	1.5996	-2.9016	-4.0061
H	0.4065	-3.3202	-2.7557
H	3.0545	-0.1842	2.1747
C	5.1657	-0.4196	2.2317
C	3.4963	-1.9245	3.2860
H	5.2427	0.1204	3.1756
H	5.9071	-1.2185	2.2121
H	5.3593	0.2696	1.4099
H	3.5883	-1.3543	4.2107
H	2.4871	-2.3310	3.2164
H	4.2151	-2.7439	3.2969

Structure **4e-N**

E_{total} = -7.39923394 a.u.

Atom	X	Y	Z
Ni	0.0357	-0.0452	-0.0468
N	1.8676	-0.0152	-0.1459
C	2.5944	1.0745	-0.1130
C	2.1022	2.4083	0.0018
C	0.6945	2.7228	-0.0195
C	0.3239	4.0994	0.0344
C	1.2600	5.0973	0.1162
C	2.6300	4.7658	0.1457
C	3.0420	3.4504	0.0869
O	-0.2378	1.8324	-0.0925
C	-0.3716	-1.9076	0.1597
C	-1.7159	-1.2878	0.0459
H	-0.0759	-2.2802	1.1495
H	-0.0802	-2.5786	-0.6582
H	-1.6236	-0.1055	0.0635
H	-2.3220	-1.4016	0.9625
C	-2.5291	-1.5764	-1.2203
C	-3.1478	-2.9746	-1.2154
H	-3.7853	-3.0854	-0.3199
H	-2.3475	-3.7288	-1.1237
C	-3.9769	-3.2453	-2.4696
H	-1.8735	-1.4579	-2.1000
H	-3.3313	-0.8251	-1.3223
H	-3.3586	-3.1635	-3.3772
H	-4.4144	-4.2541	-2.4483
H	-4.8021	-2.5218	-2.5613
H	-0.7423	4.3262	0.0121
H	3.6831	0.9806	-0.2044
H	0.9742	6.1472	0.1606
N	3.6215	5.8224	0.2283
O	4.8182	5.4932	0.2930
O	3.2129	6.9958	0.2282
H	4.1101	3.2359	0.1058
C	2.6228	-1.2277	-0.3903
C	2.4320	-1.9181	-1.6055
C	3.1824	-3.0745	-1.8728
C	4.1027	-3.5526	-0.9339
C	3.5510	-1.7106	0.5575
C	4.2834	-2.8749	0.2765
C	1.4840	-1.3709	-2.6657
H	3.0694	-3.6007	-2.8084
H	4.6757	-4.4435	-1.1447
C	3.7396	-1.0338	1.9082
H	4.9923	-3.2593	0.9948
H	0.7138	-0.7870	-2.1643
C	2.1903	-0.4353	-3.6488
C	0.7538	-2.4478	-3.4750
H	1.4653	-0.0252	-4.3521
H	2.6588	0.3828	-3.1014
H	2.9557	-0.9857	-4.1964
H	0.0071	-1.9778	-4.1154
H	1.4612	-2.9949	-4.0981

H	0.2545	-3.1420	-2.7993
H	3.0347	-0.2087	1.9889
C	5.1427	-0.4501	2.0910
C	3.4455	-1.9670	3.0853
H	5.1999	0.0756	3.0444
H	5.8832	-1.2499	2.0755
H	5.3546	0.2510	1.2838
H	3.5178	-1.4111	4.0203
H	2.4368	-2.3687	2.9860
H	4.1612	-2.7890	3.1001

Structure **4f**

E_{total} = -6.18513206 a.u.

Atom	X	Y	Z
Ni	-0.0343	0.0107	-0.0300
N	1.9062	-0.0079	0.0324
C	2.6603	1.0592	0.0479
C	2.1942	2.4040	0.1188
C	0.8013	2.7508	0.0124
C	0.4706	4.1400	0.0319
C	1.4280	5.1118	0.1643
C	2.7857	4.7450	0.2685
C	3.1599	3.4190	0.2369
O	-0.1685	1.9040	-0.1117
C	-0.2548	-1.9794	0.2096
C	-1.1537	-1.2922	1.0452
H	-1.4428	0.0809	-0.3348
H	-2.2180	-1.3196	0.7900
C	-0.8641	-1.0152	2.4935
H	-0.6229	-2.4461	-0.7087
H	0.6473	-2.4166	0.6484
H	0.2157	-0.9679	2.6924
H	-1.3246	-0.0733	2.8229
H	-1.2961	-1.8272	3.1071
H	-0.5856	4.3957	-0.0567
H	1.1670	6.1687	0.1879
N	3.8030	5.7730	0.3993
O	3.4222	6.9550	0.4229
O	4.9893	5.4111	0.4787
H	4.2184	3.1697	0.3103
H	3.7508	0.9512	-0.0224
C	2.6852	-1.2162	-0.1683
C	2.5692	-1.9172	-1.3863
C	3.3488	-3.0647	-1.6045
C	4.2233	-3.5243	-0.6139
C	3.5655	-1.6818	0.8324
C	4.3277	-2.8376	0.6004
C	1.6682	-1.3941	-2.4968
H	3.2934	-3.5987	-2.5409
H	4.8187	-4.4086	-0.7871
C	3.6654	-0.9958	2.1879
H	5.0002	-3.2085	1.3597
H	0.8687	-0.8129	-2.0400
C	2.4107	-0.4646	-3.4588
C	0.9901	-2.4922	-3.3220
H	1.7159	-0.0728	-4.2019
H	2.8437	0.3665	-2.9019
H	3.2073	-1.0139	-3.9612
H	0.2663	-2.0422	-4.0018
H	1.7321	-3.0379	-3.9047
H	0.4721	-3.1833	-2.6572
H	2.9444	-0.1812	2.2229
C	3.3170	-1.9281	3.3508
C	5.0462	-0.3890	2.4487
H	3.3213	-1.3660	4.2849
H	2.3242	-2.3499	3.1925
H	4.0458	-2.7362	3.4146
H	5.0401	0.1405	3.4016
H	5.7990	-1.1769	2.4789
H	5.2929	0.3130	1.6523

Structure **4g**

E_{total} = -6.18609085 a.u.

Atom	X	Y	Z
Ni	-0.0933	0.0304	-0.0892
N	1.8613	-0.0194	0.1298
C	2.6218	1.0421	0.1365
C	2.1648	2.3939	0.1416
C	0.7912	2.7529	-0.0907
C	0.4761	4.1451	-0.1290
C	1.4311	5.1101	0.0600
C	2.7709	4.7317	0.2805
C	3.1305	3.4013	0.3093
O	-0.1747	1.9133	-0.2864
C	-0.4300	-1.9522	0.1805
C	-1.0201	-1.2122	1.2139
H	-1.4706	0.0977	-0.5089
H	-2.0984	-1.0289	1.1713
C	-0.4013	-1.0479	2.5690
H	-1.0451	-2.3250	-0.6427
H	0.4946	-2.5037	0.3762
H	0.6860	-1.1939	2.5414
H	-0.6134	-0.0555	2.9924
H	-0.8374	-1.7964	3.2562
H	-0.5661	4.4091	-0.3102
H	1.1819	6.1699	0.0391
N	3.7884	5.7515	0.4666
O	3.4220	6.9376	0.4328
O	4.9598	5.3784	0.6471
H	4.1768	3.1431	0.4713
H	3.7136	0.9295	0.1076
C	2.6471	-1.2336	-0.0194
C	2.5380	-1.9781	-1.2131
C	3.3263	-3.1261	-1.3931
C	4.2091	-3.5423	-0.3916
C	3.5435	-1.6524	0.9903
C	4.3157	-2.8085	0.7943
C	1.6435	-1.4987	-2.3485
H	3.2737	-3.6915	-2.3112
H	4.8131	-4.4258	-0.5365
C	3.6623	-0.9133	2.3169
H	5.0011	-3.1425	1.5590
H	0.8613	-0.8707	-1.9263
C	2.4038	-0.6461	-3.3660
C	0.9345	-2.6275	-3.1031
H	1.7149	-0.2807	-4.1279
H	2.8601	0.2046	-2.8595
H	3.1837	-1.2435	-3.8388
H	0.2190	-2.2018	-3.8069
H	1.6599	-3.2265	-3.6535
H	0.4027	-3.2636	-2.3956
H	2.8978	-0.1394	2.3561
C	3.4257	-1.8192	3.5287
C	5.0187	-0.2268	2.4990
H	3.4156	-1.2183	4.4383
H	2.4662	-2.3257	3.4248
H	4.2182	-2.5641	3.6009
H	5.0238	0.3326	3.4347
H	5.8125	-0.9738	2.5214
H	5.1978	0.4603	1.6726

Structure **4h**

E_{total} = -7.33919874 a.u.

Atom	X	Y	Z
Ni	0.0096	0.0050	0.0189
N	1.9915	0.0053	0.0145
C	2.6916	1.1024	0.0096
C	2.1808	2.4378	0.0884
C	0.8412	2.7301	0.5501
C	0.5229	4.1092	0.7657
C	1.4157	5.1138	0.4960
C	2.7072	4.7984	0.0261
C	3.0852	3.4817	-0.1494
O	-0.0496	1.8421	0.8028
C	-0.1865	-1.8700	0.9361
C	-1.2359	-1.0816	1.4127
H	-1.4346	0.0719	0.1118
H	-2.2382	-1.3235	1.0368
C	-1.2143	-0.3922	2.7480
H	-0.3637	-2.6269	0.1701
H	0.6940	-2.0127	1.5613
H	-0.1875	-0.2096	3.0902
H	-1.7343	0.5742	2.7106
H	-1.7271	-1.0272	3.4910
H	-0.4785	4.3305	1.1360
H	1.1546	6.1614	0.6396
N	3.6585	5.8528	-0.2437
O	3.2887	7.0254	-0.0576
O	4.7913	5.5283	-0.6445
H	4.1036	3.2709	-0.4758
H	3.7885	1.0349	-0.0287
C	-0.4145	-0.6969	-1.9531
C	-0.2101	0.6669	-2.0031
H	-1.4267	-1.1080	-1.9537
H	0.3788	-1.4021	-2.2025
H	-1.0534	1.3595	-2.0150
H	0.7607	1.0850	-2.2777
C	2.8549	-1.1598	0.1225
C	3.3924	-1.7728	-1.0303
C	4.2597	-2.8688	-0.8952
C	4.6116	-3.3445	0.3717
C	3.2516	-1.6110	1.4013
C	4.1212	-2.7073	1.5156
C	3.1142	-1.2284	-2.4222
H	4.6831	-3.3417	-1.7687
H	5.2886	-4.1806	0.4667
C	2.8060	-0.8839	2.6642
H	4.4385	-3.0572	2.4864
H	2.2922	-0.5214	-2.3560
C	4.3074	-0.4653	-3.0008
C	2.7012	-2.3063	-3.4291
H	4.0397	-0.0458	-3.9708
H	4.5835	0.3447	-2.3256
H	5.1562	-1.1391	-3.1198
H	2.3974	-1.8352	-4.3642
H	3.5367	-2.9786	-3.6235
H	1.8649	-2.8799	-3.0295
H	1.9330	-0.2806	2.4219
C	2.3951	-1.8160	3.8092
C	3.8776	0.0690	3.1985
H	1.9790	-1.2267	4.6266
H	1.6406	-2.5205	3.4601
H	3.2610	-2.3679	4.1745
H	3.4920	0.6073	4.0646
H	4.7634	-0.4965	3.4886
H	4.1485	0.7870	2.4247

Structure **4i**

E = -7.34330559 a.u.

Atom	X	Y	Z
Ni	0.0297	0.0226	-0.0256
N	2.0836	0.0057	-0.0273
C	2.8017	1.0897	-0.0983
C	2.3364	2.4441	-0.1304
C	0.9428	2.8211	-0.2206
C	0.6599	4.2238	-0.3127
C	1.6474	5.1725	-0.3081
C	2.9981	4.7762	-0.2198
C	3.3282	3.4382	-0.1405
O	-0.0469	2.0064	-0.2307
C	-0.1929	-1.6241	-1.3036
C	-0.3377	-0.4464	-2.0247
H	-1.0728	-2.1990	-1.0085
H	0.7489	-2.1758	-1.2984
H	-1.3318	-0.0809	-2.2878
H	0.4821	-0.0019	-2.5869
C	-0.3372	-1.0770	1.7655
C	-0.5284	0.2566	2.0688
H	-1.3955	0.0443	-0.0874
H	-1.5547	0.6325	1.9951
C	0.3986	1.1672	2.8105
H	-1.1968	-1.7084	1.5371
H	0.5766	-1.6053	2.0333
H	1.4563	0.8978	2.7109
H	0.2743	2.2050	2.4710
H	0.1407	1.1439	3.8847
H	4.3827	3.1663	-0.0880
N	4.0450	5.7730	-0.2232
O	5.2246	5.3825	-0.1550
O	3.7022	6.9665	-0.2923
H	1.4180	6.2351	-0.3760
H	3.8972	1.0019	-0.1548
H	-0.3910	4.5061	-0.3881
C	2.9412	-1.1698	-0.1725
C	3.4143	-1.5466	-1.4534
C	4.2478	-2.6672	-1.5959
C	4.6504	-3.4015	-0.4787
C	3.4153	-1.8750	0.9591
C	4.2536	-2.9897	0.7952
C	3.1100	-0.7254	-2.6978
H	4.6089	-2.9583	-2.5711
H	5.3047	-4.2528	-0.5952
C	3.1371	-1.3921	2.3709
H	4.6269	-3.5261	1.6545
H	2.3821	0.0379	-2.4409
C	4.3425	0.0115	-3.2273
C	2.5229	-1.5508	-3.8472
H	4.0607	0.6351	-4.0760
H	4.7542	0.6445	-2.4411
H	5.0990	-0.7072	-3.5429
H	2.2317	-0.8872	-4.6617
H	3.2623	-2.2626	-4.2139
H	1.6452	-2.0946	-3.4995
H	2.2858	-0.7266	2.3292
C	2.7851	-2.5104	3.3575
C	4.3010	-0.5878	2.9530
H	2.4599	-2.0733	4.3018
H	1.9783	-3.1195	2.9497
H	3.6555	-3.1406	3.5390
H	4.0294	-0.2093	3.9387
H	5.1832	-1.2226	3.0389
H	4.5259	0.2535	2.2972

Structure **5a**

E_{total} = -8.58252789 a.u.

Atom	X	Y	Z
Ni	0.0120	-0.0196	-0.0899
N	1.9199	0.0244	0.0775
C	2.6447	1.1066	0.1299
C	2.1475	2.4481	0.1004
C	0.7777	2.7400	0.4347
C	0.4213	4.1210	0.6081
C	1.3066	5.1145	0.2606
C	2.6182	4.7971	-0.1408
C	3.0477	3.4850	-0.1688
C	0.0549	-1.7692	-0.9751
C	0.3449	-1.5598	-2.4585

O	-0.1244	1.8244	0.5546
H	-0.4730	-0.9903	-2.9343
H	1.2512	-0.9438	-2.5822
C	0.5307	-2.8873	-3.2069
H	0.8556	-2.3818	-0.5230
H	-0.8689	-2.3549	-0.8474
H	-0.3773	-3.5078	-3.1408
H	0.7545	-2.7203	-4.2722
H	1.3599	-3.4669	-2.7709
H	4.0853	3.2724	-0.4262
N	3.5408	5.8601	-0.4769
O	3.1166	7.0282	-0.4342
O	4.7028	5.5454	-0.7903
H	1.0571	6.1711	0.3535
H	3.7312	1.0269	0.2601
P	-2.1659	0.0098	-0.1032
C	-2.8457	0.1943	1.6098
C	-2.8444	1.5047	-0.9639
C	-3.2026	-1.3595	-0.7917
H	-3.9371	0.3295	1.5878
H	-2.5919	-0.6930	2.2049
H	-2.3703	1.0714	2.0618
H	-3.9241	1.6087	-0.7818
H	-2.3067	2.3821	-0.5831
H	-2.6584	1.4192	-2.0433
H	-4.2655	-1.0813	-0.7377
H	-2.9300	-1.5482	-1.8389
H	-3.0398	-2.2785	-0.2131
C	2.6756	-1.1833	0.3733
C	-0.9720	4.4527	1.1361
C	3.8090	-1.5657	-0.3832
C	4.5181	-2.7236	-0.0246
C	4.1160	-3.4974	1.0689
C	2.2637	-1.9751	1.4672
C	2.9920	-3.1242	1.8119
C	4.2521	-0.8060	-1.6281
H	5.3811	-3.0320	-0.5958
H	4.6720	-4.3833	1.3378
C	1.0749	-1.5637	2.3274
H	2.6989	-3.7240	2.6606
H	3.5315	-0.0175	-1.8354
C	5.6263	-0.1478	-1.4717
C	4.2978	-1.6862	-2.8800
H	5.8569	0.4355	-2.3634
H	5.6239	0.5126	-0.6052
H	6.3907	-0.9129	-1.3347
H	4.5288	-1.0723	-3.7508
H	5.0624	-2.4553	-2.7709
H	3.3292	-2.1618	-3.0268
H	0.5110	-0.7979	1.8004
C	0.0927	-2.7051	2.6047
C	1.5017	-0.9529	3.6629
H	-0.7748	-2.3179	3.1395
H	-0.2368	-3.1407	1.6616
H	0.5712	-3.4744	3.2105
H	0.6205	-0.6286	4.2167
H	2.0475	-1.6913	4.2506
H	2.1446	-0.0918	3.4785
C	-1.7548	5.4643	0.5293
C	-3.0409	5.7476	1.0254
C	-3.5520	5.0347	2.1144
C	-1.4824	3.7682	2.2663
C	-2.7754	4.0548	2.7392
H	-4.5418	5.2562	2.4867
C	-1.3252	6.1414	-0.6294
C	-2.1263	7.1213	-1.2310
C	-3.3832	7.4264	-0.6981
C	-3.8432	6.7294	0.4244
H	-0.3849	5.9119	-1.1022
H	-1.7773	7.6339	-2.1153
H	-4.0038	8.1775	-1.1640
H	-4.8255	6.9435	0.8193
C	-0.6855	2.8754	3.0122
C	-1.1943	2.2271	4.1457
C	-2.5063	2.4724	4.5646
C	-3.2918	3.3957	3.8652
H	0.3425	2.6842	2.7496
H	-0.5707	1.5410	4.6995
H	-2.9002	1.9746	5.4382
H	-4.2911	3.6156	4.2115

Structure 5b-O

E_{total} = -6.18223416 a.u.

Atom	X	Y	Z
Ni	-0.0008	-0.0007	0.0028
N	1.8309	-0.0006	-0.0199
C	2.5714	1.0794	-0.0242
C	2.0970	2.4225	0.0350
C	0.7155	2.7381	0.2972
C	0.3687	4.1239	0.5144
C	1.2973	5.1046	0.2567
C	2.6301	4.7721	-0.0575
C	3.0315	3.4563	-0.1343
C	-0.4133	-1.8021	-0.5037
C	-1.7627	-1.2119	-0.3172
O	-0.2140	1.8443	0.3510
H	-1.6711	-0.0671	-0.0173
H	-2.3132	-1.0971	-1.2655
C	-2.6358	-1.8029	0.7899
H	-0.0992	-2.0085	-1.5352
H	-0.1388	-2.5993	0.1996
H	-2.0749	-1.8693	1.7329
H	-3.5361	-1.1965	0.9640
H	-2.9524	-2.8162	0.5020
H	4.0767	3.2336	-0.3465
N	3.5954	5.8303	-0.2931
O	3.1825	7.0017	-0.2514
O	4.7731	5.5057	-0.5253
H	1.0478	6.1622	0.3389
H	3.6620	0.9669	-0.0387
C	2.5720	-1.2424	0.0794
C	-1.0940	4.5065	0.7740
C	3.4724	-1.6444	-0.9317
C	4.1904	-2.8414	-0.7804
C	4.0229	-3.6311	0.3621
C	2.3918	-2.0469	1.2237
C	3.1280	-3.2346	1.3616
C	3.6389	-0.8505	-2.2204
H	4.8767	-3.1657	-1.5485
H	4.5846	-4.5469	0.4726
C	1.4691	-1.5931	2.3489
H	3.0236	-3.8491	2.2428
H	2.9549	-0.0044	-2.2035
C	5.0517	-0.2883	-2.3971
C	3.2828	-1.6644	-3.4667
H	5.0931	0.3228	-3.2990
H	5.3103	0.3283	-1.5364
H	5.7691	-1.1047	-2.4820
H	3.3430	-1.0278	-4.3497
H	3.9738	-2.5000	-3.5789
H	2.2665	-2.0473	-3.3713
H	0.6879	-0.9697	1.9175
C	0.7545	-2.7356	3.0775
C	2.1967	-0.7435	3.3927
H	0.0230	-2.3224	3.7722
H	0.2392	-3.3672	2.3540
H	1.4739	-3.3351	3.6351
H	1.4869	-0.3956	4.1435
H	2.9735	-1.3374	3.8750
H	2.6534	0.1191	2.9071
C	-1.7698	5.4133	-0.0742
C	-3.1088	5.7536	0.1917
C	-3.7783	5.1880	1.2828
C	-1.7751	3.9468	1.8781
C	-3.1176	4.2842	2.1218
H	-4.8087	5.4486	1.4768
C	-1.1541	5.9512	-1.2209
C	-1.8437	6.8428	-2.0537
C	-3.1647	7.1996	-1.7607
C	-3.7982	6.6477	-0.6413
H	-0.1482	5.6809	-1.4985
H	-1.3567	7.2497	-2.9277
H	-3.6978	7.8841	-2.4039
H	-4.8245	6.9076	-0.4267
C	-1.1205	3.0840	2.7780
C	-1.8067	2.5327	3.8684
C	-3.1528	2.8506	4.0839
C	-3.8046	3.7331	3.2140
H	-0.0780	2.8349	2.6557
H	-1.2942	1.8665	4.5466
H	-3.6817	2.4290	4.9258
H	-4.8380	3.9924	3.3919

Structure 5b-N

E_{total} = -6.16810434 a.u.

Atom	X	Y	Z
Ni	-0.0097	-0.0085	0.0628
N	1.8835	-0.0027	-0.0879
C	2.6127	1.0809	-0.0994
C	2.1123	2.4149	-0.0119
C	0.7253	2.7157	0.2250
C	0.3581	4.0892	0.4284
C	1.2902	5.0836	0.2460
C	2.6288	4.7687	-0.0567
C	3.0400	3.4580	-0.1526
O	-0.2206	1.8285	0.2192
C	-1.9010	-0.3708	0.2349
C	-1.3295	-1.6861	-0.0404
H	-0.1004	-1.5983	-0.0874
H	-1.3859	-2.3804	0.8138
C	-1.6676	-2.3622	-1.3666
H	-2.2344	-0.1465	1.2540
H	-2.4757	0.1186	-0.5602
H	-1.5734	-1.6518	-2.1997
H	-1.0128	-3.2227	-1.5657
H	-2.7071	-2.7214	-1.3323
H	4.0899	3.2443	-0.3510
N	3.5938	5.8371	-0.2360
O	3.1810	7.0057	-0.1447
O	4.7730	5.5218	-0.4718
H	1.0507	6.1354	0.3982
H	3.7058	1.0008	-0.1459
C	2.6634	-1.2259	-0.0655
C	-1.0887	4.4157	0.8063
C	3.5658	-1.5460	-1.1059
C	4.3168	-2.7299	-1.0292
C	4.1790	-3.5907	0.0644
C	2.5086	-2.1072	1.0248
C	3.2780	-3.2801	1.0879
C	3.6965	-0.6851	-2.3562
H	5.0047	-2.9906	-1.8197
H	4.7660	-4.4957	0.1172
C	1.5872	-1.7534	2.1850
H	3.1943	-3.9484	1.9314
H	2.9900	0.1396	-2.2934
C	5.0923	-0.0778	-2.5216
C	3.3489	-1.4470	-3.6375
H	5.1059	0.5780	-3.3923
H	5.3472	0.5021	-1.6347
H	5.8292	-0.8698	-2.6558
H	3.3814	-0.7666	-4.4886
H	4.0611	-2.2565	-3.7978
H	2.3446	-1.8624	-3.5509
H	0.8267	-1.0651	1.8226
C	0.8405	-2.9536	2.7741
C	2.3261	-1.0420	3.3198
H	0.1026	-2.6046	3.4968
H	0.3309	-3.4942	1.9765
H	1.5395	-3.6232	3.2751
H	1.6182	-0.7598	4.0995
H	3.0836	-1.7043	3.7395
H	2.8079	-0.1437	2.9330
C	-1.7594	5.5119	0.2070
C	-3.0933	5.7965	0.5558
C	-3.7700	4.9946	1.4788
C	-1.7731	3.6393	1.7772
C	-3.1157	3.9213	2.0886
H	-4.7973	5.2136	1.7320
C	-1.1669	6.2825	-0.8142
C	-1.8538	7.3502	-1.4076
C	-3.1595	7.6542	-1.0099
C	-3.7819	6.8662	-0.0363
H	-0.1832	6.0623	-1.1928
H	-1.3780	7.9316	-2.1835
H	-3.6925	8.4728	-1.4705
H	-4.8024	7.0778	0.2479
C	-1.1180	2.6455	2.5339
C	-1.8083	1.8866	3.4882
C	-3.1639	2.1295	3.7305
C	-3.8111	3.1603	3.0408
H	-0.0634	2.4536	2.4192
H	-1.2893	1.1204	4.0451
H	-3.6973	1.5500	4.4695
H	-4.8460	3.3796	3.2592

Structure 5c-O

E_{total} = -7.35611003 a.u.

Atom	X	Y	Z
Ni	0.0172	0.0489	0.1079
N	1.9347	0.0553	0.1137
C	2.6801	1.1284	0.1170
C	2.2304	2.4809	0.1010
C	0.8706	2.8246	-0.2245
C	0.5500	4.2173	-0.3805
C	1.4827	5.1746	-0.0615
C	2.7909	4.8108	0.3148
C	3.1727	3.4878	0.3571
O	-0.0572	1.9412	-0.3430
C	-0.0692	-1.7514	0.8785
C	0.1327	-1.6284	2.3820
H	1.0835	-1.1163	2.6009
H	-0.6609	-1.0020	2.8245
C	0.1241	-3.0010	3.0729
H	-1.0476	-2.2072	0.6536
H	0.6972	-2.4053	0.4286
H	0.9231	-3.6461	2.6752
H	0.2761	-2.8982	4.1585
H	-0.8354	-3.5164	2.9100
H	4.2025	3.2393	0.6125
N	3.7590	5.8459	0.6253
O	4.9148	5.4920	0.9143
O	3.3708	7.0256	0.5850
H	1.2748	6.2397	-0.1577
H	3.7708	1.0161	0.0872
C	-2.0300	0.2131	0.3738
C	-1.7382	-0.2341	-0.9045
H	-2.1876	1.2775	0.5617
H	-2.3604	-0.4793	1.1511
H	-1.6631	0.4760	-1.7310
H	-1.8328	-1.2881	-1.1739
C	2.7081	-1.1614	-0.0827
C	-0.8558	4.5966	-0.8480
C	2.4617	-1.9333	-1.2384
C	3.2229	-3.0860	-1.4861
C	4.2191	-3.4808	-0.5880

C	3.7186	-1.5604	0.8243
C	4.4629	-2.7217	0.5610
C	1.4282	-1.4896	-2.2650
H	3.0576	-3.6710	-2.3784
H	4.8022	-4.3685	-0.7833
C	3.9929	-0.8054	2.1195
H	5.2331	-3.0419	1.2468
H	0.7776	-0.7523	-1.8014
C	2.0636	-0.8136	-3.4808
C	0.5202	-2.6211	-2.7547
H	1.2828	-0.4603	-4.1546
H	2.6622	0.0360	-3.1513
H	2.7032	-1.5229	-4.0066
H	-0.2575	-2.2110	-3.3994
H	1.1002	-3.3529	-3.3168
H	0.0525	-3.1097	-1.8999
H	3.2399	-0.0287	2.2394
C	3.9015	-1.6957	3.3625
C	5.3658	-0.1266	2.1388
H	3.9972	-1.0830	4.2591
H	2.9385	-2.2042	3.3796
H	4.6982	-2.4394	3.3512
H	5.4775	0.4483	3.0583
H	6.1524	-0.8797	2.0875
H	5.4598	0.5448	1.2861
C	-1.4625	3.9046	-1.9269
C	-2.7695	4.2326	-2.3302
C	-3.4626	5.2681	-1.6980
C	-1.5609	5.6587	-0.2288
C	-2.8579	5.9894	-0.6646
H	-4.4619	5.5230	-2.0202
C	-0.7531	2.9590	-2.6958
C	-1.3625	2.2914	-3.7664
C	-2.6889	2.5754	-4.1066
C	-3.3857	3.5584	-3.3955
H	0.2838	2.7378	-2.5001
H	-0.8042	1.5612	-4.3337
H	-3.1602	2.0643	-4.9330
H	-4.3950	3.8112	-3.6858
C	-1.0446	6.3455	0.8888
C	-1.7668	7.3794	1.5000
C	-3.0327	7.7313	1.0211
C	-3.5815	7.0253	-0.0546
H	-0.0960	6.0837	1.3263
H	-1.3495	7.8976	2.3507
H	-3.5928	8.5242	1.4945
H	-4.5727	7.2738	-0.4049

Structure 5c-N

E_{total} = -7.35159077a.u.

Atom	X	Y	Z
Ni	0.1014	-0.1341	-0.2882
N	2.0562	-0.0468	0.0172
C	2.7643	1.0484	0.0687
C	2.2465	2.3771	0.1238
C	0.8487	2.6676	-0.0474
C	0.4247	4.0365	0.0550
C	1.3605	5.0366	0.1665
C	2.7322	4.7311	0.2457
C	3.1700	3.4246	0.2479
O	-0.0281	1.7746	-0.3637
C	-1.7112	-0.0856	-1.0199
C	-1.5191	0.2202	-2.4925
H	-0.9091	1.1305	-2.6075
H	-0.9841	-0.6042	-2.9954
C	-2.8684	0.4356	-3.2021
H	-2.2630	-1.0252	-0.8596
H	-2.2010	0.7424	-0.4855
H	-3.4162	1.2736	-2.7449
H	-2.7135	0.6646	-4.2677
H	-3.5003	-0.4632	-3.1315
H	4.2377	3.2234	0.3317
N	3.6973	5.8094	0.3256
O	4.9009	5.5070	0.3759
O	3.2612	6.9725	0.3305
H	1.0807	6.0858	0.2569
H	3.8612	0.9890	0.0546
C	-0.0782	-2.1463	0.0406
C	-0.5203	-1.3889	1.1294
H	0.8959	-2.6400	0.0787
H	-0.7921	-2.5857	-0.6601
H	0.1422	-1.2107	1.9821
H	-1.5842	-1.2239	1.3132
C	2.9092	-1.2140	-0.1285
C	-1.0725	4.3422	-0.0230
C	2.9065	-1.9208	-1.3488
C	3.7606	-3.0224	-1.5166
C	4.6000	-3.4309	-0.4745
C	3.7555	-1.6268	0.9232
C	4.5940	-2.7380	0.7409
C	2.0407	-1.4564	-2.5114
H	3.7883	-3.5587	-2.4531
H	5.2534	-4.2803	-0.6088
C	3.7392	-0.9328	2.2782
H	5.2411	-3.0692	1.5396
H	1.2331	-0.8470	-2.1113
C	2.8125	-0.5822	-3.5009
C	1.3783	-2.5982	-3.2881
H	2.1384	-0.2261	-4.2803
H	3.2356	0.2744	-2.9757
H	3.6182	-1.1603	-3.9541
H	0.6901	-2.1860	-4.0263
H	2.1340	-3.1931	-3.8008
H	0.8223	-3.2344	-2.5996
H	2.9799	-0.1533	2.2643
C	3.3640	-1.8773	3.4226
C	5.0710	-0.2599	2.6194
H	3.2898	-1.3140	4.3531
H	2.4009	-2.3413	3.2084
H	4.1217	-2.6532	3.5319
H	4.9811	0.2721	3.5667
H	5.8571	-1.0108	2.7009
H	5.3326	0.4503	1.8350
C	-1.5464	5.4344	-0.7929
C	-2.9285	5.6889	-0.8755
C	-3.8415	4.8612	-0.2162
C	-2.0077	3.5408	0.6809
C	-3.3863	3.7924	0.5597
H	-4.9011	5.0568	-0.2954
C	-0.6823	6.2299	-1.5729
C	-1.1737	7.2922	-2.3436
C	-2.5447	7.5659	-2.3709
C	-3.4219	6.7531	-1.6455
H	0.3751	6.0343	-1.6272
H	-0.4929	7.8931	-2.9282
H	-2.9258	8.3803	-2.9692
H	-4.4846	6.9413	-1.6925
C	-1.5978	2.5490	1.5960
C	-2.5338	1.7637	2.2819
C	-3.9026	1.9762	2.0903
C	-4.3261	3.0038	1.2408
H	-0.5554	2.3780	1.8113
H	-2.1970	0.9994	2.9667
H	-4.6262	1.3754	2.6212
H	-5.3824	3.1992	1.1265

Structure 5d-O

E_{total} = -7.31897787 a.u.

Atom	X	Y	Z
Ni	0.0059	0.0139	0.0194
N	1.9521	0.0039	0.0459
C	2.7023	1.0721	0.0261
C	2.2306	2.4154	0.1398
C	0.8296	2.7409	0.1819
C	0.4582	4.1078	0.4200
C	1.4248	5.0851	0.4455
C	2.7865	4.7535	0.3118
C	3.1854	3.4401	0.1855
O	-0.1124	1.8856	-0.0551
C	-1.8989	-0.0996	-0.3886
C	-1.3514	-1.3781	-0.7431
H	-2.0295	0.6683	-1.1566
H	-2.5935	-0.0377	0.4558
H	-0.8866	-1.4556	-1.7335
H	-1.9161	-2.2866	-0.5139
C	-0.1865	-1.9741	0.7616
C	-1.2387	-2.4901	1.7335
H	-1.8551	-1.6489	2.0915
H	-1.9220	-3.1927	1.2265
C	-0.6028	-3.1935	2.9358
H	0.3356	-2.7822	0.2275
H	0.5516	-1.4118	1.3660
H	0.0073	-2.4955	3.5284
H	-1.3788	-3.6071	3.5974
H	0.0442	-4.0236	2.6123
H	4.2494	3.2134	0.1204
N	3.7832	5.8061	0.3320
O	4.9786	5.4780	0.2312
O	3.3813	6.9770	0.4453
H	1.1886	6.1310	0.6380
H	3.7911	0.9708	-0.0744
C	2.7409	-1.2131	-0.0569
C	-1.0250	4.4405	0.6019
C	2.7005	-1.9747	-1.2421
C	3.4872	-3.1324	-1.3530
C	4.2978	-3.5415	-0.2891
C	3.5585	-1.6271	1.0172
C	4.3316	-2.7921	0.8915
C	1.8816	-1.5100	-2.4357
H	3.4873	-3.7113	-2.2643
H	4.9007	-4.4329	-0.3807
C	3.5871	-0.8639	2.3344
H	4.9596	-3.1208	1.7061
H	1.1196	-0.8209	-2.0770
C	2.7259	-0.7495	-3.4596
C	1.1506	-2.6443	-3.1606
H	2.0883	-0.3890	-4.2671
H	3.2050	0.1016	-2.9751
H	3.4921	-1.4082	-3.8692
H	0.4866	-2.2255	-3.9170
H	1.8685	-3.3059	-3.6451
H	0.5604	-3.2154	-2.4438
H	2.8191	-0.0928	2.3081
C	3.2677	-1.7473	3.5429
C	4.9251	-0.1655	2.5885
H	3.2011	-1.1310	4.4397
H	2.3139	-2.2492	3.3828
H	4.0492	-2.4948	3.6791
H	4.8689	0.4102	3.5125
H	5.7202	-0.9066	2.6726
H	5.1490	0.5084	1.7618
C	-1.5835	5.5969	0.0000
C	-2.9521	5.8837	0.1635
C	-3.7723	5.0253	0.9005
C	-1.8604	3.6042	1.3880
C	-3.2323	3.8904	1.5104
H	-4.8242	5.2466	1.0096
C	-0.8334	6.4329	-0.8524
C	-1.4094	7.5607	-1.4525
C	-2.7571	7.8627	-1.2337
C	-3.5300	7.0135	-0.4353
H	0.1938	6.2209	-1.0955
H	-0.8140	8.1910	-2.0965
H	-3.2042	8.7279	-1.7005
H	-4.5798	7.2250	-0.2935
C	-1.3427	2.5367	2.1512
C	-2.1818	1.7161	2.9165
C	-3.5562	1.9689	2.9639
C	-4.0761	3.0691	2.2738
H	-0.2852	2.3306	2.1878
H	-1.7644	0.8940	3.4790
H	-4.2050	1.3418	3.5574
H	-5.1303	3.2934	2.3462

Structure 5d-N

E_{total} = -7.32935394 a.u.

Atom	X	Y	Z
Ni	0.0039	-0.0033	0.0017
N	-1.8831	-0.0016	0.0065
C	2.6663	1.0463	0.0093
C	2.2552	2.4054	0.1198
C	0.8672	2.7799	0.0603
C	0.5400	4.1714	0.1982
C	1.5438	5.1091	0.2689
C	2.8975	4.7207	0.2653
C	3.2498	3.3890	0.2057
O	-0.0673	1.9243	-0.1829
C	-0.0837	-1.8447	0.6279
C	-1.4591	-1.4890	0.5193
H	0.3905	-1.8326	1.6159
H	0.3067	-2.5944	-0.0691
H	-1.9950	-1.2373	1.4395
H	-2.0532	-2.0677	-0.1934
C	-2.0907	0.1784	-0.5250
C	-1.9990	0.0845	-2.0366
H	-1.0658	0.5483	-2.3944
H	-1.9820	-0.9718	-2.3572
C	-3.1907	0.7947	-2.6960
H	-3.0618	-0.1911	-0.1734
H	-1.9771	1.2037	-0.1501
H	-3.2155	1.8577	-2.4128
H	-3.1217	0.7346	-3.7925
H	-4.1438	0.3371	-2.3875
H	4.3052	3.1182	0.2219
N	3.9327	5.7326	0.3426
O	5.1172	5.3535	0.3492
O	3.5730	6.9214	0.3960
H	1.3343	6.1709	0.3946
H	3.7477	0.8946	-0.0981
C	2.6211	-1.2333	-0.2078
C	-0.9332	4.5812	0.2264
C	2.4197	-1.9538	-1.4036
C	3.1613	-3.1207	-1.6476
C	4.0856	-3.5805	-0.7037
C	3.5530	-1.6992	0.7459
C	4.2768	-2.8745	0.4888
C	1.4584	-1.4386	-2.4653
H	3.0358	-3.6688	-2.5691
H	4.6519	-4.4798	-0.8958
C	3.7507	-0.9952	2.0816
H	4.9873	-3.2459	1.2123
H	0.7567	-0.7605	-1.9853
C	2.1706	-0.6444	-3.5612
C	0.6165	-2.5325	-3.1287
H	1.4368	-0.2453	-4.2619
H	2.7213	0.1820	-3.1113
H	2.8664	-1.2927	-4.0944
H	-0.1154	-2.0751	-3.7948
H	1.2544	-3.2004	-3.7071
H	0.0914	-3.1046	-2.3639
H	3.0500	-0.1652	2.1485
C	3.4564	-1.9021	3.2790
C	5.1577	-0.4158	2.2486
H	3.5344	-1.3271	4.2020
H	2.4458	-2.3016	3.1918

H	4.1686	-2.7268	3.3088
H	5.2207	0.1286	3.1911
H	5.8937	-1.2200	2.2470
H	5.3717	0.2679	1.4272
C	-1.3818	5.7100	-0.5044
C	-2.7457	6.0584	-0.4917
C	-3.6664	5.2889	0.2252
C	-1.8699	3.8417	0.9924
C	-3.2332	4.1864	0.9661
H	-4.7132	5.5563	0.2190
C	-0.5191	6.4522	-1.3364
C	-0.9874	7.5524	-2.0674
C	-2.3355	7.9181	-2.0014
C	-3.2158	7.1603	-1.2222
H	0.5170	6.1863	-1.4606
H	-0.3077	8.1116	-2.6933
H	-2.6992	8.7619	-2.5691
H	-4.2639	7.4206	-1.1967
C	-1.4653	2.8207	1.8769
C	-2.4031	2.0947	2.6232
C	-3.7646	2.3986	2.5247
C	-4.1753	3.4578	1.7082
H	-0.4242	2.5794	2.0187
H	-2.0727	1.3050	3.2816
H	-4.4892	1.8435	3.1020
H	-5.2215	3.7237	1.6664

Structure **5e**

E_{total} = -7.36189907 a.u.

Atom	X	Y	Z
Ni	0.0424	-0.0105	0.0147
N	1.9428	0.0025	0.0084
C	2.6641	1.0917	0.0430
C	2.1573	2.4163	0.2012
C	0.7502	2.7135	0.2644
C	0.3605	4.0796	0.4774
C	1.3106	5.0737	0.4874
C	2.6778	4.7650	0.3598
C	3.0960	3.4584	0.2388
O	-0.1836	1.8347	0.0682
C	-1.8570	-0.3691	0.0549
C	-1.2638	-1.7007	0.1415
H	-2.3329	-0.0796	-0.8906
H	-2.3069	0.0695	0.9509
H	-0.0377	-1.6112	0.0735
H	-1.3393	-2.1534	1.1442
C	-1.5778	-2.7101	-0.9669
C	-2.9883	-3.2842	-0.8155
H	-3.0809	-3.7623	0.1760
H	-3.7169	-2.4557	-0.8313
C	-3.3269	-4.2971	-1.9072
H	-1.4828	-2.2093	-1.9452
H	-0.8445	-3.5347	-0.9491
H	-2.6283	-5.1482	-1.8903
H	-4.3442	-4.6946	-1.7767
H	-3.2707	-3.8361	-2.9057
H	4.1626	3.2481	0.1638
N	3.6582	5.8341	0.3780
O	4.8584	5.5243	0.2824
O	3.2371	6.9983	0.4863
H	1.0508	6.1175	0.6602
H	3.7535	1.0237	-0.0695
C	2.7382	-1.1903	-0.2157
C	-1.1230	4.4085	0.6524
C	2.5483	-1.9293	-1.4021
C	3.3363	-3.0665	-1.6459
C	4.2924	-3.4789	-0.7122
C	3.7012	-1.6101	0.7295
C	4.4709	-2.7554	0.4712
C	1.5647	-1.4492	-2.4617
H	3.2272	-3.6305	-2.5595
H	4.8935	-4.3551	-0.9055
C	3.8869	-0.8931	2.0607
H	5.2060	-3.0910	1.1875
H	0.7085	-1.0113	-1.9518
C	2.1594	-0.3677	-3.3670
C	1.0190	-2.5584	-3.3669
H	1.4045	-0.0251	-4.0751
H	2.4900	0.4774	-2.7637
H	3.0115	-0.7728	-3.9134
H	0.2162	-2.1600	-3.9877
H	1.8102	-2.9390	-4.0130
H	0.6276	-3.3723	-2.7571
H	3.1518	-0.0945	2.1366
C	3.6500	-1.8076	3.2651
C	5.2698	-0.2528	2.2061
H	3.7163	-1.2263	4.1850
H	2.6564	-2.2507	3.1940
H	4.3976	-2.6005	3.2871
H	5.3220	0.2979	3.1456
H	6.0397	-1.0246	2.1977
H	5.4433	0.4357	1.3793
C	-1.6912	5.5331	0.0028
C	-3.0585	5.8242	0.1673
C	-3.8663	5.0032	0.9591
C	-1.9442	3.6109	1.4897
C	-3.3140	3.9034	1.6207
H	-4.9167	5.2290	1.0731
C	-0.9504	6.3296	-0.8941
C	-1.5356	7.4254	-1.5426
C	-2.8826	7.7330	-1.3267
C	-3.6456	6.9219	-0.4802
H	0.0766	6.1094	-1.1323
H	-0.9479	8.0264	-2.2208
H	-3.3367	8.5736	-1.8303
H	-4.6943	7.1384	-0.3375
C	-1.4096	2.5855	2.2964
C	-2.2323	1.8144	3.1285
C	-3.6057	2.0703	3.1897
C	-4.1419	3.1265	2.4454
H	-0.3516	2.3797	2.3175
H	-1.8032	1.0262	3.7293
H	-4.2414	1.4796	3.8327
H	-5.1948	3.3543	2.5258

Structure **5h**

E_{total} = -7.30945002 a.u.

Atom	X	Y	Z
Ni	-0.0016	0.0012	-0.0002
N	1.9684	0.0007	0.0010
C	2.6447	1.1122	0.0007
C	2.0970	2.4263	0.1702
C	0.8484	2.6206	0.8768
C	0.5521	3.9585	1.3235
C	1.3004	5.0174	0.8683
C	2.4496	4.8056	0.0804
C	2.8762	3.5245	-0.2080
O	0.0130	1.6738	1.1036
C	-0.2530	-1.9559	0.7882
C	-1.3660	-1.2326	1.1960
H	-1.4385	0.1576	0.0236
H	-2.3054	-1.4230	0.6634
C	-1.5169	-0.6540	2.5730
H	-0.3105	-2.6370	-0.0622
H	0.5595	-2.1233	1.4944
H	-0.5415	-0.5337	3.0607
H	-2.0107	0.3266	2.5508
H	-2.1366	-1.3326	3.1837
H	3.8146	3.3885	-0.7458
N	3.2251	5.9376	-0.3739
O	4.2581	5.7107	-1.0301
O	2.8127	7.0751	-0.0845
H	1.0825	6.0459	1.1554
H	3.7407	1.0732	-0.0809
C	-0.3804	-0.4926	-2.0064
C	-0.1964	0.8792	-1.9110
H	-1.3865	-0.9130	-2.0826
H	0.4277	-1.1496	-2.3302
H	-1.0506	1.5583	-1.8916
H	0.7704	1.3335	-2.1391
C	2.8388	-1.1560	0.1131
C	-0.6542	4.1640	2.2390
C	3.4444	-1.7238	-1.0277
C	4.3167	-2.8139	-0.8789
C	4.6027	-3.3257	0.3911
C	3.1570	-1.6488	1.3973
C	4.0353	-2.7366	1.5260
C	3.2131	-1.1515	-2.4172
H	4.7901	-3.2560	-1.7429
H	5.2835	-4.1573	0.4975
C	2.6132	-0.9710	2.6508
H	4.2980	-3.1189	2.5008
H	2.4141	-0.4165	-2.3592
C	4.4431	-0.4244	-2.9645
C	2.7808	-2.2049	-3.4413
H	4.2076	0.0179	-3.9327
H	4.7361	0.3657	-2.2730
H	5.2692	-1.1265	-3.0791
H	2.5241	-1.7168	-4.3817
H	3.5907	-2.9133	-3.6154
H	1.9090	-2.7418	-3.0674
H	1.7115	-0.4242	2.3796
C	2.2172	-1.9433	3.7671
C	3.5932	0.0444	3.2426
H	1.7240	-1.3950	4.5698
H	1.5308	-2.6944	3.3769
H	3.1025	-2.4373	4.1673
H	3.1360	0.5402	4.0991
H	4.5035	-0.4638	3.5613
H	3.8447	0.7927	2.4914
C	-1.5603	5.2304	2.0176
C	-2.6653	5.4015	2.8726
C	-2.8806	4.5198	3.9359
C	-0.8585	3.3045	3.3476
C	-1.9803	3.4786	4.1780
H	-3.7348	4.6548	4.5835
C	-1.4502	6.0822	0.9000
C	-2.3699	7.1180	0.6870
C	-3.4335	7.3075	1.5751
C	-3.5860	6.4391	2.6612
H	-0.6776	5.9501	0.1613
H	-2.2640	7.7637	-0.1722
H	-4.1463	8.1017	1.4091
H	-4.4248	6.5645	3.3302
C	0.0968	2.3369	3.7213
C	-0.1066	1.5119	4.8354
C	-1.2643	1.6484	5.6079
C	-2.1942	2.6423	5.2842
H	1.0225	2.2209	3.1812
H	0.6346	0.7728	5.1007
H	-1.4228	1.0137	6.4673
H	-3.0670	2.7783	5.9061

Structure **5i**

E_{total} = -7.30948653 a.u.

Atom	X	Y	Z
Ni	0.0189	0.0232	-0.0246
N	2.0624	0.0270	-0.0413
C	2.7685	1.1219	-0.0244
C	2.3048	2.4787	-0.0222
C	0.9173	2.8542	-0.2096
C	0.6415	4.2552	-0.4353
C	1.6631	5.1737	-0.4521
C	2.9958	4.7850	-0.2199
C	3.3091	3.4578	-0.0224
O	-0.0436	2.0092	-0.2670
C	-0.2016	-1.6082	-1.3298
C	-0.3762	-0.4211	-2.0260
H	-1.0663	-2.2005	-1.0254
H	0.7491	-2.1445	-1.3545
H	-1.3790	-0.0630	-2.2646
H	0.4298	0.0460	-2.5892
C	-0.4212	-1.0971	1.7379
C	-0.4394	0.2380	2.0909
H	-1.4070	0.0768	-0.0699
H	-1.4076	0.7443	2.0301
C	0.5929	0.9789	2.8803
H	-1.3551	-1.6074	1.4987
H	0.4184	-1.7478	1.9797
H	1.5712	0.4872	2.8982
H	0.7272	2.0038	2.5077
H	0.2406	1.0646	3.9240
H	4.3552	3.1795	0.1058
N	4.0448	5.7793	-0.2245
O	3.7173	6.9622	-0.4248
O	5.2123	5.3960	-0.0279
H	1.4741	6.2373	-0.5986
H	3.8653	1.0430	-0.0665
C	2.9304	-1.1128	-0.3385
C	-0.7907	4.7091	-0.7270
C	3.4258	-1.2895	-1.6542
C	4.2759	-2.3671	-1.9495
C	4.6655	-3.2614	-0.9506
C	3.3753	-1.9922	0.6763
C	4.2299	-3.0610	0.3608
C	3.1045	-0.3111	-2.7757
H	4.6548	-2.5049	-2.9512
H	5.3305	-4.0799	-1.1832
C	3.0413	-1.7542	2.1349
H	4.5833	-3.7266	1.1337
H	2.3448	0.3833	-2.4280
C	4.3145	0.5322	-3.1853
C	2.5533	-0.9903	-4.0333
H	4.0170	1.2562	-3.9441
H	4.6995	1.0653	-2.3161
H	5.0973	-0.1113	-3.5874
H	2.2370	-0.2315	-4.7495
H	3.3211	-1.6144	-4.4905
H	1.6976	-1.6115	-3.7695
H	2.1948	-1.0836	2.1662
C	2.6404	-3.0206	2.8982
C	4.1815	-1.0716	2.8926
H	2.2819	-2.7489	3.8913
H	1.8446	-3.5358	2.3599
H	3.4970	-3.6868	2.9995
H	3.8688	-0.8614	3.9156
H	5.0572	-1.7209	2.9073
H	4.4366	-0.1345	2.3973
C	-1.0478	5.6023	-1.7975
C	-2.3661	6.0118	-2.0728
C	-3.4300	5.5362	-1.3014
C	-1.8740	4.2709	0.0736
C	-3.1873	4.6742	-0.2289
H	-4.4397	5.8509	-1.5226
C	-0.0276	6.0292	-2.6720
C	-0.3038	6.8954	-3.7385
C	-1.6119	7.3338	-3.9675
C	-2.6439	6.8801	-3.1394
H	0.9884	5.6870	-2.5676
H	0.4938	7.2155	-4.3924
H	-1.8274	7.9968	-4.7924
H	-3.6595	7.1929	-3.3336
C	-1.6662	3.5294	1.2516
C	-2.7431	3.1254	2.0525
C	-4.0509	3.4705	1.6969

C	-4.2693	4.2575	0.5611
H	-0.6712	3.2858	1.5831
H	-2.5629	2.5563	2.9524
H	-4.8820	3.1627	2.3140
H	-5.2743	4.5641	0.3102

Structure **6a**

E_{total} = -8.44380020 a.u.

Atom	X	Y	Z
Ni	-0.0083	-0.0708	-0.1865
P	2.1084	-0.1075	-0.3576
C	2.9913	1.3479	-0.2964
C	2.4044	2.6268	-0.0717
C	1.0210	2.7738	0.3310
C	0.5801	4.0800	0.7352
C	1.3739	5.1818	0.5161
C	2.6724	5.0285	0.0001
C	3.1951	3.7754	-0.2425
C	-0.1615	-2.0093	-0.5313
C	-0.0005	-2.3671	-2.0049
O	0.1516	1.8126	0.3152
H	-0.7253	-1.8078	-2.6199
H	0.9923	-2.0463	-2.3599
C	-0.1680	-3.8676	-2.2744
H	0.6197	-2.5010	0.0760
H	-1.1260	-2.3874	-0.1476
H	-1.1704	-4.2160	-1.9781
H	-0.0326	-4.0956	-3.3433
H	0.5699	-4.4540	-1.7046
H	4.2248	3.6899	-0.5871
N	3.4866	6.2040	-0.2336
O	2.9685	7.3149	-0.0240
O	4.6515	6.0363	-0.6335
H	1.0638	6.1876	0.7964
H	4.0708	1.3222	-0.4600
P	-2.2173	0.1086	-0.2579
C	-3.0530	-0.3598	1.3298
C	-2.8379	1.8222	-0.5673
C	-3.1763	-0.8712	-1.5053
H	-4.1425	-0.2264	1.2557
H	-2.8252	-1.4084	1.5653
H	-2.6576	0.2718	2.1349
H	-3.9312	1.8669	-0.4615
H	-2.3568	2.5006	0.1432
H	-2.5476	2.1309	-1.5805
H	-4.2540	-0.6970	-1.3680
H	-2.8858	-0.5569	-2.5169
H	-2.9671	-1.9426	-1.3931
C	3.3775	-1.4492	-0.5243
C	-0.7934	4.2298	1.3886
C	3.9991	-1.6975	-1.7658
C	4.9810	-2.6966	-1.8600
C	5.3383	-3.4482	-0.7354
C	3.7271	-2.2154	0.6057
C	4.7133	-3.2085	0.4931
C	3.6417	-0.8938	-3.0078
H	5.4758	-2.8898	-2.8001
H	6.0980	-4.2117	-0.8150
C	3.0662	-1.9649	1.9539
H	5.0053	-3.7924	1.3529
H	2.7386	-0.3218	-2.8051
C	4.7337	0.1049	-3.3977
C	3.3367	-1.7679	-4.2280
H	4.4042	0.6941	-4.2537
H	4.9340	0.7730	-2.5605
H	5.6483	-0.4290	-3.6570
H	2.9845	-1.1411	-5.0475
H	4.2349	-2.2978	-4.5448
H	2.5625	-2.4923	-3.9752
H	2.1346	-1.4280	1.7869
C	2.6867	-3.2468	2.7004
C	3.9280	-1.1008	2.8764
H	2.1213	-2.9925	3.5972
H	2.0693	-3.8733	2.0562
H	3.5832	-3.7953	2.9888
H	3.3897	-0.9023	3.8034
H	4.8607	-1.6182	3.1023
H	4.1519	-0.1544	2.3835
C	-1.6558	5.2917	1.0194
C	-2.9161	5.4192	1.6327
C	-3.3278	4.4996	2.6013
C	-1.2085	3.3240	2.3981
C	-2.4791	3.4586	2.9868
H	-4.2992	4.6017	3.0631
C	-1.3359	6.1813	-0.0261
C	-2.2129	7.2106	-0.3936
C	-3.4398	7.3562	0.2618
C	-3.7943	6.4506	1.2672
H	-0.4255	6.0837	-0.5936
H	-1.9461	7.8854	-1.1935
H	-4.1194	8.1454	-0.0242
H	-4.7551	6.5421	1.7524
C	-0.3427	2.3386	2.9156
C	-0.7622	1.4637	3.9264
C	-2.0506	1.5732	4.4596
C	-2.9040	2.5795	3.9945
H	0.6742	2.2441	2.5715
H	-0.0853	0.7105	4.3019
H	-2.3748	0.9028	5.2418
H	-3.8865	2.6882	4.4301

Structure **6b-O**

E = -6.03851947 a.u.

Atom	X	Y	Z
Ni	-0.0047	0.0036	0.0103
P	2.0511	0.0068	0.0069
C	2.8082	1.5337	0.0132
C	2.1180	2.7803	-0.0057
C	0.6722	2.8890	0.0355
C	0.0883	4.1963	0.1066
C	0.8787	5.3167	-0.0033
C	2.2747	5.1932	-0.1115
C	2.8840	3.9581	-0.0873
C	-0.4387	-1.8525	0.1205
C	-1.8161	-1.2667	0.1310
O	-0.1351	1.8746	-0.0458
H	-1.7654	-0.1124	-0.0390
H	-2.3929	-1.5566	-0.7627
C	-2.6158	-1.4470	1.4207
H	-0.1569	-2.4236	-0.7735
H	-0.1223	-2.3372	1.0538
H	-2.0231	-1.1309	2.2909
H	-3.5474	-0.8637	1.4056
H	-2.8739	-2.5088	1.5478
H	3.9700	3.9050	-0.1467
N	3.0878	6.3921	-0.2297
O	2.4979	7.4853	-0.2645
O	4.3209	6.2541	-0.2926
H	0.4696	6.3242	0.0574
H	3.8997	1.5717	0.0165
C	3.3749	-1.2723	0.1508
C	-1.4301	4.3152	0.2625
C	4.1684	-1.6056	-0.9661
C	5.1911	-2.5579	-0.8295
C	5.4222	-3.1779	0.4033
C	3.5979	-1.9068	1.3894
C	4.6284	-2.8532	1.5086
C	3.9498	-0.9466	-2.3199
H	5.8129	-2.8157	-1.6739
H	6.2141	-3.9057	0.5019
C	2.7528	-1.5647	2.6082
H	4.8230	-3.3356	2.4548
H	3.0513	-0.3356	-2.2722
C	5.1011	-0.0198	-2.7169
C	3.7264	-1.9563	-3.4487
H	4.8673	0.4728	-3.6609
H	5.2419	0.7365	-1.9446
H	6.0202	-0.5956	-2.8280
H	3.4946	-1.4266	-4.3730
H	4.6225	-2.5590	-3.5963
H	2.8912	-2.6083	-3.1920
H	1.8494	-1.0596	2.2726
C	2.2844	-2.7930	3.3934
C	3.4708	-0.6159	3.5698
H	1.6002	-2.4819	4.1831
H	1.7652	-3.4772	2.7218
H	3.1375	-3.3024	3.8413
H	2.8069	-0.3563	4.3947
H	4.3668	-1.0966	3.9633
H	3.7539	0.2933	3.0390
C	-2.1571	5.2718	-0.4907
C	-3.5545	5.3653	-0.3482
C	-4.2364	4.5084	0.5200
C	-2.1303	3.4843	1.1753
C	-3.5305	3.5721	1.2797
H	-5.3103	4.5793	0.6143
C	-1.5393	6.0809	-1.4663
C	-2.2787	7.0071	-2.2141
C	-3.6584	7.1259	-2.0203
C	-4.2962	6.2932	-1.0951
H	-0.4895	5.9972	-1.6911
H	-1.7835	7.6216	-2.9514
H	-4.2308	7.8348	-2.6002
H	-5.3670	6.3592	-0.9685
C	-1.4569	2.6324	2.0752
C	-2.1629	1.8188	2.9711
C	-3.5600	1.8629	3.0076
C	-4.2409	2.7539	2.1714
H	-0.3802	2.5977	2.1189
H	-1.6262	1.1640	3.6417
H	-4.1064	1.2398	3.7000
H	-5.3174	2.8223	2.2299

Structure **6b-P**

E_{total} = -6.02728522 a.u.

Atom	X	Y	Z
Ni	-0.0073	0.0041	-0.0563
P	2.1240	-0.0016	0.0016
C	2.8704	1.5322	0.0210
C	2.1643	2.7705	-0.0011
C	0.7208	2.8687	0.0515
C	0.1350	4.1750	0.1611
C	0.9151	5.3019	0.0478
C	2.3089	5.1872	-0.0913
C	2.9223	3.9545	-0.0843
O	-0.1111	1.8714	-0.0473
C	-1.9562	-0.2616	-0.1404
C	-1.3968	-1.5926	-0.0318
H	-0.1256	-1.5482	-0.0866
C	-1.6273	-2.3796	1.2537
H	-1.4676	-1.7397	2.1326
H	-0.9559	-3.2464	1.3275
H	-2.6653	-2.7438	1.2714
H	-1.5085	-2.2006	-0.9442
H	-2.4352	0.1811	0.7380
H	-2.3133	0.0949	-1.1111
H	4.0078	3.9052	-0.1584
N	3.1141	6.3905	-0.2141
O	2.5196	7.4819	-0.2125
O	4.3454	6.2588	-0.3157
H	0.5006	6.3056	0.1311
H	3.9606	1.5934	0.0411
C	3.5106	-1.2104	0.1948
C	-1.3780	4.2822	0.3642
C	3.9902	-1.9118	-0.9297
C	5.0295	-2.8437	-0.7738
C	5.6007	-3.0628	0.4845
C	4.0784	-1.4387	1.4651
C	5.1290	-2.3603	1.5986
C	3.3762	-1.6898	-2.3047
H	5.3999	-3.4024	-1.6199
H	6.4036	-3.7765	0.5963
C	3.5797	-0.7024	2.7001
H	5.5792	-2.5388	2.5638
H	2.9370	-0.6939	-2.3244
C	4.3895	-1.7287	-3.4526
C	2.2601	-2.6900	-2.6138
H	3.8975	-1.4426	-4.3825
H	5.1988	-1.0273	-3.2480
H	4.7978	-2.7333	-3.5621
H	1.8139	-2.4566	-3.5808
H	2.6672	-3.7012	-2.6370
H	1.4923	-2.6299	-1.8423
H	2.6848	-0.1425	2.4380
C	3.1803	-1.6430	3.8399
C	4.5979	0.3071	3.2346
H	2.7545	-1.0640	4.6598
H	2.4352	-2.3529	3.4802
H	4.0529	-2.1872	4.2012
H	4.1700	0.8487	4.0785
H	5.5005	-0.2117	3.5582
H	4.8536	1.0167	2.4475
C	-2.1350	5.2398	-0.3566
C	-3.5273	5.3235	-0.1665
C	-4.1738	4.4580	0.7202
C	-2.0407	3.4428	1.2966
C	-3.4366	3.5229	1.4512
H	-5.2442	4.5227	0.8525
C	-1.5536	6.0603	-1.3447
C	-2.3230	6.9868	-2.0613
C	-3.6966	7.0947	-1.8221
C	-4.2988	6.2517	-0.8823
H	-0.5105	5.9853	-1.6020
H	-1.8560	7.6103	-2.8093
H	-4.2921	7.8040	-2.3777
H	-5.3651	6.3104	-0.7198
C	-1.3302	2.5900	2.1667
C	-1.9991	1.7699	3.0852
C	-3.3942	1.8080	3.1733
C	-4.1098	2.6981	2.3653
H	-0.2526	2.5578	2.1677
H	-1.4354	1.1139	3.7320
H	-3.9121	1.1801	3.8832
H	-5.1837	2.7608	2.4633

Structure **6c-O**

E = -7.21680969 a.u.

Atom	X	Y	Z
Ni	-0.0020	-0.0002	0.0046
P	2.1159	0.0091	0.0373
C	2.9381	1.5030	-0.0123
C	2.3013	2.7706	-0.1062
C	0.8727	2.9145	-0.3136
C	0.3432	4.2461	-0.4182
C	1.1408	5.3380	-0.1733
C	2.5156	5.1727	0.0740
C	3.0916	3.9228	0.0708
O	0.0384	1.9241	-0.3467
C	-0.0319	-1.8439	0.7021
C	-0.0485	-1.7754	2.2227
H	0.8506	-1.2579	2.5935

H	-0.9081	-1.1785	2.5723
C	-0.1210	-3.1731	2.8568
H	-0.9436	-2.3281	0.3159
H	0.8296	-2.4276	0.3367
H	0.7472	-3.7827	2.5622
H	-0.1323	-3.1021	3.9552
H	-1.0311	-3.7053	2.5394
H	4.1625	3.8340	0.2482
N	3.3389	6.3438	0.3272
O	4.5575	6.1725	0.4955
O	2.7684	7.4466	0.3637
H	0.7588	6.3568	-0.2260
H	4.0278	1.5039	0.0622
C	-2.1001	0.1042	0.0663
C	-1.6806	-0.3082	-1.1818
H	-2.2844	1.1626	0.2654
H	-2.4701	-0.6121	0.8027
H	-1.5282	0.4167	-1.9824
H	-1.7071	-1.3584	-1.4772
C	3.4129	-1.2935	0.2661
C	-1.1386	4.4243	-0.7422
C	3.7312	-2.1545	-0.8041
C	4.7246	-3.1323	-0.6386
C	5.3968	-3.2592	0.5814
C	4.0810	-1.4304	1.5015
C	5.0749	-2.4117	1.6466
C	3.0207	-2.0460	-2.1453
H	4.9809	-3.7930	-1.4536
H	6.1624	-4.0115	0.7012
C	3.7568	-0.5330	2.6870
H	5.6026	-2.5202	2.5824
H	2.2419	-1.2905	-2.0725
C	3.9564	-1.6100	-3.2747
C	2.3263	-3.3458	-2.5593
H	3.3871	-1.4870	-4.1963
H	4.4221	-0.6596	-3.0128
H	4.7317	-2.3611	-3.4271
H	1.7728	-3.1866	-3.4849
H	3.0648	-4.1326	-2.7131
H	1.6316	-3.6514	-1.7766
H	2.8560	0.0334	2.4613
C	3.4690	-1.3144	3.9724
C	4.8661	0.4790	2.9831
H	3.1329	-0.6281	4.7499
H	2.6884	-2.0515	3.7851
H	4.3703	-1.8248	4.3116
H	4.5572	1.1346	3.7976
H	5.7792	-0.0446	3.2673
H	5.0596	1.0801	2.0951
C	-1.7242	3.7117	-1.8168
C	-3.0925	3.8658	-2.1031
C	-3.8752	4.7441	-1.3484
C	-1.9335	5.3350	-0.0043
C	-3.2975	5.4882	-0.3152
H	-4.9238	4.8654	-1.5788
C	-0.9461	2.9305	-2.6943
C	-1.5326	2.2602	-3.7766
C	-2.9084	2.3658	-4.0059
C	-3.6852	3.1785	-3.1731
H	0.1222	2.8470	-2.5744
H	-0.9206	1.6608	-4.4344
H	-3.3623	1.8481	-4.8380
H	-4.7399	3.2953	-3.3752
C	-1.4230	6.0357	1.1069
C	-2.2318	6.9149	1.8395
C	-3.5742	7.0928	1.4889
C	-4.1078	6.3691	0.4171
H	-0.4082	5.9012	1.4424
H	-1.8204	7.4480	2.6839
H	-4.1999	7.7663	2.0558
H	-5.1515	6.4839	0.1633

Structure **6c-P**

E = -7.21034203 a.u.

Atom	X	Y	Z
Ni	0.0935	-0.1401	-0.2047
P	2.2212	-0.0190	0.3966
C	2.9496	1.5140	0.5603
C	2.2816	2.7435	0.3029
C	0.8630	2.8109	0.0338
C	0.2700	4.1054	-0.1415
C	1.0572	5.2326	-0.1870
C	2.4431	5.1394	0.0282
C	3.0407	3.9278	0.2934
O	0.0876	1.7787	-0.1121
C	-1.7585	0.0491	-0.8867
C	-1.7439	0.7224	-2.2414
H	-1.1816	1.6662	-2.1800
H	-1.2317	0.0862	-2.9843
C	-3.1708	1.0121	-2.7385
H	-2.2782	-0.9216	-0.9128
H	-2.1930	0.6874	-0.1011
H	-3.7083	1.6594	-2.0293
H	-3.1454	1.5182	-3.7157
H	-3.7487	0.0814	-2.8495

H	4.1142	3.8939	0.4742
N	3.2547	6.3462	-0.0147
O	4.4738	6.2328	0.1912
O	2.6759	7.4179	-0.2572
H	0.6355	6.2275	-0.3242
H	4.0032	1.5766	0.8409
C	0.0860	-2.0619	-0.8882
C	-0.3353	-2.0193	0.4410
H	1.1088	-2.3533	-1.1409
H	-0.6364	-2.1405	-1.7038
H	0.3516	-2.2729	1.2525
H	-1.3970	-2.0530	0.6949
C	3.5494	-1.1850	0.9701
C	-1.2431	4.1931	-0.3394
C	4.4766	-1.7080	0.0466
C	5.4989	-2.5585	0.4971
C	5.5944	-2.8947	1.8520
C	3.6371	-1.5329	2.3330
C	4.6663	-2.3842	2.7662
C	4.4032	-1.3510	-1.4306
H	6.2255	-2.9552	-0.1961
H	6.3856	-3.5462	2.1924
C	2.6466	-0.9835	3.3493
H	4.7563	-2.6474	3.8095
H	3.4470	-0.8702	-1.6256
C	5.4966	-0.3666	-1.8504
C	4.4643	-2.5716	-2.3528
H	5.3671	-0.0985	-2.8991
H	5.4282	0.5342	-1.2401
H	6.4777	-0.8214	-1.7116
H	4.3116	-2.2573	-3.3855
H	5.4352	-3.0595	-2.2679
H	3.6799	-3.2760	-2.0750
H	1.7989	-0.5602	2.8145
C	2.0714	-2.0551	4.2795
C	3.2448	0.1347	4.2051
H	1.2994	-1.6144	4.9107
H	1.6307	-2.8546	3.6835
H	2.8577	-2.4665	4.9122
H	2.4825	0.5331	4.8749
H	4.0764	-0.2539	4.7933
H	3.6051	0.9346	3.5578
C	-1.7889	5.0144	-1.3566
C	-3.1828	5.0676	-1.5443
C	-4.0349	4.3079	-0.7377
C	-2.1208	3.4625	0.5001
C	-3.5093	3.5102	0.2820
H	-5.1031	4.3468	-0.8951
C	-0.9716	5.7152	-2.2662
C	-1.5304	6.5022	-3.2822
C	-2.9193	6.5848	-3.4242
C	-3.7436	5.8559	-2.5604
H	0.1029	5.6499	-2.2289
H	-0.8865	7.0365	-3.9652
H	-3.3513	7.1861	-4.2105
H	-4.8155	5.8934	-2.6886
C	-1.6521	2.7572	1.6274
C	-2.5320	2.0403	2.4492
C	-3.9037	2.0389	2.1756
C	-4.3918	2.7878	1.0993
H	-0.6088	2.7629	1.8997
H	-2.1510	1.4949	3.2999
H	-4.5843	1.4902	2.8097
H	-5.4550	2.8211	0.9116

Structure **6d-O**

E_{total} = -7.17671612 a.u.

Atom	X	Y	Z
Ni	0.0139	0.0276	0.0546
P	2.1982	0.0150	0.0961
C	2.9535	1.5466	0.0383
C	2.2628	2.7951	0.0294
C	0.8237	2.9026	0.1228
C	0.2430	4.2069	0.2781
C	1.0282	5.3306	0.1714
C	2.4149	5.2108	-0.0263
C	3.0228	3.9746	-0.0683
O	-0.0063	1.9087	0.0268
C	-1.7660	-0.0345	-0.7941
C	-1.1993	-1.3501	-0.9181
H	-1.6520	0.6924	-1.6022
H	-2.6338	0.1119	-0.1444
H	-0.4965	-1.5123	-1.7462
H	-1.8557	-2.2176	-0.7955
C	-0.4944	-1.8703	0.8441
C	-1.7719	-2.2033	1.5974
H	-2.3621	-1.2854	1.7518
H	-2.4006	-2.8952	1.0107
C	-1.4626	-2.8348	2.9584
H	0.0686	-2.7558	0.5176
H	0.1545	-1.2896	1.5344
H	-0.9019	-2.1394	3.6012
H	-2.3931	-3.1024	3.4809
H	-0.8629	-3.7507	2.8427
H	4.1051	3.9225	-0.1777

N	3.2205	6.4106	-0.1595
O	4.4422	6.2717	-0.3394
O	2.6386	7.5072	-0.0901
H	0.6289	6.3360	0.2999
H	4.0439	1.5996	0.0023
C	3.6222	-1.1530	0.3342
C	-1.2676	4.3032	0.5171
C	4.3514	-1.6133	-0.7808
C	5.4050	-2.5227	-0.5915
C	5.7398	-2.9610	0.6946
C	3.9542	-1.5999	1.6292
C	5.0170	-2.5007	1.8005
C	3.9891	-1.1645	-2.1893
H	5.9647	-2.8993	-1.4342
H	6.5515	-3.6598	0.8327
C	3.1730	-1.1375	2.8504
H	5.2802	-2.8524	2.7872
H	3.4648	-0.2133	-2.1211
C	5.2006	-0.9164	-3.0926
C	3.0545	-2.1509	-2.8927
H	4.8682	-0.4875	-4.0382
H	5.8813	-0.2182	-2.6049
H	5.7214	-1.8530	-3.2916
H	2.7774	-1.7609	-3.8723
H	3.5555	-3.1117	-3.0134
H	2.1533	-2.2883	-2.2946
H	2.4078	-0.4327	2.5338
C	2.4481	-2.2849	3.5579
C	4.0454	-0.4047	3.8721
H	1.8415	-1.8890	4.3726
H	1.8003	-2.7981	2.8471
H	3.1732	-2.9930	3.9594
H	3.4233	-0.0365	4.6882
H	4.8008	-1.0811	4.2723
H	4.5372	0.4399	3.3889
C	-2.0388	5.2948	-0.1419
C	-3.4302	5.3565	0.0646
C	-4.0645	4.4312	0.8977
C	-1.9196	3.4032	1.4015
C	-3.3161	3.4566	1.5620
H	-5.1350	4.4760	1.0367
C	-1.4761	6.1737	-1.0901
C	-2.2594	7.1348	-1.7433
C	-3.6303	7.2203	-1.4824
C	-4.2159	6.3191	-0.5875
H	-0.4374	6.1208	-1.3681
H	-1.8051	7.8025	-2.4605
H	-4.2368	7.9559	-1.9899
H	-5.2810	6.3589	-0.4122
C	-1.2012	2.5037	2.2174
C	-1.8608	1.6069	3.0681
C	-3.2563	1.6195	3.1534
C	-3.9804	2.5607	2.4139
H	-0.1232	2.4887	2.2251
H	-1.2898	0.9129	3.6673
H	-3.7677	0.9337	3.8126
H	-5.0551	2.6036	2.5138

Structure **6d-P**

E = -7.18553465 a.u.

Atom	X	Y	Z
Ni	0.000	0.000	0.000
P	2.093	0.000	0.000
C	2.944	1.475	0.000
C	2.322	2.756	-0.037
C	0.888	2.926	0.066
C	0.371	4.264	0.103
C	1.201	5.341	-0.104
C	2.583	5.150	-0.265
C	3.137	3.890	-0.203
O	0.031	1.949	0.072
C	-0.074	-1.968	-0.056
C	-1.440	-1.598	0.027
H	0.415	-2.373	0.837
H	0.316	-2.341	-1.009
H	-1.939	-1.716	0.992
H	-2.071	-1.803	-0.841
C	-2.136	0.423	-0.211
C	-2.222	0.891	-1.648
H	-1.304	1.426	-1.932
H	-2.321	0.026	-2.327
C	-3.426	1.825	-1.849
H	-3.060	-0.076	0.103
H	-1.912	1.223	0.503
H	-3.333	2.720	-1.218
H	-3.489	2.153	-2.897
H	-4.370	1.321	-1.589
H	4.216	3.783	-0.305
N	3.441	6.302	-0.478
O	4.663	6.105	-0.578
O	2.898	7.417	-0.551
H	0.835	6.367	-0.082
H	4.036	1.450	-0.009
C	3.372	-1.325	0.154
C	-1.126	4.469	0.334

C	4.004	-1.836	-0.998
C	5.000	-2.816	-0.865
C	5.360	-3.292	0.400
C	3.724	-1.815	1.428
C	4.724	-2.794	1.542
C	3.639	-1.331	-2.386
H	5.502	-3.207	-1.738
H	6.130	-4.044	0.496
C	3.051	-1.282	2.685
H	5.017	-3.167	2.512
H	2.737	-0.728	-2.313
C	4.727	-0.442	-2.992
C	3.323	-2.458	-3.374
H	4.395	-0.060	-3.958
H	4.923	0.397	-2.324
H	5.644	-1.017	-3.126
H	2.982	-2.031	-4.318
H	4.212	-3.061	-3.555
H	2.535	-3.089	-2.963
H	2.134	-0.772	2.396
C	2.635	-2.380	3.668
C	3.921	-0.266	3.428
H	2.069	-1.939	4.488
H	2.008	-3.109	3.154
H	3.516	-2.879	4.071
H	3.375	0.127	4.286
H	4.838	-0.746	3.771
H	4.174	0.555	2.758
C	-1.857	5.391	-0.455
C	-3.237	5.560	-0.240
C	-3.897	4.815	0.741
C	-1.798	3.755	1.357
C	-3.183	3.917	1.539
H	-4.960	4.943	0.892
C	-1.264	6.085	-1.529
C	-2.009	6.975	-2.314
C	-3.370	7.170	-2.056
C	-3.985	6.451	-1.025
H	-0.231	5.937	-1.797
H	-1.534	7.502	-3.129
H	-3.947	7.850	-2.665
H	-5.042	6.577	-0.846
C	-1.100	2.948	2.279
C	-1.779	2.245	3.283
C	-3.167	2.360	3.404
C	-3.866	3.210	2.540
H	-0.026	2.860	2.248
H	-1.227	1.620	3.970
H	-3.692	1.822	4.180
H	-4.932	3.332	2.659

Structure 6e

E_{total} = -7.22178268 a.u.

Atom	X	Y	Z
Ni	0.0124	0.0008	-0.0517
P	2.1446	0.0279	-0.1113
C	2.8720	1.5475	0.1571
C	2.1534	2.7552	0.3972
C	0.7121	2.8182	0.5222
C	0.1184	4.0786	0.8696
C	0.8844	5.2189	0.9358
C	2.2748	5.1506	0.7438
C	2.8978	3.9456	0.5072
O	-0.1121	1.8373	0.2890
C	-1.9361	-0.2818	-0.0939
C	-1.3570	-1.5733	-0.3969
H	-2.3585	0.3139	-0.9100
H	-2.3558	-0.0977	0.8987
H	-0.0891	-1.5367	-0.2773
H	-1.5059	-2.3264	0.3952
C	-1.5247	-2.1479	-1.8035
C	-2.9291	-2.7186	-2.0153
H	-3.1261	-3.4907	-1.2502
H	-3.6718	-1.9194	-1.8504
C	-3.1072	-3.3179	-3.4084
H	-1.3233	-1.3531	-2.5417
H	-0.7783	-2.9419	-1.9760
H	-2.3921	-4.1371	-3.5822
H	-4.1213	-3.7230	-3.5382
H	-2.9443	-2.5585	-4.1889
H	3.9805	3.9260	0.3912
N	3.0669	6.3660	0.8241
O	4.2970	6.2697	0.6772
O	2.4635	7.4321	1.0341
H	0.4617	6.1863	1.2040
H	3.9610	1.6261	0.1359
C	3.5584	-1.1598	-0.2236
C	-1.3892	4.1336	1.1241
C	3.9806	-1.6281	-1.4843
C	5.0428	-2.5435	-1.5639
C	5.6940	-2.9744	-0.4029
C	4.2078	-1.6014	0.9475
C	5.2803	-2.5020	0.8472
C	3.2815	-1.1742	-2.7579
H	5.3695	-2.9258	-2.5191
H	6.5144	-3.6735	-0.4717
C	3.7758	-1.1172	2.3241
H	5.7931	-2.8416	1.7349
H	2.8010	-0.2175	-2.5611
C	4.2298	-0.9376	-3.9370
C	2.1914	-2.1509	-3.2034
H	3.6748	-0.5045	-4.7695
H	5.0182	-0.2468	-3.6372
H	4.6745	-1.8791	-4.2589
H	1.6723	-1.7519	-4.0751
H	2.6381	-3.1129	-3.4554
H	1.4760	-2.2891	-2.3931
H	2.8494	-0.5561	2.2241
C	3.4833	-2.2603	3.2996
C	4.8005	-0.1796	2.9663
H	3.0974	-1.8534	4.2346
H	2.7369	-2.9258	2.8654
H	4.3942	-2.8231	3.5032
H	4.4177	0.1854	3.9196
H	5.7373	-0.7118	3.1329
H	4.9815	0.6685	2.3058
C	-2.1704	5.1884	0.5890
C	-3.5579	5.2251	0.8234
C	-4.1758	4.2196	1.5721
C	-2.0220	3.1462	1.9220
C	-3.4138	3.1858	2.1225
H	-5.2427	4.2507	1.7395
C	-1.6189	6.1662	-0.2638
C	-2.4121	7.1895	-0.8001
C	-3.7801	7.2419	-0.5144
C	-4.3531	6.2499	0.2882
H	-0.5817	6.1458	-0.5533
H	-1.9680	7.9325	-1.4461
H	-4.3939	8.0264	-0.9318
H	-5.4153	6.2701	0.4834
C	-1.2830	2.1710	2.6230
C	-1.9220	1.2074	3.4145
C	-3.3145	1.2163	3.5433
C	-4.0573	2.2170	2.9076
H	-0.2055	2.1506	2.5903
H	-1.3371	0.4618	3.9327
H	-3.8093	0.4770	4.1557
H	-5.1286	2.2519	3.0418

Structure 6h

E_{total} = -7.17534679 a.u.

Atom	X	Y	Z
Ni	-0.0057	0.0216	-0.0073
P	2.2352	-0.0032	0.0032
C	3.0088	1.5151	0.0058
C	2.3347	2.7640	0.1551
C	1.0310	2.8213	0.7943
C	0.5724	4.1125	1.2334
C	1.2075	5.2551	0.8056
C	2.3936	5.1753	0.0515
C	2.9796	3.9539	-0.2159
O	0.2959	1.7846	1.0029
C	-0.0014	-1.2445	1.7654
C	-1.3255	-0.9864	1.4796
H	-1.4215	0.3276	-0.0910
H	-1.8673	-1.7232	0.8783
C	-2.1616	-0.0331	2.2894
H	0.4693	-2.1693	1.4280
H	0.5054	-0.6821	2.5530
H	-1.5828	0.8590	2.5529
H	-3.0635	0.2827	1.7495
H	-2.4807	-0.5334	3.2193
H	3.9394	3.9290	-0.7308
N	3.0391	6.3948	-0.3914
O	4.0997	6.2939	-1.0338
O	2.4907	7.4746	-0.1062
H	0.8670	6.2499	1.0906
H	4.0951	1.5444	-0.1124
C	-0.3454	-0.9499	-1.7772
C	-0.2081	0.4245	-2.0162
H	-1.3373	-1.4085	-1.7721
H	0.4868	-1.6331	-1.9633
H	-1.0894	1.0423	-2.1975
H	0.7380	0.8404	-2.3698
C	3.6288	-1.2181	0.1665
C	-0.6559	4.1803	2.1394
C	4.1629	-1.8443	-0.9777
C	5.2294	-2.7470	-0.8398
C	5.7613	-3.0275	0.4237
C	4.1653	-1.4990	1.4400
C	5.2320	-2.4039	1.5588
C	3.6215	-1.5470	-2.3677
H	5.6529	-3.2280	-1.7090
H	6.5840	-3.7203	0.5219
C	3.6244	-0.8236	2.6925
H	5.6574	-2.6217	2.5272
H	2.7472	-0.9077	-2.2740
C	4.6271	-0.7952	-3.2421
C	3.1653	-2.8026	-3.1150
H	4.1700	-0.5523	-4.2016
H	4.9222	0.1280	-2.7428
H	5.5100	-1.4127	-3.4086
H	2.7119	-2.5187	-4.0649
H	4.0167	-3.4562	-3.3047
H	2.4286	-3.3353	-2.5132
H	2.7374	-0.2535	2.4290
C	3.1942	-1.8168	3.7749
C	4.6168	0.1668	3.3045
H	2.7352	-1.2779	4.6041
H	2.4683	-2.5155	3.3586
H	4.0587	-2.3704	4.1413
H	4.1570	0.6673	4.1571
H	5.5125	-0.3600	3.6342
H	4.8915	0.9127	2.5584
C	-1.6713	5.1424	1.9166
C	-2.7912	5.1907	2.7679
C	-2.9127	4.2888	3.8293
C	-0.7674	3.3033	3.2475
C	-1.9052	3.3514	4.0731
H	-3.7795	4.3277	4.4730
C	-1.6490	6.0038	0.8014
C	-2.6748	6.9340	0.5863
C	-3.7567	7.0044	1.4700
C	-3.8184	6.1223	2.5540
H	-0.8623	5.9580	0.0669
H	-2.6361	7.5897	-0.2711
H	-4.5509	7.7168	1.3022
H	-4.6685	6.1546	3.2197
C	0.2843	2.4403	3.6207
C	0.1613	1.5831	4.7223
C	-1.0070	1.5929	5.4912
C	-2.0332	2.4894	5.1731
H	1.2197	2.4260	3.0854
H	0.9735	0.9201	4.9820
H	-1.1031	0.9358	6.3429
H	-2.9183	2.5271	5.7911

Structure 6i

E_{total} = -7.17553427 a.u.

Atom	X	Y	Z
Ni	0.0490	0.0868	0.0686
P	2.3397	-0.0114	0.2670
C	3.1140	1.5101	0.2275
C	2.4687	2.7833	0.1764
C	1.0676	2.9483	0.5237
C	0.5614	4.2922	0.6217
C	1.3437	5.3617	0.2524
C	2.6832	5.1725	-0.1304
C	3.2438	3.9119	-0.1379
O	0.2622	1.9678	0.7458
C	-0.1606	-0.6410	-1.9438
C	0.1417	0.7033	-1.9806
H	-1.1899	-0.9848	-2.0557
H	0.6150	-1.3961	-2.0795
H	-0.6452	1.4515	-2.0917
H	1.1644	1.0483	-2.1479
C	-0.5934	-1.6918	0.9553
C	-0.6151	-0.6997	1.9265
H	-1.3570	0.3538	-0.0918
H	-1.5537	-0.1600	2.0906
C	0.3958	-0.5865	3.0234
H	-1.5047	-1.9774	0.4280
H	0.2195	-2.4242	0.9397
H	1.2660	-1.2292	2.8277
H	0.7413	0.4477	3.1585
H	-0.0616	-0.9126	3.9743
H	4.2948	3.8044	-0.4038
N	3.4908	6.3209	-0.4879
O	2.9489	7.4401	-0.4615
O	4.6775	6.1217	-0.8011
H	0.9806	6.3878	0.3022
H	4.2069	1.5286	0.2262
C	3.7591	-1.1675	0.6238
C	-0.8885	4.5041	1.0613
C	4.1780	-2.0863	-0.3613
C	5.2410	-2.9628	-0.0915
C	5.9003	-2.9188	1.1407
C	4.4247	-1.1255	1.8695
C	5.4958	-2.0000	2.1140
C	3.4927	-2.1588	-1.7168
H	5.5617	-3.6782	-0.8339
H	6.7216	-3.5914	1.3393
C	4.0236	-0.1451	2.9631
H	6.0183	-1.9720	3.0586
H	2.8428	-1.2941	-1.8246
C	4.4702	-2.1067	-2.8940
C	2.6198	-3.4069	-1.8639
H	3.9127	-2.0671	-3.8300
H	5.0911	-1.2145	-2.8109
H	5.1068	-2.9915	-2.8946
H	2.1066	-3.3857	-2.8255
H	3.2395	-4.3019	-1.8046
H	1.8797	-3.4284	-1.0636
H	3.0959	0.3422	2.6745
C	3.7639	-0.8206	4.3130

C	5.0630	0.9572	3.1821
H	3.3676	-0.0890	5.0174
H	3.0389	-1.6244	4.1870
H	4.6908	-1.2339	4.7104
H	4.6956	1.6654	3.9251
H	5.9989	0.5206	3.5313
H	5.2422	1.4843	2.2455
C	-1.7240	5.4108	0.3617
C	-3.0589	5.5950	0.7683
C	-3.5727	4.8797	1.8535
C	-1.4099	3.8185	2.1872
C	-2.7536	3.9981	2.5635
H	-4.6006	5.0213	2.1544
C	-1.2920	6.0746	-0.8047
C	-2.1397	6.9516	-1.4948
C	-3.4472	7.1641	-1.0465
C	-3.9085	6.4738	0.0793
H	-0.3115	5.9117	-1.2195
H	-1.7862	7.4552	-2.3824
H	-4.1037	7.8351	-1.5805
H	-4.9282	6.6117	0.4081
C	-0.5888	3.0374	3.0251
C	-1.1151	2.3825	4.1469
C	-2.4709	2.5108	4.4641
C	-3.2859	3.3318	3.6777
H	0.4701	2.9445	2.8439
H	-0.4707	1.7850	4.7745
H	-2.8773	2.0087	5.3297
H	-4.3230	3.4686	3.9472