N-H activation in N-nitropropionamide: Coordination chemistry of a primary nitroamide.

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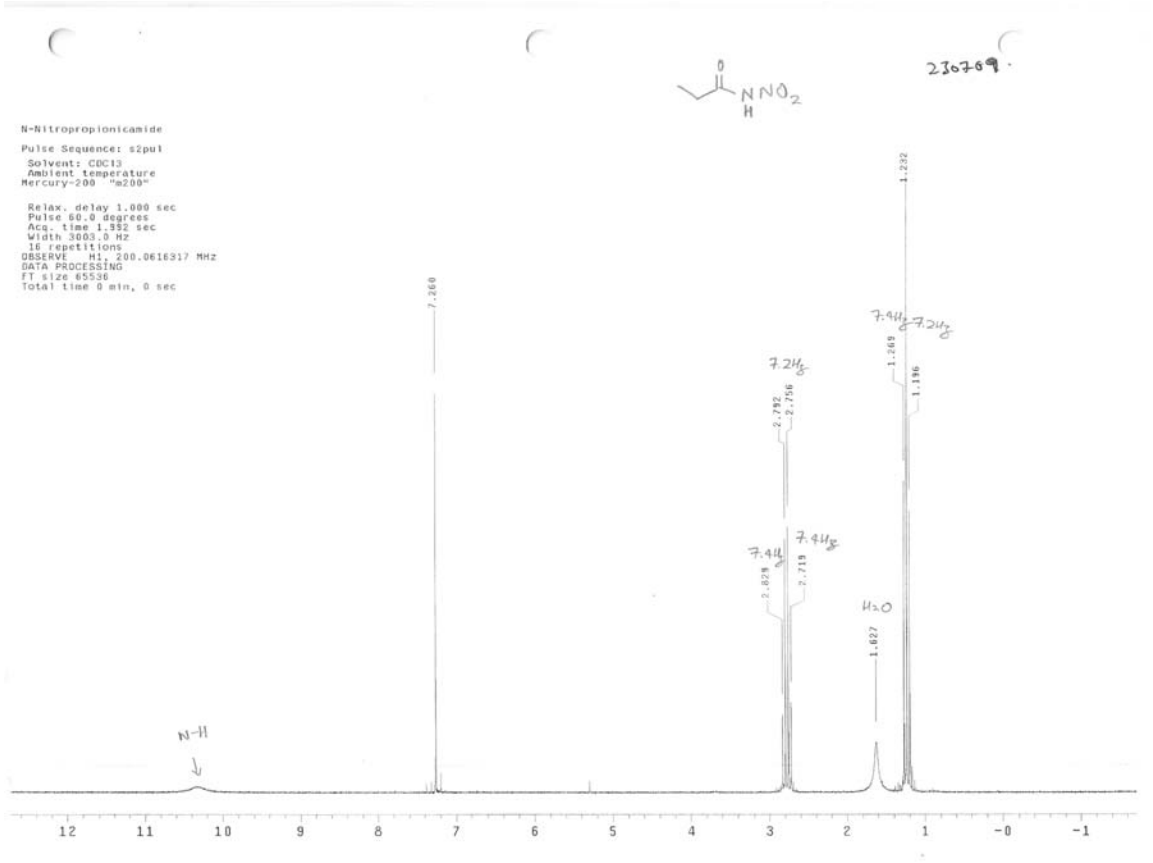
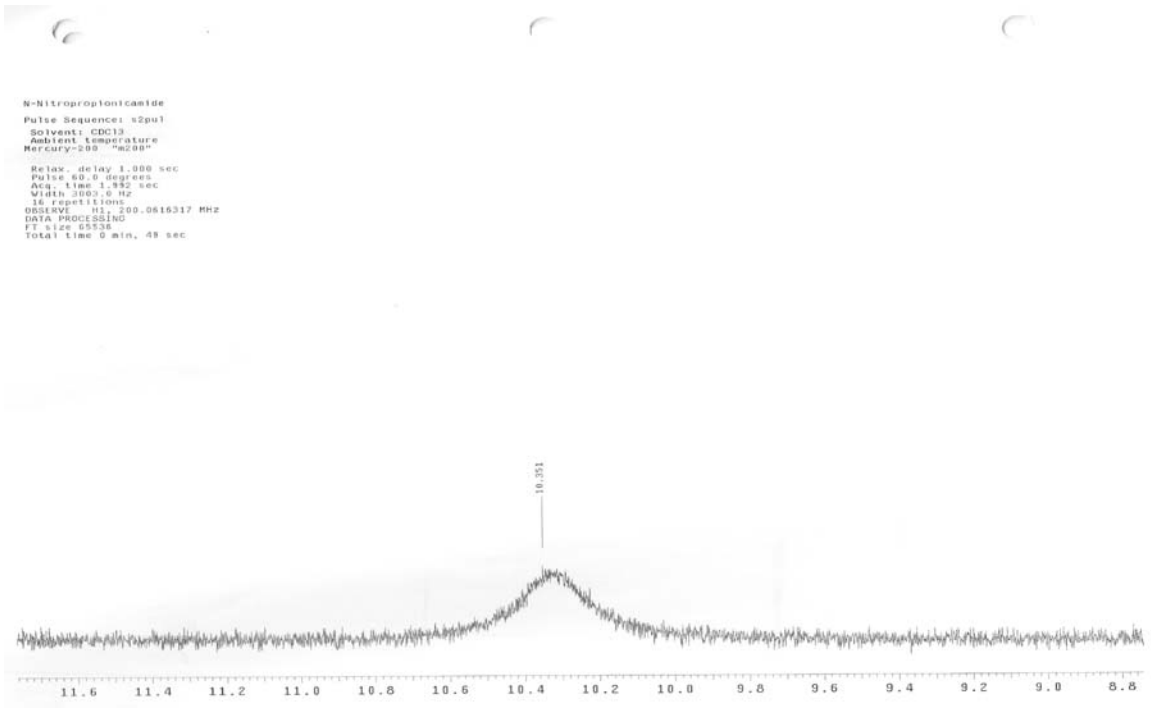
1. NMR spectrums of N-nitropropionamide, 1.

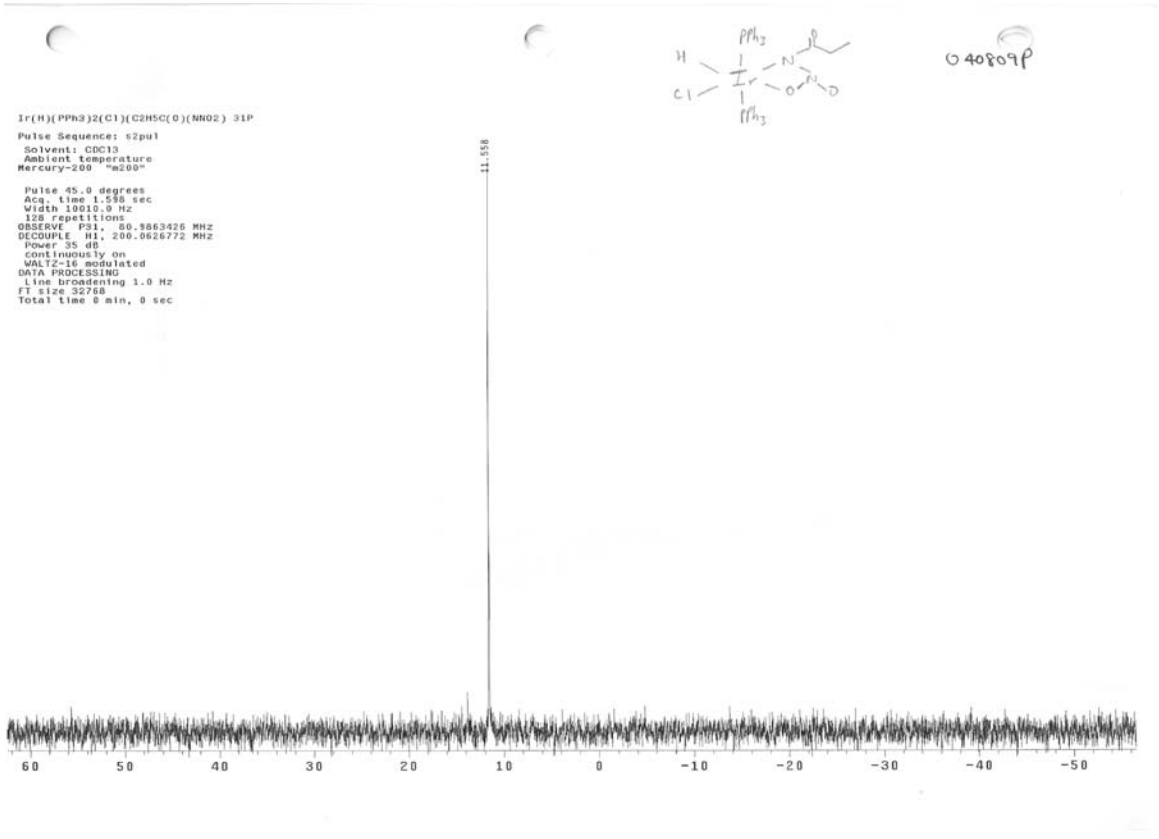
^{1}H
NMR



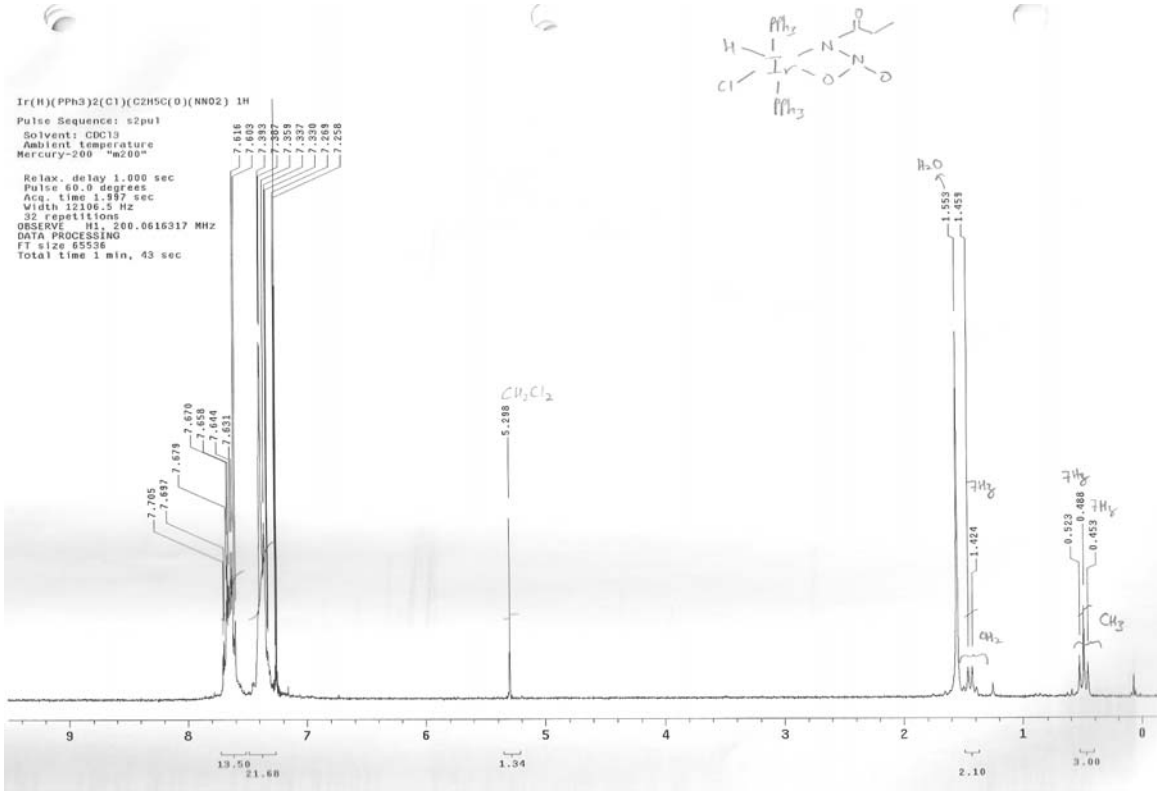


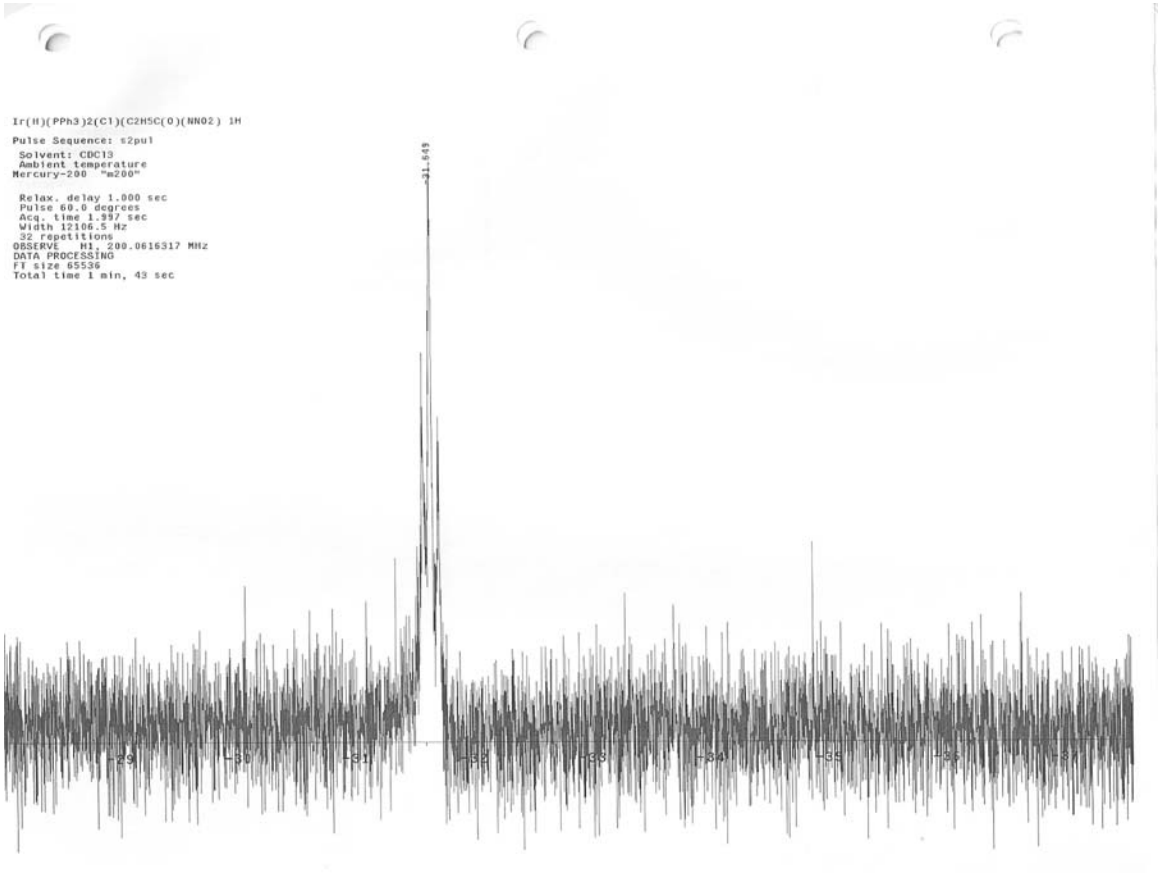
2. NMR spectrums of *trans*-Ir(η^2-$C_2H_5C(O)NNO_2$)(H)(Cl)(PPh_3)$_2$, 2.

^{31}P NMR



^{1}H NMR


Ir(H)(PPh3)2(Cl)(C2H5C(O)(NNO2) 1H
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-200 "m200"
Relax. delay 1.000 sec
Pulse 60.0 degrees
Acq. time 1.997 sec
Width 12106.5 Hz
32 repetitions
OBSERVE H1, 200.0616317 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 43 sec
7.705
7.697
7.679
7.670
7.658
7.644
7.631
7.616
7.603
7.393
7.387
7.359
7.337
7.330
7.284
7.258
5.298
1.553
1.459
1.424
0.523
0.488
0.453
13.50
21.60
1.34
2.10
3.00


Ir(H)(PPh3)2(Cl)(C2H5C(O)(NNO2) 1H
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-200 "m200"
Relax. delay 1.000 sec
Pulse 60.0 degrees
Acq. time 1.997 sec
Width 12106.5 Hz
32 repetitions
OBSERVE H1, 200.0616317 MHz
DATA PROCESSING
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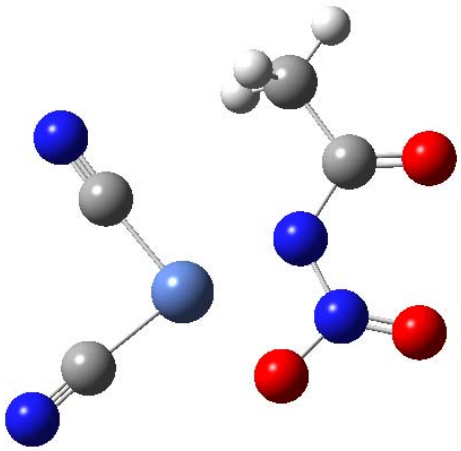
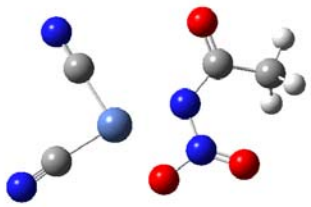
Total time 1 min, 43 sec
-31.649

3. Geometry of optimized nitramide complexes of $Ni(CN)_2$



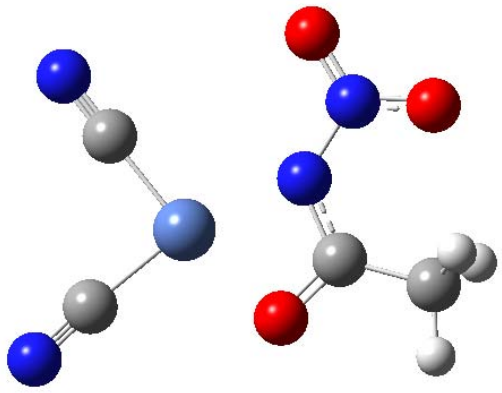
Isomer A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.918935	-0.104045	0.002253
2	6	0	-2.710398	-0.581118	-0.006537
3	6	0	-1.373883	1.684354	-0.005324
4	7	0	-3.814725	-0.944609	-0.011818
5	7	0	-1.590897	2.826881	-0.013774
6	7	0	1.050249	-0.098451	0.011704
7	7	0	1.107199	-1.444874	0.009743
8	6	0	2.224114	0.677037	-0.010025
9	6	0	1.918271	2.156248	0.039398
10	1	0	1.255217	2.449124	-0.776134
11	1	0	1.388038	2.408319	0.960286
12	1	0	2.858909	2.702353	-0.015699
13	8	0	3.353020	0.233881	-0.061346
14	8	0	2.077188	-2.160540	0.017671
15	8	0	-0.103130	-1.903128	0.005227



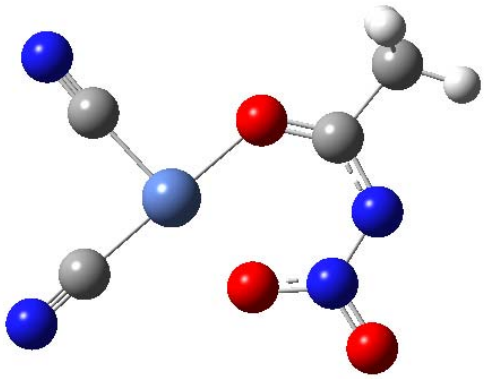
Isomer B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	0.968225	-0.080012	-0.024288
2	6	0	2.725563	-0.652821	0.073414
3	6	0	1.526949	1.675096	0.038261
4	7	0	3.800763	-1.091411	0.132825
5	7	0	1.868151	2.784372	0.102240
6	7	0	-1.004955	0.006904	-0.112884
7	7	0	-1.122025	-1.321834	-0.091134
8	6	0	-2.126553	0.864065	-0.052976
9	6	0	-3.449257	0.357826	0.494864
10	1	0	-3.978734	-0.217483	-0.266614
11	1	0	-3.318968	-0.296941	1.357518
12	1	0	-4.036682	1.234988	0.764531
13	8	0	-1.984033	2.015002	-0.395817
14	8	0	-2.143404	-1.986350	-0.149168
15	8	0	0.048729	-1.852582	-0.044274



Isomer C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.949429	-0.117848	0.000000
2	6	0	-2.653385	-0.833382	0.000002
3	6	0	-1.669475	1.578091	0.000000
4	7	0	-3.689637	-1.360845	0.000004
5	7	0	-2.104475	2.655969	0.000000
6	7	0	1.029345	0.108975	-0.000001
7	7	0	2.059183	1.023190	0.000001
8	6	0	1.221443	-1.231747	-0.000002
9	6	0	2.502870	-2.009325	-0.000005
10	1	0	3.105155	-1.757827	-0.873980
11	1	0	3.105147	-1.757846	0.873981
12	1	0	2.244785	-3.068101	-0.000016
13	8	0	0.114007	-1.832573	-0.000001
14	8	0	3.231935	0.618864	0.000014
15	8	0	1.736471	2.197544	-0.000008

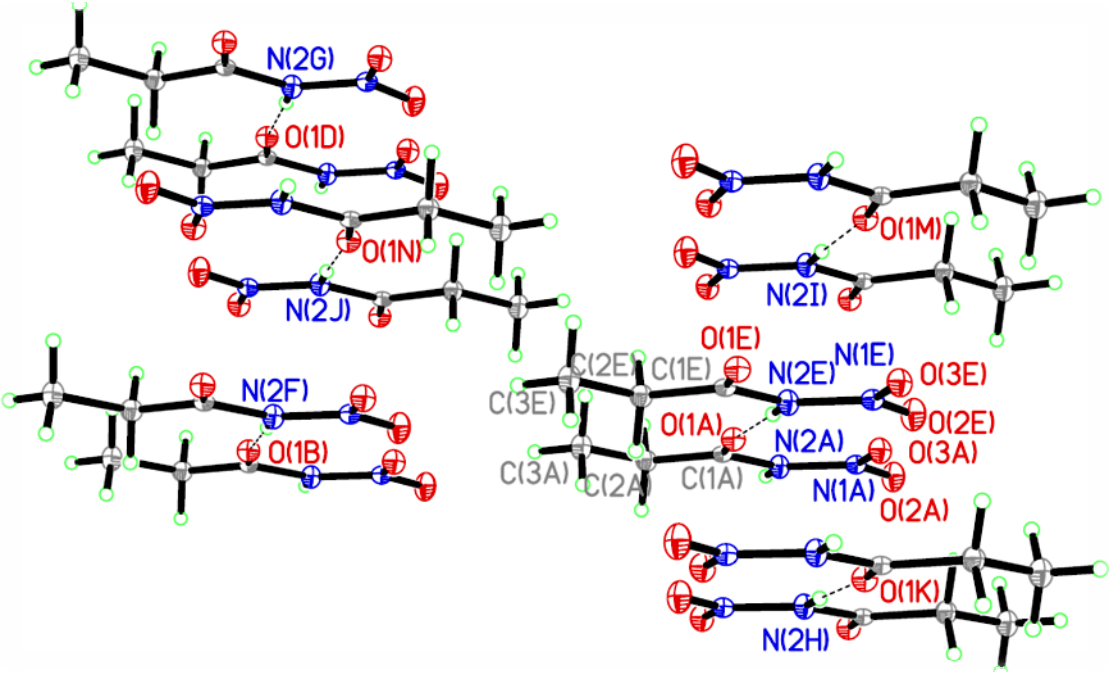


Isomer D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	28	0	-0.866315	0.032239	0.004221
2	6	0	-2.117817	1.394993	0.005799
3	6	0	-2.261056	-1.189832	0.004688
4	7	0	-2.858857	2.290095	-0.019515
5	7	0	-3.105598	-1.988294	0.001865
6	7	0	2.435032	-0.188944	-0.006756
7	7	0	1.714031	-1.336963	-0.004294
8	6	0	1.802588	1.000370	-0.000536
9	6	0	2.756364	2.173059	0.002782
10	1	0	3.792084	1.843179	-0.048055
11	1	0	2.522107	2.822292	-0.844001
12	1	0	2.594373	2.754881	0.913969
13	8	0	0.578772	1.274701	0.006809
14	8	0	0.439968	-1.400810	-0.005828
15	8	0	2.353202	-2.377120	-0.002930

4. Crystal Packing Diagrams of 1 and 2.

Packing for **1**.



Packing for **2**.