

## ***Supporting Information***

# **Structural disassembly, dangling bond and hydrogen storage of $\text{Ni}_n\text{S}_n$ ( $n=2-10$ ) clusters**

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and Meng Zhang<sup>1\*</sup>

### AUTHOR INFORMATION

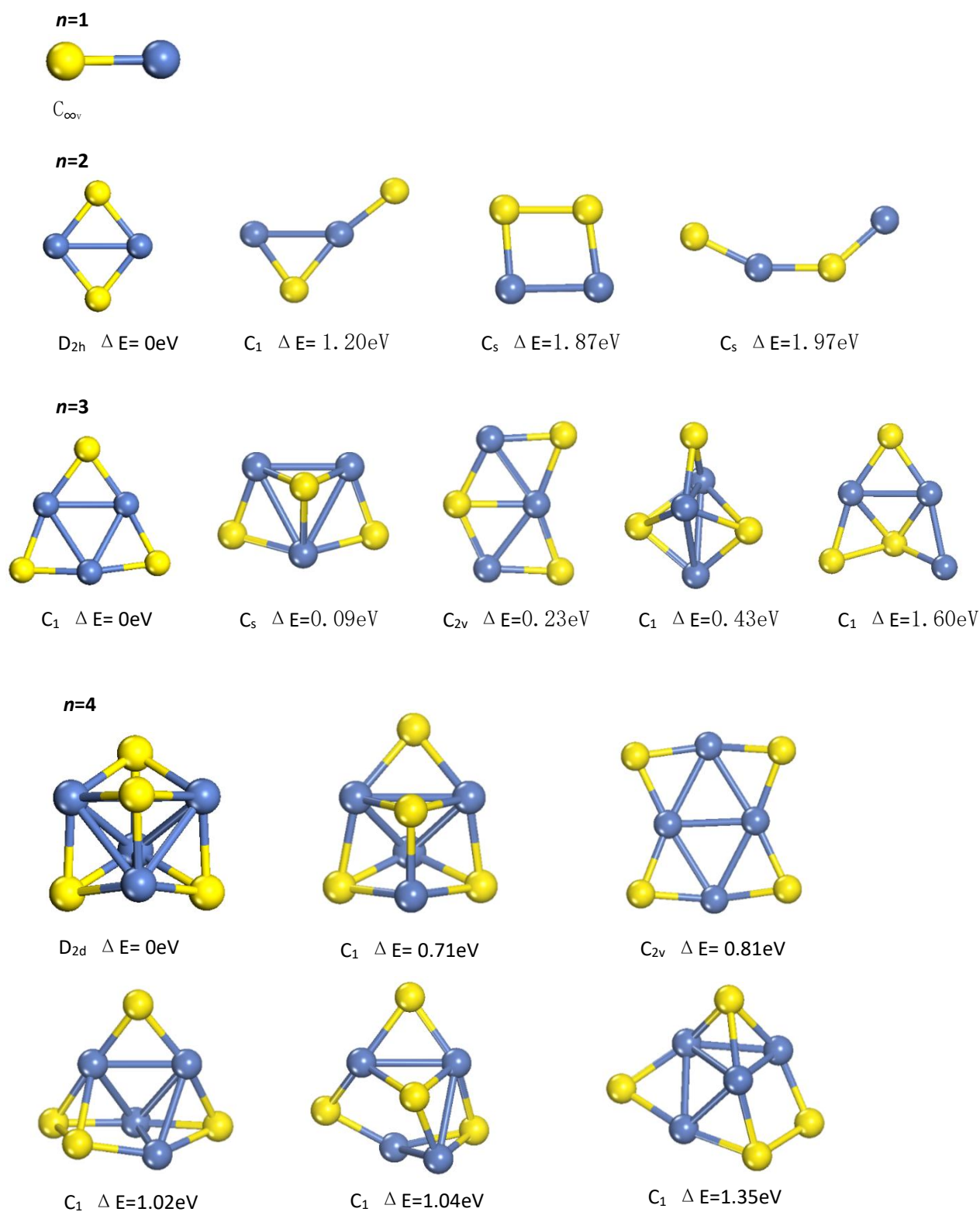
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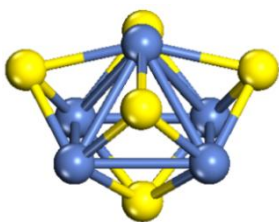
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1. Figure S1. Lowest-energy structures and low-lying isomers with relative energies (in eV) of  $\text{Ni}_n\text{S}_n$  ( $n=1-10$ ) clusters. Yellow and blue circles represent nickel and sulphur atoms, respectively. The symmetry type is given at 0.1 Å tolerances.
2. Figure S2. The shortest and average Ni-S bond lengths in Angstroms of the  $\text{Ni}_n\text{S}_n$  clusters ( $n=1-10$ ) and  $\beta$ -NiS bulk phase for the lowest-energy structures.
3. Table S1. Calculated bond distance  $d$  (Å) and vibrational frequency  $\omega_e$  ( $\text{cm}^{-1}$ ) of the  $\text{S}_2$  and  $\text{Ni}_2$  dimers optimized using different density functional methods.
4. Table S2. The x,y,z coordinates of the proposed structures of the neutral  $\text{Ni}_n\text{S}_n$  ( $n=1-10$ ) clusters collected in Figure S1.
5. Table S3. The x,y,z coordinates of the proposed structures of the  $\text{Ni}_4\text{S}_4$  cluster with adsorbed hydrogen atoms.

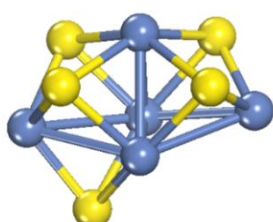
Figure S1. Lowest-energy structures and low-lying isomers with relative energies (in eV) of  $\text{Ni}_n\text{S}_n$  ( $n=1-10$ ) clusters. Yellow and blue circles represent nickel and sulphur atoms, respectively. The symmetry is given at 0.1 Å tolerances.



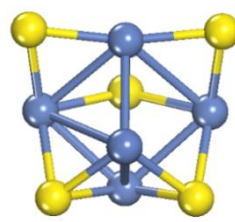
***n=5***



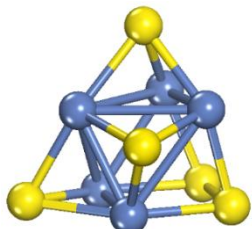
$C_{4v}$   $\Delta E = 0\text{eV}$



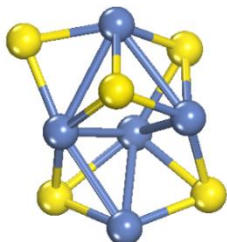
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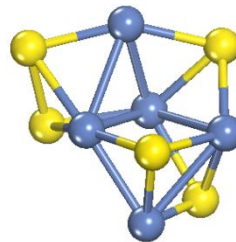
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$C_1$   $\Delta E = 1.31\text{eV}$

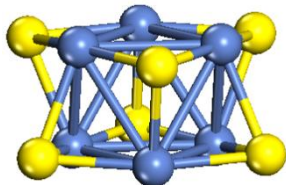


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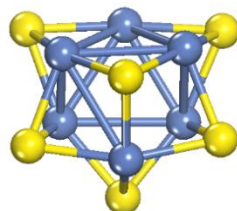


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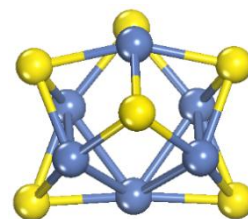
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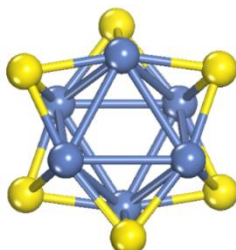
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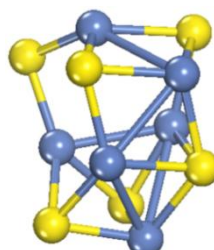
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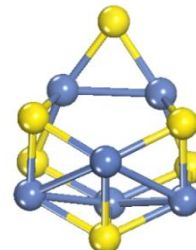
$C_{2v}$   $\Delta E = 0.42\text{eV}$



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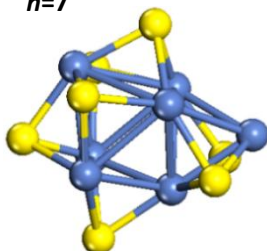


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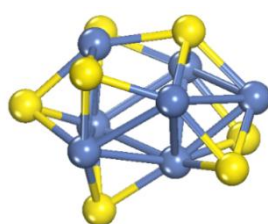


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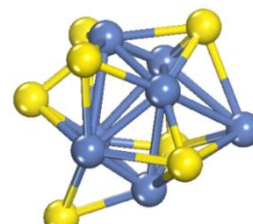
***n=7***



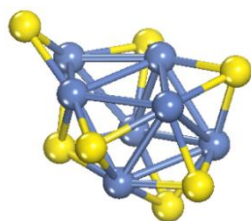
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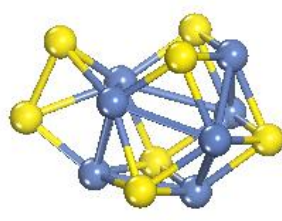
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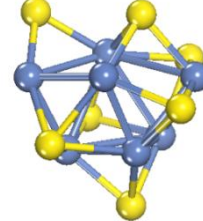
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$C_1$   $\Delta E = 0.40\text{eV}$

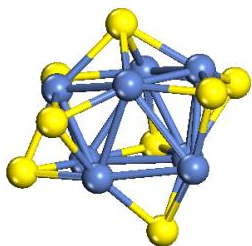


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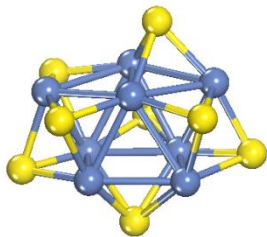


$C_1$   $\Delta E = 0.72\text{eV}$

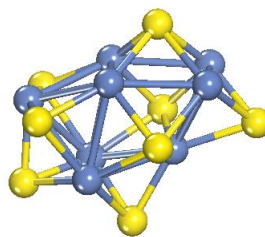
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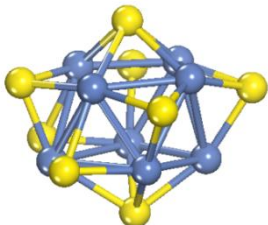
$C_s \Delta E= 0\text{eV}$



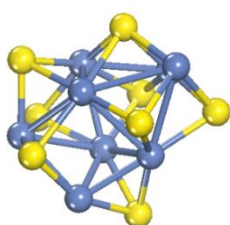
$C_1 \Delta E= 0.04\text{eV}$



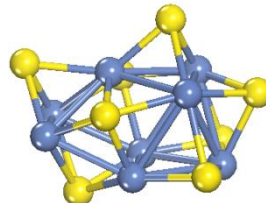
$C_s \Delta E= 0.09\text{eV}$



$C_s \Delta E= 0.17\text{eV}$

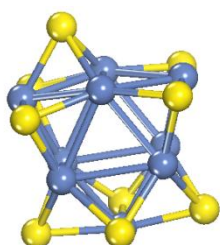


$C_1 \Delta E= 0.36\text{eV}$

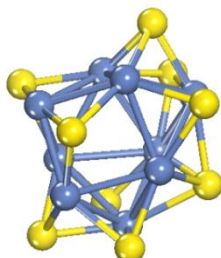


$C_s \Delta E= 0.38\text{eV}$

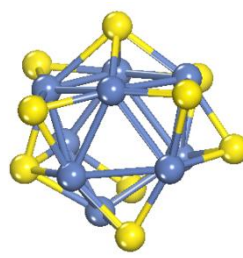
**$n=9$**



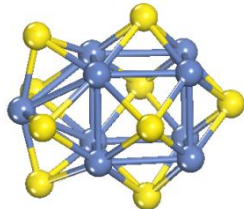
$C_s \Delta E= 0\text{eV}$



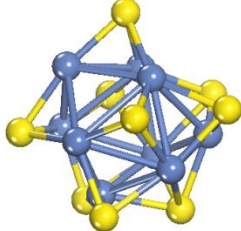
$C_s \Delta E= 0.23\text{eV}$



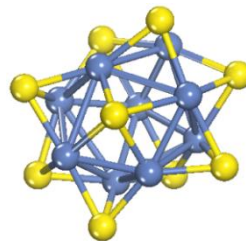
$C_1 \Delta E= 0.34\text{eV}$



$C_{4v} \Delta E= 0.36\text{eV}$

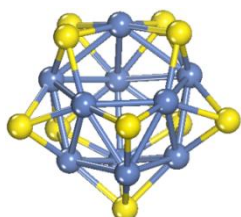


$C_s \Delta E= 0.48\text{eV}$

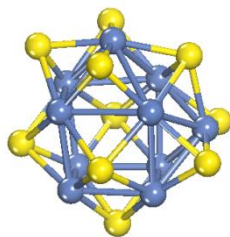


$C_s \Delta E= 0.49\text{eV}$

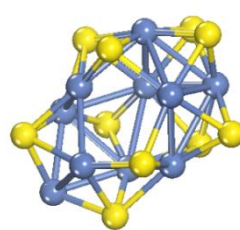
**$n=10$**



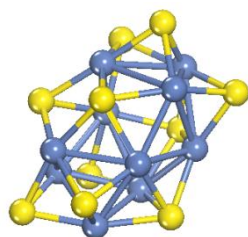
$C_s \Delta E= 0\text{eV}$



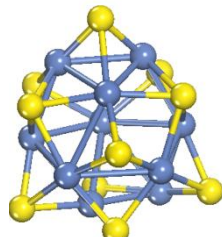
$C_s \Delta E= 0.07\text{eV}$



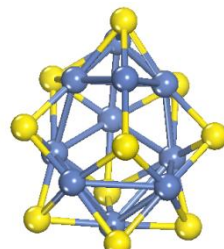
$C_1 \Delta E= 0.39\text{eV}$



$C_1 \Delta E= 0.48\text{eV}$



$C_1 \Delta E= 0.49\text{eV}$



$C_s \Delta E= 0.50\text{eV}$

Figure S2. The shortest and average Ni-S bond lengths in Angstroms of the  $\text{Ni}_n\text{S}_n$  clusters ( $n=1-10$ ) and  $\beta$ -NiS bulk phase for the lowest-energy structures.

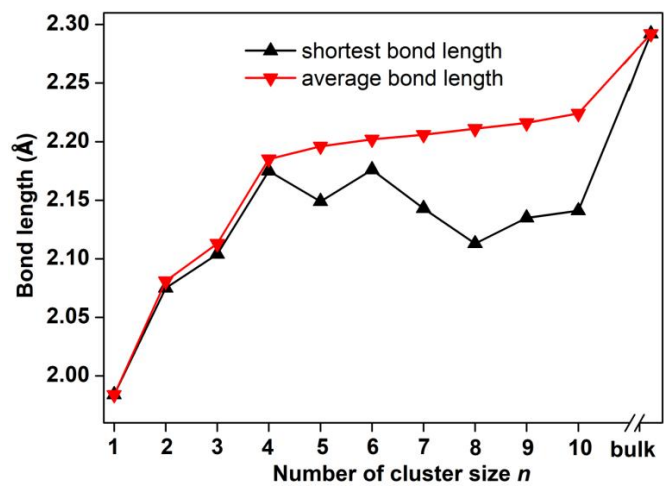


Table S1. Calculated bond distance  $d$  (Å) and vibrational frequency  $\omega_e$  (cm<sup>-1</sup>) of the S<sub>2</sub> and Ni<sub>2</sub> dimers optimized using different density functional methods. a) Ref. [70-72].

methods	S <sub>2</sub>		Ni <sub>2</sub>	
	$d$	$\omega_e$	$d$	$\omega_e$
BP	1.937	691.1	2.102	333.8
BLYP	1.958	656.6	2.144	334.1
PW91	1.937	690.6	2.096	338.9
PBE	1.936	694.6	2.112	333.2
expt. <sup>a)</sup>	1.89	725.65	2.15	325

Table S2. The x,y,z coordinates of the proposed structures of the neutral Ni<sub>n</sub>S<sub>n</sub> (n=1-10) clusters collected in Figure S1.

**Coordinates (Angstroms) of Ni<sub>n</sub>S<sub>n</sub> (n=1-10) Clusters**

System	ATOM	X	Y	Z
-----				
Isomer 1-1				
1	Ni	9.265021	14.109239	10.805929
2	S	7.616033	13.515477	11.735125
Isomer 2-1				
1	Ni	9.154717	13.361306	11.045676
2	S	7.465848	14.414645	11.688243
3	Ni	8.594415	14.106393	13.402159
4	S	10.283316	13.053040	12.759619
Isomer 2-2				
1	Ni	8.969493	13.637448	11.871735
2	S	7.244997	14.204939	11.043060
3	Ni	11.249345	14.189519	11.789014
4	S	10.505717	12.552311	12.801612
Isomer 2-3				
1	S	-5.981820	3.391323	-0.015709
2	Ni	-4.601389	1.855476	0.014455
3	S	-4.267577	4.710117	-0.022573
4	Ni	-2.829480	3.264333	0.017132
Isomer 2-4				
1	S	-5.585594	3.712296	-0.115136
2	Ni	-4.154350	2.343397	0.054792
3	S	-2.684746	1.004953	0.214320
4	Ni	-6.988504	5.057695	-0.280448
Isomer 3-1				
1	Ni	9.002523	13.232218	11.648298
2	S	7.241735	14.291349	11.180035
3	Ni	8.939850	12.284323	13.917584
4	S	10.674128	12.708754	12.802974
5	Ni	6.818710	12.857800	12.702619
6	S	7.009376	11.534940	14.363865
Isomer 3-2				
1	Ni	9.672146	12.872057	11.385737
2	S	7.978020	14.506128	11.618272
3	Ni	8.724423	14.131720	13.522622
4	S	9.373399	12.171018	13.357294

5	Ni	9.801164	15.502029	11.713529
6	S	11.068568	14.263712	10.638397
Isomer 3-3				
1	Ni	8.973648	13.385044	11.801304
2	S	7.219590	14.424934	11.290619
3	Ni	10.925749	14.728261	11.590347
4	S	10.805161	12.910542	12.729288
5	Ni	8.936567	15.354653	10.441845
6	S	10.667970	16.599383	10.608993
Isomer 3-4				
1	Ni	9.045722	13.102880	11.102432
2	S	7.747792	14.836127	11.666720
3	Ni	8.410171	13.569190	13.392359
4	S	10.529530	13.711327	12.707851
5	Ni	9.776658	15.442850	11.730438
6	S	7.765795	11.843304	12.233677
Isomer 3-5				
1	Ni	8.879500	13.326354	11.986141
2	S	7.491670	14.506874	10.843580
3	Ni	11.039060	14.306672	11.585453
4	S	10.693076	12.606131	12.821852
5	Ni	10.530130	16.009144	10.126948
6	S	9.242562	15.518421	11.679428
Isomer 4-1				
1	Ni	9.271726	13.837066	11.542523
2	S	7.127505	13.447304	11.569499
3	Ni	7.550419	14.846732	13.197053
4	S	9.673580	15.329356	13.092387
5	Ni	8.067293	12.010269	12.932587
6	S	7.344248	13.195097	14.623835
7	Ni	9.474124	13.604035	14.418271
8	S	10.217345	12.316953	12.804874
Isomer 4-2				
1	Ni	8.446629	13.379197	11.209631
2	S	8.264735	15.601860	11.073540
3	Ni	10.062010	13.354503	13.523576
4	S	10.671989	13.304243	11.377897
5	Ni	10.232574	15.341030	11.889435
6	S	7.933756	13.124531	13.315334
7	Ni	8.245392	15.302671	13.273473
8	S	9.587375	14.915034	14.923317

Isomer 4-3				
1	Ni	11.853375	8.850724	7.983161
2	Ni	8.846681	11.848623	7.985096
3	Ni	11.203001	11.201972	7.806799
4	Ni	9.487590	9.487539	7.800213
5	S	13.131903	10.440585	7.538804
6	S	7.561041	10.269812	7.537853
7	S	10.440016	13.143266	7.612136
8	S	10.271252	7.547095	7.610264
Isomer 4-4				
1	Ni	9.152024	14.277160	11.746035
2	S	8.410521	12.345540	10.985549
3	Ni	8.445030	14.563885	14.050920
4	S	9.304220	16.086344	12.845714
5	Ni	7.260980	12.584226	12.873452
6	S	7.268770	12.955469	15.034045
7	Ni	9.505444	12.140177	12.921479
8	S	9.468997	12.784989	14.962614
Isomer 4-5				
1	Ni	8.782587	13.223548	11.111836
2	S	6.976934	14.318655	11.207367
3	Ni	10.714601	14.545118	12.017703
4	S	10.258474	12.512858	12.502267
5	Ni	9.933137	16.068862	10.015749
6	S	10.020706	16.654326	12.094452
7	Ni	8.023160	16.107203	11.466404
8	S	10.430170	14.015490	9.854366
Isomer 4-6				
1	Ni	8.937704	12.665114	11.075589
2	S	7.319165	14.070920	10.646753
3	Ni	9.106471	12.865439	13.784008
4	S	10.708221	12.331132	12.427502
5	Ni	7.072386	13.007536	12.551992
6	S	7.266351	12.071383	14.449687
7	Ni	10.018357	14.397428	12.107482
8	S	8.640669	15.708312	11.196247
Isomer 5-1				
1	Ni	7.490401	8.557174	9.169749
2	Ni	9.507122	9.851507	10.369447
3	Ni	7.496244	11.136109	9.149750
4	Ni	7.603523	11.156878	11.725510

5	Ni	7.595047	8.579288	11.746546
6	S	6.312943	9.860846	10.497936
7	S	9.081958	9.870095	12.608221
8	S	8.900211	9.835485	8.171858
9	S	8.984451	7.631756	10.408887
10	S	8.996662	12.074651	10.371825
Isomer 5-2				
1	Ni	10.014593	8.294615	10.550362
2	Ni	7.839748	8.365509	8.352968
3	Ni	10.430896	8.998064	8.147954
4	Ni	8.972805	10.403750	9.614017
5	S	10.162656	10.403157	11.471121
6	S	9.500731	7.069993	8.749172
7	S	8.654583	10.143542	7.411918
8	S	7.838787	8.678129	10.461986
9	Ni	11.629962	10.552165	9.947356
10	S	12.072976	8.520173	9.548689
Isomer 5-3				
1	Ni	9.839328	9.639813	11.616072
2	Ni	10.107584	9.886764	8.010990
3	Ni	8.301740	9.141860	9.541453
4	Ni	10.876309	8.130399	9.837928
5	Ni	9.574923	11.584778	9.972044
6	S	11.287936	10.245149	10.113688
7	S	7.997158	10.631642	11.078641
8	S	9.086263	7.725566	10.969335
9	S	10.970570	7.970698	7.755477
10	S	9.469467	11.899029	7.909486
Isomer 5-4				
1	Ni	9.954314	10.943602	8.089494
2	Ni	9.134383	10.905280	10.426262
3	Ni	8.384251	8.672233	10.421076
4	Ni	9.133725	8.773255	7.822693
5	S	7.299303	7.925373	8.695804
6	S	10.344827	8.179882	9.576855
7	S	11.140602	10.268528	9.807171
8	S	8.411627	10.492429	6.577105
9	Ni	7.316715	10.187725	8.510610
10	S	7.012631	10.374493	10.717229
Isomer 5-5				
1	Ni	9.037681	14.011893	11.632544
2	S	8.513962	11.835265	11.421180

3	Ni	8.312238	13.849173	14.365018
4	S	7.331350	14.935437	12.657908
5	Ni	6.858295	12.825341	12.389861
6	S	6.482733	12.697668	14.439838
7	Ni	9.753854	12.305246	13.166166
8	S	10.150442	13.067935	15.256339
9	Ni	10.687284	14.614025	13.858160
10	S	11.150296	13.666205	12.015716

Isomer 5-6

1	Ni	11.561991	8.909656	10.488420
2	Ni	8.548128	7.957932	10.050024
3	Ni	7.816703	9.284656	8.255955
4	Ni	10.610378	7.656441	8.436378
5	Ni	9.617337	10.124848	9.793408
6	S	11.342865	9.743995	8.537573
7	S	8.517048	7.256596	7.903362
8	S	8.041382	9.695654	11.348776
9	S	10.542208	7.070616	10.590781
10	S	7.485731	10.918074	9.631961

Isomer 6-1

1	Ni	10.724477	9.313635	9.177799
2	Ni	8.872769	11.220549	9.422822
3	Ni	8.816459	7.443813	9.337504
4	Ni	8.620827	9.414905	7.500187
5	Ni	9.068298	9.250273	11.259467
6	Ni	6.964285	9.350643	9.581759
7	S	10.250985	10.843064	7.702374
8	S	10.549423	7.698848	10.627244
9	S	7.187458	7.840959	7.946057
10	S	7.138815	10.966594	8.131930
11	S	10.502828	10.824128	10.814602
12	S	7.435963	7.821389	11.057019

Isomer 6-2

1	Ni	10.771250	9.040397	8.938269
2	Ni	9.053134	11.126688	9.513632
3	Ni	8.949480	7.435601	8.946105
4	Ni	8.643737	9.610597	7.523750
5	Ni	9.268999	8.915301	11.279892
6	Ni	7.097029	9.382199	9.519798
7	S	10.783564	10.428304	10.640026
8	S	10.613578	7.394751	10.389335
9	S	10.070316	7.995254	7.118716
10	S	7.263584	11.161836	8.200868

11	S	7.809764	10.557614	11.227981
12	S	7.583166	7.582787	10.655857
Isomer 6-3				
1	Ni	8.325600	11.014485	9.085712
2	Ni	10.929879	8.225825	9.086205
3	Ni	8.325615	8.225819	9.085649
4	Ni	10.929869	11.014470	9.086152
5	Ni	9.628067	9.620149	7.579274
6	Ni	9.627448	9.620154	11.179780
7	S	9.627435	11.763917	10.681186
8	S	9.627290	7.476382	10.681189
9	S	7.485099	9.620119	10.565628
10	S	11.770004	9.620179	10.566189
11	S	9.628083	7.432464	7.451086
12	S	9.628012	11.807836	7.451086
Isomer 6-4				
1	Ni	9.340397	14.614140	12.448934
2	S	7.302517	15.076638	11.839646
3	Ni	9.419575	13.385661	14.865668
4	S	11.047578	13.687533	13.440383
5	Ni	7.072575	14.242705	13.844399
6	S	7.434075	13.244313	15.757199
7	Ni	9.692074	11.983789	12.875541
8	S	9.333466	12.972306	10.957100
9	Ni	7.429089	11.608224	14.271985
10	S	9.468312	11.143824	14.879482
11	Ni	7.349568	12.838447	11.855298
12	S	5.720828	12.533807	13.280411
Isomer 6-5				
1	Ni	10.357576	9.256024	8.885631
2	Ni	7.321729	9.285803	11.418454
3	Ni	11.274556	9.305959	11.620872
4	Ni	9.315919	7.783320	11.116691
5	Ni	9.416254	10.930649	10.534893
6	Ni	7.494812	9.483750	8.854466
7	S	9.257547	9.620013	12.339392
8	S	8.952797	9.576307	7.355812
9	S	7.510474	7.666404	9.990303
10	S	11.556861	10.756104	10.045070
11	S	11.266423	7.717250	10.204394
12	S	7.267638	11.137615	10.308043
Isomer 6-6				

1	Ni	11.414281	9.579573	10.388602
2	Ni	8.757650	11.015301	9.391320
3	Ni	9.168528	7.708656	9.361628
4	Ni	8.421722	9.339057	7.506275
5	Ni	8.712803	9.342661	11.308937
6	S	9.991213	11.054841	11.147179
7	S	7.545112	9.176554	9.485596
8	S	10.296668	7.871087	11.224059
9	S	9.988789	7.854297	7.340871
10	S	9.709630	11.052747	7.469259
11	Ni	11.231973	9.565258	7.969620
12	S	12.774831	10.548072	9.062840

Isomer 7-1

1	Ni	9.917613	9.200540	9.266685
2	Ni	11.557592	11.207469	9.415021
3	Ni	12.373831	9.085805	8.733141
4	Ni	9.160872	11.664712	9.779842
5	Ni	9.033895	9.767778	11.798850
6	Ni	10.973696	11.745035	11.757616
7	Ni	11.674602	9.283914	11.163142
8	S	8.809835	11.921097	11.914169
9	S	10.840326	10.000177	13.083987
10	S	10.899782	10.149833	7.571029
11	S	10.830300	13.131283	10.017293
12	S	9.950803	7.909782	11.055136
13	S	7.901796	9.869708	9.882791
14	S	13.390833	10.251385	10.234227

Isomer 7-2

1	Ni	9.687819	8.536293	9.387902
2	Ni	12.295789	11.181818	9.250701
3	Ni	12.187531	8.651704	8.710389
4	Ni	9.447056	11.392384	9.491529
5	Ni	9.234821	9.770227	11.583929
6	Ni	11.176357	11.720796	11.488530
7	Ni	11.639403	9.299434	10.992500
8	S	9.020966	11.926746	11.614072
9	S	10.989255	10.030448	12.908061
10	S	10.662390	10.119610	8.105505
11	S	11.076181	12.923336	9.618168
12	S	11.298881	7.283972	10.123502
13	S	7.939263	9.761466	9.779238
14	S	13.606010	9.629335	10.012590

Isomer 7-3

1	Ni	9.590869	8.733993	9.384783
2	Ni	12.130572	11.442422	9.358404
3	Ni	12.067839	8.943848	8.660592
4	Ni	9.285525	11.562102	9.672193
5	Ni	9.166518	9.809333	11.662570
6	Ni	11.050264	11.821522	11.646444
7	Ni	11.571030	9.443110	10.988097
8	S	8.894877	11.952945	11.831581
9	S	10.946937	10.041589	12.954673
10	S	10.497604	10.413756	8.183237
11	S	10.875127	13.132004	9.859201
12	S	11.242878	7.476024	10.011446
13	S	7.824476	9.875299	9.892616
14	S	13.501490	9.879545	9.979424

Isomer 7-4

1	Ni	9.888586	9.197650	9.199948
2	Ni	11.628347	11.165278	9.708408
3	Ni	12.282305	9.026074	8.731002
4	Ni	9.221109	11.861159	9.816164
5	Ni	9.094861	9.721729	11.562803
6	Ni	11.011303	11.738927	11.960220
7	Ni	11.762246	8.978377	11.121112
8	S	8.830821	11.847005	11.981189
9	S	10.867549	9.775858	12.957168
10	S	10.752547	8.169752	7.579560
11	S	9.925983	7.814727	10.900173
12	S	10.961075	13.167103	10.224297
13	S	7.947961	10.085573	9.635940
14	S	13.454120	10.073416	10.232032

Isomer 7-5

1	Ni	9.097896	14.389630	12.008756
2	Ni	10.485939	12.817201	13.040302
3	Ni	7.213525	15.628268	13.411454
4	Ni	8.429701	11.597100	13.769360
5	Ni	6.554725	13.257736	14.683427
6	Ni	6.859765	13.291804	12.054325
7	Ni	8.915936	14.143944	14.523340
8	S	5.408938	14.445953	13.279510
9	S	7.314738	15.170314	15.566394
10	S	7.327307	15.350164	11.243561
11	S	11.213565	14.499975	11.962391
12	S	8.780144	12.160522	11.713531
13	S	6.293601	11.517446	13.381902
14	S	9.967231	12.335642	15.116158

## Isomer 7-6

1	Ni	9.131670	9.231333	8.384207
2	Ni	11.314894	11.640555	9.094557
3	Ni	11.671948	9.014255	8.315916
4	Ni	8.965842	11.687162	8.472269
5	Ni	9.448480	11.385150	10.824098
6	Ni	11.486715	8.956694	10.859354
7	Ni	8.952735	8.727917	10.867065
8	S	12.835101	10.192172	9.700953
9	S	7.797062	10.275765	9.801890
10	S	9.745386	13.585982	9.061791
11	S	10.297222	7.750578	9.454412
12	S	10.502519	10.550277	7.287958
13	S	10.126690	9.885768	12.259140
14	S	10.904511	13.054073	10.768147

## Isomer 8-1

1	Ni	8.068506	10.005751	9.522966
2	Ni	9.829465	9.634766	8.060347
3	Ni	9.378652	11.393507	11.141348
4	Ni	9.216955	8.932983	11.612107
5	Ni	11.602856	10.125030	11.899166
6	Ni	11.434522	8.489572	9.805753
7	Ni	11.513693	10.966321	9.365459
8	S	9.838560	10.390195	13.119613
9	S	11.437358	12.199149	11.208411
10	S	7.415414	10.306535	11.522051
11	S	10.473700	7.174680	11.261616
12	S	8.001730	8.495345	7.992863
13	S	11.920693	9.382014	7.784787
14	S	9.411920	11.690956	8.872945
15	Ni	9.160813	7.562016	9.567294
16	S	13.112798	9.757418	10.407712

## Isomer 8-2

1	Ni	10.062001	14.870405	12.561070
2	S	8.076805	15.062487	11.609942
3	Ni	9.959497	13.203123	14.484538
4	S	11.689378	14.357295	13.911240
5	Ni	6.073324	14.375515	14.327007
6	S	6.240464	12.317095	13.685721
7	Ni	7.882247	15.098478	16.142332
8	S	9.489172	13.683231	16.628917
9	Ni	8.084427	15.712202	13.720605
10	S	6.511511	16.404664	15.037210

11	Ni	10.235816	15.392007	15.276401
12	S	9.968110	16.802854	13.659794
13	Ni	7.770969	12.526908	15.312253
14	S	6.237201	13.692831	16.417048
15	Ni	8.007124	13.226386	12.791280
16	S	8.985670	11.450687	13.776442

Isomer 8-3

1	Ni	11.205582	9.678393	11.634998
2	Ni	8.769423	8.003746	8.962664
3	Ni	10.893004	9.403667	9.045841
4	Ni	11.787406	11.710069	9.886608
5	Ni	9.357115	11.576365	8.947583
6	Ni	7.349824	10.020160	8.899107
7	Ni	9.628967	11.864247	11.565126
8	S	9.434296	10.106971	12.913609
9	S	9.215465	9.786100	7.666399
10	S	10.298586	7.867687	10.504611
11	S	12.797476	9.786459	10.025134
12	S	10.289503	13.286064	9.918965
13	S	7.668114	11.593419	10.360418
14	S	6.975367	8.284688	10.119859
15	Ni	8.682269	9.526492	10.955968
16	S	11.761716	11.752570	12.069242

Isomer 8-4

1	Ni	9.518920	9.016219	9.092669
2	Ni	12.206510	11.395361	9.674837
3	Ni	11.845379	8.959162	9.109675
4	Ni	9.262908	11.466364	9.643221
5	Ni	8.951004	9.809853	11.463932
6	Ni	10.722978	11.895207	11.918172
7	Ni	12.396661	9.726403	11.496935
8	S	8.531815	11.941780	11.717999
9	S	10.655178	9.588662	12.903378
10	S	10.732785	10.626927	8.061672
11	S	10.767163	13.031835	10.039726
12	Ni	10.627266	8.039960	11.267375
13	S	7.642507	9.898229	9.677735
14	S	13.747403	9.746306	9.733290
15	S	12.916383	11.837120	11.766609
16	S	10.633320	7.200502	9.297197

Isomer 8-5

1	Ni	9.700856	8.136251	9.597039
2	Ni	12.150378	11.242507	9.205544

3	Ni	12.294882	8.680576	8.760400
4	Ni	9.622051	11.867865	9.627794
5	Ni	9.246056	9.848757	11.393432
6	Ni	11.223359	11.619282	11.837005
7	Ni	11.639773	9.320903	11.000576
8	S	9.053517	11.981232	11.762845
9	S	10.798169	9.761536	12.937898
10	Ni	10.108551	9.977676	8.222060
11	S	11.451746	13.040639	10.210017
12	S	11.532814	7.269369	10.301011
13	S	8.219406	9.912404	9.459467
14	S	13.579728	9.881669	10.127235
15	S	10.624452	8.004587	7.540274
16	S	10.675160	11.941585	7.664115

Isomer 8-6

1	Ni	9.889203	8.895145	9.097224
2	Ni	11.657030	10.706148	8.462218
3	Ni	12.398468	8.285117	9.028270
4	Ni	9.622730	11.449373	9.537825
5	Ni	9.209164	9.737122	11.642580
6	Ni	11.336233	11.376612	11.623097
7	Ni	11.499368	8.914525	11.197256
8	S	9.235461	11.938456	11.660812
9	S	10.891481	9.793130	13.068028
10	S	9.764100	10.504548	7.528795
11	S	11.824960	12.485827	9.815071
12	S	10.783248	7.165092	10.068658
13	S	8.063632	9.850172	9.791155
14	Ni	13.256056	10.677722	10.148348
15	S	13.620276	8.677752	10.838561
16	S	13.576093	9.827422	8.061942

Isomer 9-1

1	Ni	9.196211	10.000916	8.923744
2	Ni	11.292163	11.358574	8.436948
3	Ni	11.567296	9.125526	9.596543
4	Ni	9.737664	12.278933	10.202093
5	Ni	9.411229	8.767473	11.148923
6	Ni	9.949001	10.991922	12.393361
7	Ni	11.775241	9.165844	12.095818
8	S	8.506108	12.563549	11.969390
9	S	12.057444	11.189286	12.978104
10	S	10.857397	9.411947	7.577893
11	S	11.714561	13.109272	9.663642
12	S	11.120957	7.411465	10.885433

13	S	7.615648	8.892192	9.928394
14	S	13.446243	9.556566	10.660184
15	Ni	12.132924	11.319869	10.803271
16	S	9.251737	12.036188	8.050150
17	S	9.913977	8.976903	13.286139
18	Ni	7.931825	10.754908	10.952879

Isomer 9-2

1	Ni	9.225490	10.145852	8.532659
2	Ni	11.311482	11.799166	8.483943
3	Ni	11.747704	9.386624	9.170348
4	Ni	9.296705	12.023341	10.259296
5	Ni	8.943696	10.173231	11.956214
6	Ni	11.007642	11.823780	12.322094
7	Ni	11.562335	9.394808	11.728411
8	S	8.825886	12.307285	12.368241
9	S	10.442991	10.008008	13.504739
10	S	10.946253	9.985443	7.225532
11	S	11.155013	13.191784	10.391289
12	S	11.669475	7.634302	10.452478
13	S	7.862032	9.631628	10.149516
14	S	13.347925	10.885966	8.673459
15	Ni	9.683091	8.433109	10.308900
16	S	13.044857	10.906812	12.481377
17	Ni	12.580470	11.525352	10.524487
18	S	9.158446	12.278314	8.100717

Isomer 9-3

1	Ni	9.430520	14.499250	11.837649
2	S	7.608947	15.760521	11.895087
3	Ni	8.850048	14.096096	15.822320
4	S	11.532317	13.936396	12.229861
5	Ni	6.664376	13.718161	14.357395
6	S	7.249084	12.562560	16.125618
7	Ni	10.269749	12.251418	12.942467
8	S	8.954202	12.466364	11.136977
9	Ni	8.618812	11.768510	14.655328
10	S	9.357517	10.249045	13.277824
11	Ni	7.141413	13.679541	11.839767
12	S	5.821947	12.333824	12.920332
13	Ni	8.544371	15.931104	13.831562
14	S	10.060022	15.967834	15.455073
15	Ni	7.651805	11.322129	12.426160
16	S	10.517007	12.600594	15.413742
17	Ni	10.573467	14.387681	14.100610
18	S	7.188081	15.538133	15.466273

## Isomer 9-4

1	Ni	7.980632	9.562094	10.336028
2	Ni	9.761429	9.883974	8.492389
3	Ni	9.537523	11.547251	10.576986
4	Ni	9.739648	8.207925	11.763055
5	Ni	11.316457	10.147183	11.810345
6	Ni	11.691205	8.269168	9.376465
7	Ni	11.712778	11.070581	9.346644
8	Ni	8.914683	10.340550	12.613096
9	S	11.542860	12.258182	11.193174
10	S	7.536852	11.427074	11.377278
11	S	10.849244	6.710795	10.590535
12	S	7.905740	8.823753	8.240524
13	S	11.788979	9.620214	7.680112
14	S	9.926488	12.081958	8.485248
15	Ni	9.239720	7.578818	9.397606
16	S	12.974774	9.641872	10.466675
17	S	7.780252	7.457699	11.014055
18	S	10.456737	9.166633	13.550319

## Isomer 9-5

1	Ni	9.338523	9.407133	8.094431
2	Ni	10.905648	11.504995	7.856457
3	Ni	11.808584	9.299427	8.753780
4	Ni	8.578817	11.666683	8.911078
5	Ni	10.058404	11.623400	11.173232
6	Ni	11.075863	9.233326	11.154683
7	Ni	8.782111	9.517942	10.418962
8	S	13.141985	9.074605	10.566886
9	S	7.345446	9.865407	8.854334
10	S	8.512629	13.087212	10.585897
11	S	10.168987	7.930233	9.561538
12	S	10.959723	9.602817	6.693604
13	S	9.464444	9.928981	12.424332
14	S	11.748438	13.103437	11.117858
15	Ni	12.656307	11.213692	10.621052
16	S	9.488332	13.127294	7.491330
17	Ni	10.376809	13.309751	9.441946
18	S	12.977835	11.168928	8.468394

## Isomer 9-6

1	Ni	10.413834	15.072278	12.538456
2	S	8.652333	15.136654	11.238039
3	Ni	9.954118	13.103430	14.408605
4	S	11.492323	14.715632	14.415707

5	Ni	5.973143	14.939181	14.805796
6	Ni	6.375190	12.576089	14.130607
7	Ni	7.617818	14.686659	16.656171
8	S	9.578439	13.726885	16.599390
9	Ni	7.843097	15.760441	13.219671
10	S	7.432087	16.456678	15.391184
11	Ni	9.526736	15.502447	15.100868
12	S	9.712133	16.954394	13.417626
13	Ni	8.022280	12.328209	15.971845
14	S	6.090042	13.260447	16.150222
15	Ni	8.258478	13.362225	12.524567
16	S	8.293347	11.540427	13.955190
17	S	10.430545	12.902974	12.244612
18	S	6.142362	14.247810	12.747350

Isomer 10-1

1	Ni	9.311456	15.351501	11.887446
2	Ni	10.122796	12.131429	13.082196
3	Ni	7.323888	15.635676	13.696823
4	Ni	7.606019	11.630008	12.695711
5	Ni	6.615063	13.283119	14.325414
6	Ni	6.857583	14.514852	11.309676
7	Ni	8.845400	14.306428	15.204440
8	S	5.482126	14.641679	13.033508
9	S	6.867762	14.935686	15.767300
10	S	7.476042	16.618500	11.740169
11	S	10.967654	13.689068	11.676042
12	S	9.329327	10.767005	11.619306
13	S	6.481622	11.142826	14.454896
14	S	10.454357	12.746545	15.221048
15	Ni	8.957039	12.858102	10.948542
16	S	9.527979	16.155834	14.070160
17	S	6.816462	12.375159	10.791084
18	Ni	8.489098	11.801880	15.006083
19	S	8.576321	14.732853	9.879061
20	Ni	10.671300	14.340916	13.729055

Isomer 10-2

1	Ni	9.349905	14.990106	12.307388
2	Ni	10.124185	12.775538	13.339078
3	Ni	7.272543	15.796477	13.602771
4	Ni	8.078831	11.027098	12.659199
5	Ni	6.480660	13.391438	14.541077
6	Ni	7.023404	14.327220	11.538512
7	Ni	8.797042	14.380912	14.891036
8	S	5.396074	14.552296	12.993517

9	S	6.924655	15.167610	15.713754
10	S	7.763944	16.337643	11.496407
11	S	10.892699	13.689990	11.536394
12	S	8.289464	10.859570	10.517736
13	S	6.469056	11.206463	14.239192
14	S	10.230458	12.940424	15.552805
15	Ni	8.990418	12.903809	10.955014
16	S	9.389132	16.316595	14.065478
17	S	6.805077	12.513592	10.282444
18	Ni	8.516499	11.778130	14.919419
19	S	9.935970	10.592233	13.694577
20	Ni	6.115622	12.319028	12.356367

Isomer 10-3

1	Ni	9.771668	8.791580	9.345250
2	Ni	11.482281	11.733669	8.298118
3	Ni	11.816890	9.424515	8.074928
4	Ni	9.380821	11.498161	9.614369
5	Ni	9.136220	9.848888	11.721585
6	Ni	10.930029	11.843120	11.806883
7	Ni	11.408615	8.506354	11.486013
8	S	8.755644	12.032700	11.698823
9	S	10.863276	9.995958	13.199278
10	S	9.884281	10.375761	7.641105
11	S	11.040881	13.094970	9.908847
12	S	11.810825	7.714898	9.381914
13	S	7.925814	9.865495	9.881816
14	S	13.599162	8.356692	11.909014
15	Ni	12.982134	11.960332	10.203828
16	S	13.480613	10.830176	8.352710
17	Ni	13.367975	9.276032	9.948039
18	S	13.016248	12.493051	12.311694
19	Ni	12.849442	10.351799	12.190471
20	S	9.386786	7.701529	11.278868

Isomer 10-4

1	Ni	9.320075	10.004513	8.259472
2	Ni	11.229177	11.924344	8.432202
3	Ni	11.923847	9.547589	8.631409
4	Ni	9.300003	11.745452	10.230383
5	Ni	8.928528	9.996251	12.292299
6	Ni	10.868411	11.931682	12.292292
7	Ni	11.585401	9.333801	12.268496
8	S	8.658304	12.171156	12.298406
9	S	10.432833	10.402532	13.821067
10	S	10.938118	10.305224	6.879350

11	S	10.826897	13.374815	10.400239
12	S	12.226156	8.039649	10.261354
13	S	8.142712	9.717204	10.128691
14	S	13.420468	11.216679	8.757964
15	Ni	10.143393	8.735284	10.266743
16	S	13.036896	11.102158	12.384505
17	Ni	12.553298	12.150966	10.511119
18	S	9.051608	12.155847	8.076361
19	S	9.819453	7.972799	12.289330
20	Ni	13.283655	9.911726	10.558852

Isomer 10-5

1	Ni	10.152051	9.241181	11.981606
2	Ni	9.655025	8.969488	8.884550
3	Ni	11.871845	8.798274	10.076202
4	Ni	11.168476	11.017538	8.835949
5	Ni	9.170892	12.315012	8.976224
6	Ni	7.611759	10.413704	9.285994
7	Ni	7.978755	10.661089	11.954192
8	S	10.044241	11.239183	13.000528
9	S	9.356555	10.680848	7.554130
10	S	10.133046	7.467217	10.459258
11	S	13.104922	10.489111	9.610425
12	S	11.095644	13.008191	9.865992
13	S	7.554877	12.375890	10.460293
14	S	7.597823	8.279810	8.641674
15	Ni	11.740982	11.210881	11.249425
16	S	8.248380	8.677569	12.944396
17	Ni	9.582206	12.415614	11.295686
18	S	12.354141	9.267722	12.149724
19	S	6.333226	9.635038	10.912603
20	Ni	7.952240	8.176592	10.827229

Isomer 10-6

1	Ni	9.008536	10.318144	8.774283
2	Ni	11.527808	11.083972	8.650323
3	Ni	10.817729	8.620881	9.597312
4	Ni	9.479302	12.625958	9.910580
5	Ni	9.862464	8.548555	11.824777
6	Ni	10.987574	11.796307	11.749950
7	Ni	12.334142	9.170244	11.697190
8	S	9.012593	12.536488	12.052310
9	Ni	10.800793	10.142128	13.452757
10	S	10.608286	9.342551	7.561591
11	S	11.733768	12.951369	9.945083
12	S	11.471949	7.224512	11.215412

13	S	8.537299	8.487523	10.068608
14	S	12.897692	9.474908	9.567943
15	Ni	13.025882	11.347019	10.706072
16	S	9.776234	12.127290	7.774895
17	S	8.737576	9.493095	13.378199
18	Ni	8.478413	10.468616	11.364000
19	S	7.511172	11.621293	9.743646
20	S	12.755888	11.005810	12.877178

Table S3. The x,y,z coordinates of the proposed structures of the Ni<sub>4</sub>S<sub>4</sub> cluster with adsorbed hydrogen atoms.

**Coordinates (Angstroms) of Ni<sub>4</sub>S<sub>4</sub> Cluster with adsorbed hydrogen atoms**

System	ATOM	X	Y	Z
Isomer Ni <sub>4</sub> S <sub>4</sub> @1H				
1	Ni	-0.969246	-0.969322	0.833229
2	S	-1.104409	-1.114437	-1.337387
3	Ni	1.017924	-0.991697	-0.794352
4	S	1.145074	-1.085541	1.367465
5	Ni	-1.002271	1.013515	-0.810259
6	S	1.088720	1.093735	-1.465984
7	Ni	1.012618	1.043481	0.817727
8	S	-1.122577	1.146003	1.350105
9	H	1.371546	1.410022	2.196163
Isomer Ni <sub>4</sub> S <sub>4</sub> @2H				
1	Ni	-0.858938	-0.904259	0.841856
2	S	-0.864512	-1.292335	-1.303991
3	Ni	1.267858	-0.777116	-0.904737
4	S	1.280835	-1.055289	1.232580
5	Ni	-1.097914	0.829552	-0.924387
6	S	0.976303	1.410301	-1.350378
7	Ni	1.098441	1.059555	0.862428
8	S	-1.108204	1.227508	1.203965
9	H	1.301224	1.243246	2.314316
10	H	1.601012	-2.209173	-0.997030
Isomer Ni <sub>4</sub> S <sub>4</sub> @3H				
1	Ni	-0.540321	-1.021285	1.011754
2	S	-1.146227	-1.250117	-1.093151
3	Ni	1.009020	-0.932873	-1.113017
4	S	1.633628	-0.788600	0.976638
5	Ni	-0.678786	0.852752	-0.931932
6	S	1.462014	1.467568	-1.318259
7	Ni	0.823489	1.262189	0.983136
8	S	-1.332614	1.028510	1.117910
9	H	1.003347	1.354412	2.429912
10	H	1.356887	-2.352447	-1.152575
11	H	0.960138	2.388985	-2.210464
Isomer Ni <sub>4</sub> S <sub>4</sub> @4H				
1	Ni	-0.751142	-0.892366	0.834764
2	S	-0.927274	-1.214531	-1.357891
3	Ni	1.180497	-0.814537	-1.029705

4	S	1.438432	-0.932969	1.127910
5	Ni	-0.867965	0.912339	-1.071774
6	S	1.626384	1.445036	-1.330503
7	Ni	0.968082	1.177605	0.870158
8	S	-1.197355	1.272113	1.022001
9	H	1.005852	1.338147	2.320559
10	H	1.376019	-2.260568	-1.092078
11	H	0.652546	2.101468	-2.063109
12	H	-2.286693	1.032379	-1.385340

Isomer Ni<sub>4</sub>S<sub>4</sub>@5H

1	Ni	-1.096183	-0.776999	1.068554
2	S	-1.246882	-1.201192	-1.034398
3	Ni	0.906324	-0.985429	-0.834671
4	S	1.069180	-1.237284	1.395285
5	Ni	-0.995307	0.940587	-0.811965
6	S	1.205858	1.229975	-1.338738
7	Ni	1.009896	0.857760	1.008314
8	S	-1.077814	1.422537	1.357133
9	H	-1.366202	1.034699	-2.235085
10	H	-1.567813	-2.145908	1.332330
11	H	1.808250	1.312645	2.156898
12	H	0.935829	-1.260141	-2.291481
13	H	1.841545	1.913821	-0.227419

Isomer Ni<sub>4</sub>S<sub>4</sub>@6H

1	Ni	-0.780020	-0.733601	0.829987
2	S	-1.047869	-1.161196	-1.350600
3	Ni	1.083600	-0.905717	-1.189315
4	S	1.444324	-1.006751	0.945420
5	Ni	-0.769022	0.976328	-1.286728
6	S	1.440228	1.264346	-1.955767
7	Ni	1.112253	1.073261	0.577707
8	S	-0.960026	1.537910	0.796197
9	H	1.435211	1.471735	1.944653
10	H	1.265037	-2.355960	-1.271452
11	H	-2.214264	1.162195	-1.436649
12	H	-1.642260	-1.867967	1.780033
13	H	-2.063619	-1.180689	1.865397
14	H	2.127179	1.990972	-0.994017

Isomer Ni<sub>4</sub>S<sub>4</sub>@7H

1	Ni	-0.846324	-0.749791	0.805736
2	S	-1.150494	-1.139684	-1.388977
3	Ni	0.985820	-0.892581	-1.228418
4	S	1.338333	-1.187870	0.914003

5	Ni	-0.805912	0.983712	-1.327441
6	S	1.360959	1.217733	-2.046030
7	Ni	0.883912	0.897128	1.140188
8	S	-1.161550	1.459046	0.780554
9	H	1.142220	-2.348387	-1.332427
10	H	-2.248483	1.189342	-1.492811
11	H	-1.613316	-2.000284	1.657655
12	H	-2.184104	-1.420367	1.604828
13	H	1.979717	1.861094	-1.018460
14	H	1.991888	2.013219	1.477528
15	H	1.733223	1.697769	2.223901

Isomer Ni<sub>4</sub>S<sub>4</sub>@8H

1	Ni	-0.971417	-0.851842	0.803380
2	S	-1.137494	-0.829255	-1.372295
3	Ni	1.016079	-0.965116	-0.892026
4	S	1.233443	-1.175062	1.266120
5	Ni	-1.045710	1.274907	-0.700051
6	S	1.229701	1.356569	-1.440832
7	Ni	0.969219	0.917549	0.863084
8	S	-1.043584	1.323666	1.478944
9	H	-1.715237	-2.161782	1.462803
10	H	-2.281658	-1.548814	1.503510
11	H	2.064783	2.048579	-0.569161
12	H	1.688859	-1.692382	-2.194647
13	H	1.608372	-2.299800	-1.616826
14	H	-1.805977	2.158644	-1.842480
15	H	-2.360030	2.072298	-1.213251
16	H	1.505134	1.343745	2.147920

Isomer Ni<sub>4</sub>S<sub>4</sub>@9H

1	Ni	-0.964372	-0.778663	1.042380
2	S	-0.743009	-1.442449	-1.036410
3	Ni	1.139999	-0.658230	-1.632937
4	S	1.079401	-1.124792	2.038490
5	Ni	-0.777856	0.792640	-1.011480
6	S	1.337454	1.506272	-1.507544
7	Ni	1.048902	0.660023	0.747650
8	S	-0.988609	1.424927	1.099454
9	H	-2.146341	1.383658	-1.698423
10	H	-1.674798	1.162418	-2.349621
11	H	-2.015802	-1.863814	1.707010
12	H	-2.504633	-1.250415	1.432153
13	H	1.853099	1.436841	1.681297
14	H	1.983983	1.727025	-0.208925
15	H	2.053118	-1.910535	-2.017677

16	H	2.491703	-1.224304	-2.287148
17	H	1.578507	-2.046663	1.168109

Isomer Ni<sub>4</sub>S<sub>4</sub>@10H

1	Ni	-0.851118	-0.948567	1.227196
2	S	-1.357806	-1.306290	-1.018347
3	Ni	0.910293	-0.880246	-0.727421
4	S	1.237626	-1.276935	1.443190
5	Ni	-0.995721	0.889833	-0.663356
6	S	1.151378	1.343371	-1.216165
7	Ni	0.995322	0.926775	1.218402
8	S	-1.282949	1.378739	1.533547
9	H	-1.784262	0.191421	2.204379
10	H	-1.046587	-1.875214	2.349525
11	H	1.608430	2.071845	2.149568
12	H	1.842657	1.326288	2.507307
13	H	1.634720	-2.149519	-1.383632
14	H	2.139499	-1.487940	-1.559663
15	H	-2.194648	1.465574	-1.582634
16	H	-1.610675	2.073186	-1.581195
17	H	-1.754412	-1.974058	0.264534
18	H	1.843376	1.796617	-0.029034

Isomer Ni<sub>4</sub>S<sub>4</sub>@11H

1	Ni	-0.838553	-0.846287	0.966086
2	S	-1.184096	-1.377168	-1.115160
3	Ni	0.985271	-0.963638	-0.963864
4	S	1.395276	-1.198315	1.397686
5	Ni	-0.863092	0.809150	-1.093224
6	S	1.362215	1.274426	-1.195270
7	Ni	0.943375	0.979147	1.204152
8	S	-1.255738	1.385491	1.254328
9	H	2.102857	-1.606275	0.196695
10	H	1.845896	1.852372	0.056861
11	H	-1.540111	2.008450	-0.016683
12	H	-1.461058	-1.387779	2.360791
13	H	-1.762408	-1.901396	1.754194
14	H	1.551111	-2.106462	-1.936256
15	H	1.496652	-1.401620	-2.420192
16	H	1.262838	1.400757	2.710873
17	H	1.765491	1.908748	2.236635
18	H	-1.274457	1.301780	-2.558556
19	H	-2.009994	1.236493	-2.120586

Isomer Ni<sub>4</sub>S<sub>4</sub>@12H

1	Ni	-0.886123	-0.877549	1.068691
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2	S	-1.114536	-1.306333	-1.231821
3	Ni	1.086494	-0.873963	-0.924618
4	S	1.331845	-1.216126	1.396727
5	Ni	-0.769421	0.923394	-1.084611
6	S	1.452600	1.356377	-1.065657
7	Ni	0.893131	0.991813	1.204774
8	S	-1.338342	1.339093	1.166259
9	H	1.913904	1.892033	0.236580
10	H	-1.737315	-1.835579	0.001103
11	H	-1.791456	1.853075	-0.142329
12	H	2.028091	-1.695445	0.179704
13	H	-0.949020	1.249784	-2.651606
14	H	-1.588810	1.658143	-2.265539
15	H	-1.289287	-1.200007	2.596877
16	H	-1.793370	-1.696861	2.119431
17	H	1.923973	-1.809784	-1.948460
18	H	1.549689	-1.219495	-2.434780
19	H	1.088520	1.325772	2.772652
20	H	1.589704	1.880712	2.362378

Isomer Ni<sub>4</sub>S<sub>4</sub>@13H

1	Ni	-1.456973	-0.930011	0.609353
2	S	-0.530189	-1.122861	-1.155924
3	Ni	1.162817	-0.617888	-1.170295
4	S	1.758712	-0.754117	0.769008
5	Ni	-0.578674	1.246094	-0.850140
6	S	1.652236	1.599228	-1.022557
7	Ni	1.122606	0.730645	0.910293
8	S	-1.762046	1.076330	0.690381
9	H	-1.461969	2.083111	1.727440
10	H	1.421898	-2.239605	1.240758
11	H	-1.301745	-0.850435	2.309855
12	H	1.099959	1.049002	2.466139
13	H	0.474592	2.502334	-1.223485
14	H	1.576469	-0.896432	-2.755836
15	H	2.073719	-1.398405	-2.322586
16	H	-1.031353	1.135416	-2.282907
17	H	0.942307	1.760772	2.027024
18	H	-1.755872	1.396149	-2.041294
19	H	-1.159241	-1.620470	1.930495
20	H	-0.504512	-2.479220	-1.040164
21	H	-1.619758	-1.751164	-1.876065

Isomer Ni<sub>4</sub>S<sub>4</sub>@14H

1	Ni	-0.887430	-1.279998	1.254224
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2	S	-1.073119	-1.123743	-0.931041
3	Ni	0.584695	-0.883720	-1.307214
4	S	1.574559	-1.936560	1.661910
5	Ni	-1.231521	1.302696	-0.366138
6	S	1.785364	1.440809	-0.859344
7	Ni	0.964625	0.807677	1.171794
8	S	-1.168438	1.172299	1.715579
9	H	-2.316258	1.968177	0.124283
10	H	2.000594	-1.901829	0.744649
11	H	-2.243958	-1.539903	1.997147
12	H	-1.565996	-2.188737	2.153961
13	H	2.069951	1.497736	2.211202
14	H	1.564453	2.120670	2.003936
15	H	1.690201	-1.348075	-1.704284
16	H	1.343913	-1.052834	-2.413837
17	H	-1.606474	1.730431	-1.787270
18	H	-0.949861	1.046113	-1.887296
19	H	2.893789	1.306235	-1.681533
20	H	1.340684	2.505912	-1.592671
21	H	-0.864061	-2.193488	-1.493518
22	H	-2.188781	-1.469642	-1.817257

Isomer Ni<sub>4</sub>S<sub>4</sub>@15H

1	Ni	-0.806824	-0.403459	1.176482
2	S	-1.307147	-0.833833	-0.785346
3	Ni	1.067204	-0.829822	-1.046421
4	S	1.052930	-1.074137	0.758075
5	Ni	-1.369171	0.767217	-0.942267
6	S	1.685512	1.266850	-1.474371
7	Ni	0.765888	1.511156	0.400304
8	S	-1.363092	1.837685	0.990086
9	H	-1.410368	1.850598	-1.992158
10	H	-2.221637	1.621634	-1.845566
11	H	1.725432	-1.446157	-1.922225
12	H	2.332408	-1.321214	-1.364281
13	H	3.005653	1.589858	-1.687784
14	H	1.334462	1.857046	-2.664355
15	H	-1.582298	-2.305195	-1.424418
16	H	-1.527595	-1.127939	-2.171423
17	H	1.139780	-2.272938	1.142004
18	H	2.170892	-1.054816	1.853161
19	H	-1.402570	0.939713	2.153311
20	H	1.382914	1.640875	1.875348
21	H	2.058884	1.703168	1.338768
22	H	-2.245642	-1.083965	1.121251
23	H	-1.806137	-1.521502	1.732127

Isomer Ni<sub>4</sub>S<sub>4</sub>@16H

1	Ni	-0.713323	-1.401081	0.815274
2	S	-1.296877	-1.416693	-1.286081
3	Ni	0.860804	-0.777518	-0.942796
4	S	1.331764	-1.165339	1.405996
5	Ni	-0.918315	0.934057	-0.391323
6	S	1.326164	1.431697	-1.346024
7	Ni	1.459109	0.873933	0.753169
8	S	-1.415915	1.498536	1.662574
9	H	1.298125	2.822600	-1.313665
10	H	2.654509	1.508387	-1.739309
11	H	-2.685826	-1.427200	-1.237454
12	H	-1.330744	-2.775118	-1.570104
13	H	-1.449013	2.873010	1.689115
14	H	-2.790669	1.492301	1.707425
15	H	2.313327	-2.081331	1.110342
16	H	1.596186	-1.374286	2.761949
17	H	1.704854	1.639700	2.106768
18	H	1.633875	2.260211	1.471951
19	H	2.104040	-1.310775	-1.699175
20	H	1.485761	-1.979800	-1.695987
21	H	-2.073547	-1.528092	1.584345
22	H	-1.428238	-1.590723	2.198523
23	H	-1.444705	1.322909	-1.837131
24	H	-1.879276	1.833988	-1.255006