

Article

Selective Hydrogenation of Acetylene Catalysed by a B₁₂N₁₂ Cluster Doped with a Single Nickel Atom: A DFT Study

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Table S1. The Cartesian coordinates of B₁₂N₁₂ cluster.

Atom	X	Y	Z
B	0.000000	0.961353	1.971395
B	0.000000	-0.961353	1.971395
B	-0.961353	1.971395	0.000000
B	1.971395	0.000000	0.961353
B	0.961353	1.971395	0.000000
B	0.000000	0.961353	-1.971395
B	1.971395	0.000000	-0.961353
B	0.000000	-0.961353	-1.971395
B	-0.961353	-1.971395	0.000000
B	0.961353	-1.971395	0.000000
N	0.000000	2.124351	1.123613
N	-2.124351	1.123613	0.000000
N	-2.124351	-1.123613	0.000000
N	0.000000	-2.124351	1.123613
N	2.124351	1.123613	0.000000
N	0.000000	2.124351	-1.123613
N	1.123613	0.000000	-2.124351
N	-1.123613	0.000000	-2.124351
N	0.000000	-2.124351	-1.123613
N	2.124351	-1.123613	0.000000
B	-1.971395	0.000000	-0.961353
N	1.123613	0.000000	2.124351
N	-1.123613	0.000000	2.124351
B	-1.971395	0.000000	0.961353

Table S2. The Cartesian coordinates of B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	1.857115	0.791628	0.000000
B	-1.817291	0.582934	0.922740
B	0.485257	0.413626	-1.895363
B	-1.817291	0.582934	-0.922740
B	-1.825456	-1.682353	0.000000
B	-0.480137	-1.236475	-1.932532
B	-0.144514	-2.623150	0.000000

B	1.718780	-1.422956	0.955638
B	1.718780	-1.422956	-0.955638
N	-1.661961	1.708331	0.000000
N	-0.957362	0.169065	2.026471
N	0.972047	-0.977818	2.104410
N	2.428132	-0.539679	0.000000
N	-0.957362	0.169065	-2.026471
N	-2.452204	-0.401917	0.000000
N	-1.054238	-2.276415	-1.122592
N	-1.054238	-2.276415	1.122592
N	1.287895	-2.476131	0.000000
N	0.972047	-0.977818	-2.104410
B	-0.480137	-1.236475	1.932532
N	1.208256	1.429952	-1.149496
N	1.208256	1.429952	1.149496
B	0.485257	0.413626	1.895363
Ni	0.068689	2.476317	0.000000

Table S3. The Cartesian coordinates of B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.0855160	0.8376760	1.9089440
B	0.9005710	-0.8298980	1.9367550
B	-1.5448870	1.5377880	0.0000010
B	2.1440120	0.9878740	0.9592990
B	0.3146030	2.1994750	0.0000020
B	-0.0855140	0.8376790	-1.9089420
B	2.1440130	0.9878750	-0.9592960
B	0.9005730	-0.8298950	-1.9367550
B	0.6484050	-2.2074450	-0.0000020
B	2.2814100	-1.2227060	0.0000000
N	-0.6080000	1.9090070	1.1195900
N	-0.7915950	-2.0838650	-0.0000020
N	1.5273740	-1.8457890	1.1248130
N	1.7443530	2.0451070	0.0000030
N	-0.6079990	1.9090090	-1.1195870
N	1.3725180	0.5575490	-2.0958380
N	-0.5636270	-0.5721670	-2.0424950
N	1.5273750	-1.8457870	-1.1248150
N	2.8477700	0.0937310	0.0000010
B	-1.3379350	-1.1206930	-0.9542550
N	1.3725160	0.5575450	2.0958410
N	-0.5636290	-0.5721710	2.0424930
B	-1.3379360	-1.1206940	0.9542510
Ni	-2.6967280	-0.0482270	-0.0000010

Table S4. The Cartesian coordinates of acetylene adsorption on B₁₂N₁₂ cluster.

Atom	X	Y	Z
B	0.399751	-0.446463	1.965937
B	-1.304634	0.443951	1.968929
B	1.770015	-0.062442	-0.000019
B	-1.367892	-1.746715	0.960743
B	0.844734	-1.759209	-0.000013
B	0.399701	-0.446452	-1.965941
B	-1.367916	-1.746709	-0.960710
B	-1.304683	0.443962	-1.968885
B	-1.755347	1.764843	0.000032
B	-2.646717	0.060696	0.000038
N	1.430583	-0.985196	1.121782
N	1.524622	1.363380	-0.000011
N	-0.465994	2.404446	0.000017
N	-2.337505	0.984052	1.123013
N	-0.444472	-2.403870	0.000002
N	1.430555	-0.985189	-1.121815
N	-0.973770	-0.995896	-2.123668
N	0.066841	0.993581	-2.123568
N	-2.337532	0.984059	-1.122939
N	-2.435512	-1.363568	0.000031
B	0.458548	1.743090	-0.958753
N	-0.973716	-0.995909	2.123695
N	0.066895	0.993568	2.123581
B	0.458572	1.743084	0.958760
C	4.635310	0.610215	-0.000122
H	4.569925	1.674919	-0.000184
C	4.685133	-0.597544	-0.000075
H	4.729788	-1.663326	-0.000067

Table S5. The Cartesian coordinates of acetylene adsorption on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.307135	-1.874090	-0.316959
B	-0.131527	1.858838	-0.924327
B	-0.348809	-0.695574	1.703422
B	-0.469021	1.676021	0.876750
B	1.921209	1.876873	0.397468
B	1.214181	0.344266	2.100502
B	2.940640	0.244041	0.434549
B	2.029296	-1.572210	-0.864429
B	1.700077	-1.744523	1.009388
N	-1.387019	1.561862	-0.250066
N	0.522757	1.132368	-2.006332
N	1.751437	-0.746659	-2.010976
N	1.034908	-2.398348	-0.143325
N	-0.211941	0.745749	1.973026
N	0.630189	2.449169	0.216184
N	2.348156	1.033957	1.544497
N	2.752555	1.234632	-0.656657
N	2.878254	-1.188105	0.293852

N	1.020879	-1.126246	2.119050
B	1.906902	0.695671	-1.688987
N	-1.177507	-1.408891	0.758240
N	-0.769253	-1.124201	-1.492240
B	0.322285	-0.320586	-2.007910
Ni	-2.155375	-0.218077	-0.476971
C	-4.185895	0.769012	0.388618
H	-4.082693	1.812601	0.179889
C	-4.282953	-0.413600	0.650446
H	-4.398109	-1.439564	0.926791

Table S6. The Cartesian coordinates of acetylene adsorption on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.760179	1.411264	-0.915299
B	-0.759946	1.412758	0.913468
B	-1.552783	-1.438175	0.000766
B	0.090395	-0.758364	-1.884668
B	1.394388	2.134495	-0.001611
B	1.366698	0.705046	-1.920760
B	2.275814	-1.305245	-0.958865
B	2.805264	0.845573	-0.000669
B	2.275754	-1.303803	0.960671
B	0.090462	-0.755368	1.885774
B	1.366836	0.707990	1.919701
N	-0.120740	0.712134	-2.000798
N	-0.603361	-1.740885	-1.113802
N	-0.603433	-1.738606	1.115924
N	-0.120516	0.715310	2.000065
N	2.180682	1.594893	-1.126848
N	1.576850	-0.745904	-2.084229
N	3.126679	-0.551165	0.000359
N	1.703001	-2.281347	0.001656
N	1.576855	-0.742792	2.085218
N	2.180843	1.596613	1.124444
B	0.279125	-2.159868	0.001446
N	-0.040612	2.292662	-0.001669
Ni	-2.464627	0.780855	-0.000114
C	-3.138577	-1.372078	0.000038
C	-3.994609	-0.336150	0.000324
H	-3.469067	-2.427913	-0.000735
H	-5.075157	-0.444562	-0.000237

Table S7. The Cartesian coordinates of hydrogen adsorption on B₁₂N₁₂ cluster.

Atom	X	Y	Z
B	0.383130	0.015555	2.169436
B	1.719075	0.912633	1.117480
B	-0.803148	-1.738877	1.011857
B	-0.473306	1.905878	0.937871
B	-1.799325	-0.099720	1.144907
B	-1.583307	-0.912152	-1.117478
B	-1.433144	1.453841	-0.665179

B	-0.247752	-0.015219	-2.169399
B	1.934637	0.100286	-1.145004
B	0.938583	1.739178	-1.011904
N	-0.848522	-0.727227	2.099178
N	0.388493	-2.335440	0.467281
N	1.948499	-1.287499	-0.761721
N	2.104394	1.256069	-0.226492
N	-1.812661	1.287721	0.761689
N	-1.969015	-1.256014	0.226543
N	-1.574209	0.456986	-1.694458
N	-0.410846	-1.457470	-1.850138
N	0.983770	0.727540	-2.099328
N	-0.253116	2.335885	-0.467551
B	0.608879	-1.905860	-0.938188
N	0.546384	1.457623	1.850074
N	1.709645	-0.456958	1.694579
B	1.568209	-1.453640	0.665257
H	-5.025915	0.331270	0.012990
H	-4.726451	-0.349305	-0.008874

Table S8. The Cartesian coordinates of hydrogen adsorption on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.412904	2.063227	0.114341
B	0.402228	1.291981	-1.570034
B	0.411859	0.396658	1.931119
B	-1.853035	1.595000	-0.679897
B	-1.307676	1.188195	1.624377
B	-1.347559	-1.214631	1.606018
B	-2.689003	0.013586	0.032255
B	-1.376239	-1.999309	-0.150457
B	0.327469	-1.214188	-1.630460
B	-1.372320	-0.391482	-1.928583
N	0.053082	1.761032	1.493480
N	1.428525	-0.489115	1.452467
N	1.467309	-1.577604	-0.737182
N	0.009986	0.059021	-2.254359
N	-2.387258	1.313907	0.676137
N	-0.953749	-0.057228	2.348095
N	-2.440875	-1.289319	0.599305
N	-0.409761	-2.172787	0.958584
N	-1.030026	-1.790510	-1.534179
N	-2.422835	0.408261	-1.378945
B	0.874707	-1.561577	0.695364
N	-0.605584	2.217550	-0.973591
N	1.517804	1.524700	-0.673276
H	3.604867	-0.821657	0.578880
H	1.953539	-2.436190	-0.992704
Ni	2.587092	0.109471	0.012781

Table S9. The Cartesian coordinates of hydrogen adsorption on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.048360	0.862995	1.900480
B	0.948060	-0.852486	1.927612
B	-1.367644	1.770368	0.001432
B	2.287829	0.898813	0.957955
B	0.535886	2.193984	-0.001983
B	0.042431	0.859091	-1.900614
B	2.284803	0.896937	-0.965030
B	0.941996	-0.856236	-1.927136
B	0.635864	-2.245173	0.002042
B	2.308076	-1.317833	-0.001412
N	-0.419014	1.964393	1.115879
N	-0.796061	-2.055936	0.004064
N	1.527874	-1.902420	1.125338
N	1.945898	1.979075	-0.004034
N	-0.422426	1.961739	-1.116263
N	1.482683	0.508189	-2.094242
N	-0.508616	-0.513810	-2.008248
N	1.524373	-1.904578	-1.124598
N	2.937823	-0.029458	-0.003639
B	-1.270695	-1.017019	-0.896700
N	1.489147	0.512301	2.090406
N	-0.502365	-0.509760	2.012253
B	-1.266962	-1.014247	0.903275
Ni	-2.908558	-0.103526	0.001228
H	-4.432279	0.218523	-0.014975
H	-2.583342	1.716083	0.002570

Table S10. The Cartesian coordinates of CO on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.265485	1.111173	-1.757757
B	-1.466887	-0.401179	-1.979650
B	1.460118	1.496647	0.073898
B	-2.410952	1.369717	-0.656740
B	-0.389855	2.140694	0.333900
B	-0.057499	0.433775	1.941226
B	-2.306943	1.043096	1.230130
B	-1.284910	-1.061493	1.802829
B	-1.347196	-2.130341	-0.339363
B	-2.808993	-0.933876	-0.058186
N	0.424843	2.001527	-0.890002
N	0.090727	-2.218429	-0.424880
N	-2.208125	-1.451590	-1.322139
N	-1.820732	2.190587	0.430850
N	0.567431	1.534083	1.289187
N	-1.532259	0.332123	2.210598
N	0.204975	-1.029316	1.831956
N	-2.100313	-1.835633	0.894208
N	-3.183145	0.425304	0.196300
B	0.807916	-1.494560	0.611160

N	-1.756957	1.041233	-1.896659
N	0.019338	-0.310686	-2.101055
B	0.737901	-1.130468	-1.158874
Ni	2.476765	-0.644691	-0.089803
C	2.982856	1.450343	-0.189672
C	3.867711	0.616938	0.415159
H	3.301367	2.058047	-1.049673
H	4.953651	0.654341	0.378885
H	3.814569	-1.782052	0.117618
H	3.201050	-2.253025	-0.026696

Table S11. The Cartesian coordinates of TS1 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.283153	1.279055	-1.663251
B	-1.506328	-0.199219	-1.988027
B	1.491625	1.478722	0.135131
B	-2.396976	1.451254	-0.488881
B	-0.342129	2.102563	0.513203
B	0.006510	0.235532	1.944632
B	-2.250166	0.947194	1.355349
B	-1.249687	-1.217862	1.709817
B	-1.371296	-2.078172	-0.522620
B	-2.809177	-0.894637	-0.097233
N	0.440316	2.088387	-0.740983
N	0.063191	-2.178657	-0.649278
N	-2.244940	-1.299522	-1.416951
N	-1.767621	2.159309	0.655414
N	0.631887	1.383775	1.370931
N	-1.461968	0.138777	2.244059
N	0.237366	-1.221620	1.715272
N	-2.096021	-1.890524	0.749635
N	-3.159531	0.439673	0.291397
B	0.818467	-1.614063	0.455032
N	-1.778250	1.233676	-1.770611
N	-0.023427	-0.113129	-2.127378
B	0.705318	-1.022295	-1.279152
Ni	2.413056	-0.663469	-0.157933
C	2.991557	1.349180	-0.210547
C	3.918929	0.553083	0.420453
H	3.298507	1.908206	-1.102516
H	4.991189	0.541287	0.243520
H	3.638920	-0.966867	0.777131
H	3.090835	-1.840451	0.624005

Table S12. The Cartesian coordinates of IM1 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.243690	0.768253	-1.938843
B	-1.530337	-0.667165	-1.902333
B	1.530589	1.362036	-0.151808
B	-2.354398	1.332421	-0.862705
B	-0.280446	2.105917	-0.017496

B	-0.040538	0.685863	1.886372
B	-2.247682	1.312497	1.053999
B	-1.340704	-0.708234	1.986747
B	-1.391935	-2.051614	0.025837
B	-2.846729	-0.824149	0.107120
N	0.524252	1.731184	-1.202287
N	0.043992	-2.169936	-0.033421
N	-2.274068	-1.559946	-1.050051
N	-1.699230	2.280070	0.075857
N	0.641802	1.599657	1.030467
N	-1.516447	0.743442	2.151204
N	0.134397	-0.778128	2.082448
N	-2.166280	-1.580015	1.193756
N	-3.161485	0.578620	0.136664
B	0.802092	-1.592879	1.089166
N	-1.744176	0.787682	-2.042209
N	-0.067339	-0.697718	-2.093177
B	0.722883	-1.378507	-1.079131
Ni	2.481026	-0.782044	-0.315276
C	3.079828	1.251703	-0.226625
C	3.862067	0.836420	0.820221
H	3.569267	1.441258	-1.186978
H	4.936003	0.706663	0.722255
H	3.445438	0.722664	1.819026
H	2.025721	-1.768675	1.182459

Table S13. The Cartesian coordinates of TS2 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.404348	0.970149	-1.875938
B	-1.557592	-0.593817	-1.895084
B	1.383729	1.596892	-0.165100
B	-2.503923	1.246952	-0.679862
B	-0.473899	2.177112	0.125646
B	0.016750	0.625397	1.856336
B	-2.288807	1.091541	1.220365
B	-1.147994	-0.912802	1.913654
B	-1.265689	-2.160566	-0.120704
B	-2.768397	-1.010520	0.136139
N	0.295140	1.961526	-1.122853
N	0.170403	-2.194992	-0.276258
N	-2.211040	-1.612187	-1.108287
N	-1.895310	2.183459	0.298392
N	0.554658	1.693339	1.078614
N	-1.435473	0.500258	2.214132
N	0.336680	-0.828658	1.868388
N	-1.971811	-1.795046	1.121322
N	-3.187928	0.351493	0.292618
B	0.936001	-1.435616	0.707735
N	-1.900474	0.839403	-1.920192
N	-0.091212	-0.465926	-2.113108
B	0.738489	-1.181801	-1.174785
Ni	2.554070	-0.775910	-0.203568

C	2.859930	1.312749	-0.386715
C	3.729397	0.884798	0.626577
H	3.259126	1.412263	-1.398711
H	4.793169	0.767595	0.445494
H	3.439462	0.974316	1.669093
H	3.491271	-1.107277	0.973469

Table S14. The Cartesian coordinates of IM2 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.266738	0.419330	-2.015570
B	-1.629480	-0.939468	-1.693104
B	1.634554	1.319086	-0.459215
B	-2.322821	1.260110	-1.011401
B	-0.185899	2.115549	-0.402876
B	0.113679	1.032341	1.653058
B	-2.127335	1.574159	0.865157
B	-1.237625	-0.310588	2.069499
B	-1.550494	-2.025744	0.434361
B	-2.876732	-0.656936	0.343597
N	0.547342	1.463321	-1.506344
N	-0.133306	-2.298722	0.332404
N	-2.411293	-1.627165	-0.690090
N	-1.603193	2.333748	-0.291362
N	0.773918	1.827861	0.682639
N	-1.345213	1.151793	1.997373
N	0.251027	-0.419611	2.013675
N	-2.180869	-1.257998	1.519757
N	-3.119849	0.737170	0.134292
B	0.728880	-1.353027	1.035399
N	-1.769287	0.469397	-2.078750
N	-0.157429	-1.075037	-1.905450
B	0.536226	-1.655256	-0.793952
Ni	2.332861	-1.025535	-0.139975
C	3.042896	0.842845	-0.503254
C	4.010244	1.072020	0.658205
H	3.509253	0.753953	-1.491964
H	4.749951	0.268357	0.780309
H	4.585406	1.997273	0.512805
H	3.472441	1.175125	1.606663

Table S15. The Cartesian coordinates of TS3 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.309452	0.906361	-1.878506
B	-1.543304	-0.591285	-1.893438
B	1.480140	1.472768	-0.144697
B	-2.411868	1.323629	-0.731324
B	-0.347466	2.162106	0.095597
B	0.022733	0.623824	1.863925
B	-2.241019	1.196703	1.174240
B	-1.221081	-0.851016	1.927888
B	-1.367979	-2.130359	-0.081850

B	-2.813167	-0.898466	0.122971
N	0.427433	1.878265	-1.133233
N	0.062649	-2.247202	-0.209909
N	-2.267328	-1.554403	-1.098443
N	-1.771527	2.246346	0.239579
N	0.634847	1.651815	1.084572
N	-1.439937	0.582187	2.197292
N	0.266043	-0.843462	1.905718
N	-2.078573	-1.703449	1.139098
N	-3.162930	0.487353	0.244993
B	0.859880	-1.482437	0.749284
N	-1.808829	0.858549	-1.951103
N	-0.070521	-0.548484	-2.092602
B	0.706448	-1.295495	-1.123950
Ni	2.422370	-0.749402	-0.206203
C	2.944931	1.180031	-0.371114
C	3.870889	0.401492	0.674939
H	3.404196	1.327371	-1.347386
H	4.907604	0.225247	0.406962
H	3.738444	1.672334	0.476229
H	3.619881	0.434910	1.732508

Table S16. The Cartesian coordinates of IM3 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.170569	0.830963	-1.871915
B	-1.478556	-0.599144	-1.936129
B	1.551847	1.345125	-0.018179
B	-2.307229	1.386119	-0.855674
B	-0.253171	2.135645	0.083770
B	-0.067930	0.646199	1.901120
B	-2.254620	1.296193	1.059805
B	-1.381407	-0.778786	1.910475
B	-1.484377	-2.106296	-0.078785
B	-2.867968	-0.791972	0.017907
N	0.576092	1.754520	-1.081034
N	-0.054306	-2.291555	-0.124959
N	-2.290376	-1.503943	-1.157165
N	-1.676130	2.297599	0.131333
N	0.642878	1.629060	1.149172
N	-1.547974	0.668539	2.142474
N	0.106145	-0.830928	1.962102
N	-2.233628	-1.608057	1.091091
N	-3.153205	0.611253	0.091356
B	0.704278	-1.478586	0.819272
N	-1.660953	0.862200	-2.029133
N	0.006018	-0.635015	-2.061182
B	0.662348	-1.376845	-1.011424
Ni	2.368917	-0.804501	-0.056256
C	3.175374	1.383712	-0.105668
C	4.058988	0.169360	0.181546
H	3.384489	1.784654	-1.101204
H	4.846030	-0.026990	-0.547426

H	3.353820	2.157432	0.658521
H	4.414654	0.073717	1.210398

Table S17. The Cartesian coordinates of CO2 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.716951	1.986488	-0.178217
B	-1.053845	0.048227	0.994349
B	-0.995905	-0.875195	-1.312093
B	0.813377	0.995135	-1.866652
B	0.933188	1.371895	1.589705
B	1.742974	1.985796	-0.557070
B	2.828627	-0.112632	-1.044973
B	2.643364	0.626589	1.240790
B	2.495833	-1.546284	0.190985
B	0.149426	-2.009437	0.570525
B	0.985547	-0.977501	1.959628
N	0.383107	2.187628	-1.095284
N	0.142596	-0.246990	-2.073382
N	-0.203742	-2.061388	-0.812205
N	-0.439963	-1.117646	1.596849
N	2.074672	1.943145	0.844664
N	2.286112	1.096697	-1.596720
N	3.296810	-0.301731	0.356486
N	2.304881	-1.476440	-1.281728
N	1.538778	-2.069602	1.129298
N	1.634009	0.267069	2.271658
B	0.892921	-1.413697	-1.559741
N	-0.442377	1.375835	1.138109
H	-2.176095	-0.939209	-1.753341
H	-1.863002	2.169176	-0.516244
Ni	-2.676401	0.043311	-0.311404
C	-4.606370	-0.505683	0.198781
C	-4.261026	0.502046	0.837406
H	-5.144148	-1.334789	-0.215539
H	-4.290114	1.340989	1.506917

Table S18. The Cartesian coordinates of TS1 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.770635	1.981119	-0.068332
B	-0.873992	0.193190	1.311314
B	-1.113907	-0.876739	-0.819136
B	0.457278	0.812294	-1.933149
B	1.181913	1.518722	1.427016
B	1.587126	1.900946	-0.883706
B	2.581968	-0.242607	-1.365809
B	2.797001	0.705823	0.840884
B	2.469020	-1.552383	0.039039
B	0.230159	-1.934715	0.865327
B	1.292391	-0.794125	1.988667
N	0.150437	2.052588	-1.188656
N	-0.234890	-0.447981	-1.940674

N	-0.353109	-2.099382	-0.435829
N	-0.176527	-0.940220	1.886139
N	2.168942	1.988927	0.430705
N	1.949692	0.919659	-1.923579
N	3.282510	-0.311311	-0.055270
N	2.029301	-1.617689	-1.382164
N	1.689126	-1.968760	1.175870
N	1.990552	0.459104	2.064262
B	0.595355	-1.574974	-1.444580
N	-0.248343	1.514912	1.239368
H	-2.842232	-1.036870	-0.862113
H	-1.955010	2.195630	-0.186373
Ni	-2.520759	0.145159	0.124554
C	-4.303039	-0.673845	-0.487791
C	-4.455790	0.303790	0.321237
H	-4.749145	-1.432724	-1.109687
H	-5.221614	0.898161	0.791116

Table S19. The Cartesian coordinates of IM1 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.862700	1.824118	-0.544032
B	0.782832	-0.444808	-1.119415
B	0.895083	-0.657773	0.980250
B	-0.457049	1.480709	1.500248
B	-1.088786	0.947999	-1.841774
B	-1.505347	2.212973	0.126901
B	-2.656797	0.442967	1.302852
B	-2.787726	0.549711	-1.100315
B	-2.671150	-1.290931	0.466649
B	-0.504635	-2.178687	-0.097285
B	-1.435480	-1.401497	-1.586807
N	-0.066413	2.394183	0.405086
N	0.140354	0.231087	1.900047
N	0.090522	-1.892370	1.179297
N	0.011262	-1.642788	-1.382649
N	-2.047448	1.837756	-1.152924
N	-1.936236	1.677727	1.430823
N	-3.364583	-0.032957	0.084174
N	-2.216122	-0.871830	1.821901
N	-1.953055	-2.167937	-0.424331
N	-1.990333	-0.188867	-2.113712
B	-0.781555	-0.935045	1.898723
N	0.330749	0.878964	-1.552278
H	4.581772	1.819366	0.161071
H	2.050922	1.932362	-0.411469
Ni	2.575965	-0.400436	-0.072437
C	5.123909	0.873333	0.121485
C	4.485673	-0.308694	0.015051
H	6.211758	0.965305	0.175639
H	5.119712	-1.202110	-0.014236

Table S20. The Cartesian coordinates of TS2 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	1.229975	0.837564	-1.051292
B	0.542991	-1.140000	-1.144049
B	0.928872	-0.852293	1.183613
B	0.196238	1.575410	1.080209
B	-1.012719	0.488117	-2.091885
B	-0.755274	2.202181	-0.446498
B	-2.206092	1.239756	1.232669
B	-2.609169	0.783581	-1.098386
B	-2.777018	-0.565804	0.901645
B	-0.973392	-2.115599	0.483168
B	-1.877138	-1.516448	-1.112088
N	0.692884	1.938136	-0.272598
N	0.481984	0.409668	1.871267
N	-0.199223	-1.713894	1.619401
N	-0.518311	-2.089588	-0.929904
N	-1.565984	1.744547	-1.548785
N	-1.159695	2.190441	0.973704
N	-3.160218	0.703287	0.226727
N	-2.084407	0.026473	2.075910
N	-2.408516	-1.793420	0.243608
N	-2.197536	-0.378535	-1.931170
B	-0.716754	-0.420241	2.125499
N	0.364913	0.066561	-1.960861
H	3.879490	1.590610	1.232351
H	2.884966	0.593477	-0.900517
Ni	2.254521	-0.700735	-0.196604
C	4.565173	0.980784	0.647250
C	4.115339	0.094680	-0.258471
H	5.627297	1.121848	0.847468
H	4.824757	-0.445002	-0.891187

Table S21. The Cartesian coordinates of IM2 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-1.009042	-1.388325	0.424467
B	-0.649912	-0.826390	-1.390854
B	-1.124440	1.356031	-0.059992
B	-0.025985	0.332978	1.947655
B	1.198569	-2.118622	-0.432900
B	1.052770	-1.248085	1.787824
B	2.309766	0.787454	1.459366
B	2.751087	-1.135862	0.072658
B	2.637360	1.235042	-0.379624
B	0.634272	1.266908	-1.736657
B	1.696503	-0.334484	-1.941032
N	-0.422530	-1.082423	1.720455
N	-0.488599	1.524106	1.292696
N	-0.098265	2.107481	-0.837608
N	0.259173	-0.082709	-2.234768
N	1.865474	-2.021237	0.879074

N	1.399141	0.084500	2.323420
N	3.223406	0.161183	0.466937
N	2.001184	2.026305	0.704783
N	2.113476	1.066280	-1.710673
N	2.235292	-1.495375	-1.277249
B	0.585299	2.134906	0.476999
N	-0.223751	-2.011416	-0.646144
H	-3.923791	1.458561	1.133931
H	-4.141531	-1.015740	1.437934
Ni	-2.288172	-0.160640	-0.446880
C	-4.250149	0.815857	0.322414
C	-4.375061	-0.538567	0.491176
H	-4.612050	1.311803	-0.575028
H	-4.831812	-1.165054	-0.271739

Table S22. The Cartesian coordinates of IM3 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.829687	1.737888	0.110493
B	-0.857177	0.013351	1.691746
B	-0.996835	-0.851742	-0.974898
B	0.479138	0.892910	-1.911003
B	1.181349	1.404372	1.542784
B	1.512645	1.970866	-0.732707
B	2.663223	-0.036109	-1.389906
B	2.836605	0.753814	0.885687
B	2.624153	-1.446978	-0.086573
B	0.396443	-1.969736	0.739949
B	1.439216	-0.916433	1.936967
N	0.065074	2.003223	-1.008836
N	-0.121494	-0.395763	-2.101257
N	-0.170301	-2.027999	-0.573964
N	-0.019477	-1.149183	1.911672
N	2.112803	2.014605	0.575282
N	1.954712	1.124373	-1.857664
N	3.373008	-0.160949	-0.087668
N	2.193634	-1.439197	-1.505487
N	1.866686	-1.982658	1.013395
N	2.070360	0.365394	2.099586
B	0.758731	-1.468130	-1.583661
N	-0.247550	1.322237	1.413423
H	-4.485363	-1.112394	-1.291060
H	-5.005821	1.171005	-0.411071
Ni	-2.515972	0.148139	-0.081140
C	-4.389233	-0.881051	-0.232506
C	-4.687280	0.370482	0.252177
H	-4.262268	-1.732922	0.431167
H	-4.788580	0.555708	1.317997
H	-2.086030	-0.064594	1.738784
H	-2.046839	1.959784	0.074318

Table S23. The Cartesian coordinates of TS3 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.589977	-1.478751	1.354198
B	-0.781797	-1.560935	-0.948380
B	-1.376115	1.055201	0.134157
B	0.364572	0.789525	1.952274
B	1.449180	-2.005563	0.036852
B	1.672342	-0.594185	1.927287
B	2.409054	1.377614	0.766959
B	2.907385	-0.804671	-0.140259
B	2.249337	1.290319	-1.145704
B	0.042414	0.622322	-1.920623
B	1.342939	-0.770647	-1.983348
N	0.230569	-0.663401	2.229717
N	-0.455764	1.648254	1.150943
N	-0.641384	1.560973	-1.080118
N	-0.128391	-0.852608	-2.033342
N	2.380034	-1.501423	1.063307
N	1.859309	0.866811	1.993129
N	3.198866	0.601297	-0.228736
N	1.704625	2.275015	-0.179561
N	1.508860	0.676365	-2.213700
N	2.191151	-1.602170	-1.171638
B	0.286034	2.088773	-0.054980
N	0.015483	-2.104943	0.163705
H	-3.477405	1.352801	1.414017
H	-5.012569	-0.040005	0.016700
Ni	-2.471268	-0.597147	0.086508
C	-3.246004	1.216283	0.357077
C	-4.135571	0.404431	-0.449005
H	-2.921820	2.162557	-0.101688
H	-4.217110	0.592851	-1.516312
H	-2.016921	-1.825463	-0.984254
H	-1.789575	-1.621096	1.552790

Table S24. The Cartesian coordinates of IM4 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.752511	-1.723360	-0.938464
B	0.777959	-1.373747	1.388296
B	1.458656	1.684024	-0.250201
B	-0.219955	0.456061	-1.982297
B	-1.360577	-2.023150	0.315152
B	-1.465836	-0.987608	-1.798185
B	-2.419399	1.101292	-1.109988
B	-2.874375	-0.898237	0.160082
B	-2.403899	1.383062	0.788524
B	-0.187473	1.018381	1.775598
B	-1.432255	-0.417782	2.034376
N	0.005848	-1.022047	-1.961307
N	0.457051	1.539754	-1.353402
N	0.468462	1.881447	0.853479

N	0.041582	-0.404806	2.168753
N	-2.217253	-1.771127	-0.852800
N	-1.715044	0.411684	-2.154881
N	-3.246088	0.474188	-0.040488
N	-1.859098	2.215074	-0.310859
N	-1.681312	1.024848	1.976790
N	-2.199392	-1.440251	1.371808
B	-0.437408	2.083021	-0.299154
N	0.076752	-2.100376	0.315534
H	3.381682	1.931177	-1.270546
H	4.607035	0.571789	0.401139
Ni	2.664118	-0.909499	-0.130312
C	2.988875	1.929321	-0.247661
C	3.523010	0.702731	0.540507
H	3.265716	2.886498	0.219883
H	3.330109	0.813817	1.614200
H	1.970564	-1.566802	1.536417
H	1.918004	-2.131343	-1.116518

Table S25. The Cartesian coordinates of TS4 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.797925	-1.652793	-0.914949
B	0.885901	-1.096153	1.105836
B	1.374235	1.540273	-0.409776
B	-0.340091	0.394652	-2.032186
B	-1.254690	-2.081815	0.443675
B	-1.505746	-1.086482	-1.705657
B	-2.490580	1.005976	-1.055598
B	-2.794147	-0.956035	0.320572
B	-2.377373	1.370235	0.826615
B	-0.113478	1.137691	1.690578
B	-1.277443	-0.353967	2.079106
N	-0.050564	-1.055185	-1.942004
N	0.343934	1.527287	-1.481533
N	0.476027	1.984270	0.700463
N	0.199764	-0.262949	2.069153
N	-2.177899	-1.856316	-0.689078
N	-1.835648	0.293257	-2.114043
N	-3.224298	0.396702	0.087374
N	-1.924266	2.175269	-0.336764
N	-1.584370	1.086864	1.990714
N	-2.043292	-1.431602	1.512704
B	-0.498775	2.117834	-0.410431
N	0.180884	-2.132874	0.354836
H	3.320396	1.245285	-1.455207
H	4.668120	0.451863	0.504939
Ni	2.530993	-0.823301	-0.086701
C	2.951618	1.523195	-0.458734
C	3.612255	0.693681	0.661551
H	3.227332	2.587410	-0.337298
H	3.483669	1.150803	1.643172
H	2.504627	-0.481407	1.322306
H	1.994220	-1.972926	-1.218867

Table S26. The Cartesian coordinates of IM5 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.304615	-2.109345	0.668569
B	-0.662162	-1.121374	-1.308021
B	-1.647585	0.867811	0.593356
B	0.368286	-0.104082	2.070331
B	1.668808	-1.746221	-0.797554
B	1.837975	-1.177793	1.506014
B	2.273868	1.171631	1.232282
B	2.956118	-0.381102	-0.482081
B	2.019469	1.843123	-0.547331
B	-0.155961	1.299954	-1.483976
B	1.285367	0.192484	-2.123450
N	0.438030	-1.563658	1.780035
N	-0.579848	0.878974	1.669460
N	-0.896330	1.779386	-0.359566
N	-0.173514	-0.037059	-2.134249
N	2.591985	-1.565687	0.341955
N	1.847487	0.147063	2.143149
N	3.089939	0.965511	0.003177
N	1.426033	2.280736	0.741550
N	1.285466	1.623295	-1.761837
N	2.271817	-0.784145	-1.739193
B	0.047352	1.874618	0.771995
N	0.267196	-2.082078	-0.694206
H	-3.634950	0.011348	1.366827
H	-5.146866	1.359341	-0.140740
Ni	-2.290317	-1.093333	-0.167470
C	-3.234785	0.900332	0.836943
C	-4.089121	1.247259	-0.397872
H	-3.346682	1.688643	1.598815
H	-3.735158	2.178380	-0.848486
H	-4.030691	0.481878	-1.188074
H	-1.445777	-2.536698	0.833807

Table S27. The Cartesian coordinates of TS5 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.377522	-1.679218	-0.903226
B	0.546058	-1.576825	1.030927
B	1.766366	1.345540	-0.345290
B	-0.189458	0.578854	-1.966744
B	-1.778839	-1.924414	0.238170
B	-1.681165	-0.665894	-1.784851
B	-2.204063	1.516769	-0.945495
B	-2.982977	-0.446355	0.222877
B	-2.047766	1.648385	0.960239
B	0.101441	0.791523	1.758536
B	-1.394183	-0.406744	2.034596
N	-0.223925	-0.916550	-1.958030
N	0.695569	1.528361	-1.381828
N	0.865317	1.567349	0.845323

N	0.069383	-0.670438	2.044942
N	-2.560442	-1.361525	-0.876073
N	-1.681320	0.776866	-2.061587
N	-3.086610	0.979744	0.127690
N	-1.411277	2.450112	-0.110228
N	-1.348761	1.062157	2.068590
N	-2.395881	-1.204812	1.364125
B	-0.035320	2.073218	-0.214776
N	-0.389520	-2.314001	0.163239
H	3.727694	1.508180	-1.353452
H	5.142440	1.463615	0.776174
Ni	2.176534	-1.531083	-0.163413
C	3.288902	1.719195	-0.373440
C	4.117086	1.080244	0.753341
H	3.311353	2.815619	-0.250043
H	3.663720	1.262861	1.733509
H	4.189086	-0.009421	0.617651
H	2.471023	-0.522187	-1.235646

Table S28. The Cartesian coordinates of IM6 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	0.103977	1.874493	-0.850691
B	-0.081382	1.738872	1.003067
B	-2.120975	-0.759191	-0.345692
B	0.066963	-0.430307	-1.949551
B	2.242039	1.582413	0.283074
B	1.831138	0.428068	-1.771174
B	1.806438	-1.838801	-0.976739
B	3.029079	-0.153274	0.232917
B	1.614605	-1.979792	0.912911
B	-0.303791	-0.698303	1.713301
B	1.447915	0.145557	2.022397
N	0.468898	1.035024	-1.935796
N	-1.007116	-1.139535	-1.385784
N	-1.230158	-1.293079	0.840723
N	0.072631	0.744702	2.004437
N	2.853305	0.869860	-0.844576
N	1.479136	-0.956256	-2.065383
N	2.796089	-1.555158	0.104679
N	0.816002	-2.575866	-0.172358
N	1.062748	-1.260802	2.030905
N	2.627485	0.702637	1.392303
B	-0.463770	-1.904682	-0.254091
N	0.994447	2.320595	0.212200
H	-4.002284	-1.139282	-1.470095
H	-5.485237	-1.632750	0.530667
Ni	-1.779675	1.914816	-0.094944
C	-3.555396	-1.448922	-0.514834
C	-4.512764	-1.140307	0.646170
H	-3.403908	-2.536766	-0.589215
H	-4.083708	-1.466226	1.601079
H	-4.702939	-0.060447	0.725882
H	-2.477516	0.485892	-0.295993

Table S29. The Cartesian coordinates of TS6 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.133416	-1.921475	-0.758697
B	0.104512	-1.672760	1.094895
B	1.866185	0.326445	-0.364888
B	-0.139511	0.248576	-2.014844
B	-2.246757	-1.518780	0.416122
B	-1.900135	-0.517937	-1.727686
B	-1.761700	1.790861	-1.067810
B	-3.007910	0.226341	0.277700
B	-1.520007	2.045504	0.812565
B	0.335719	0.748981	1.695875
B	-1.412848	-0.004005	2.068437
N	-0.576541	-1.177760	-1.909969
N	0.995824	0.918396	-1.476436
N	1.277552	1.213466	0.734546
N	-0.064099	-0.637977	2.083222
N	-2.891878	-0.862394	-0.734512
N	-1.513941	0.845709	-2.122949
N	-2.726904	1.613310	0.053425
N	-0.715329	2.531849	-0.329495
N	-0.985824	1.401855	1.982725
N	-2.607400	-0.562789	1.478378
B	0.530699	1.809019	-0.393326
N	-1.011173	-2.266892	0.358919
H	4.301335	0.727337	-1.480437
H	5.395718	1.820840	0.612728
Ni	1.697256	-1.730576	-0.059266
C	3.758370	1.114302	-0.613902
C	4.542905	1.134798	0.681583
H	3.275706	2.057758	-0.869881
H	3.906350	1.465961	1.507671
H	4.940323	0.142956	0.930327
H	3.013587	-0.174589	-0.463759

Table S30. The Cartesian coordinates of IM7 on B₁₂N₁₁Ni cluster.

Atom	X	Y	Z
B	-0.476466	1.307053	-1.073656
B	-0.744379	1.362706	0.826080
B	-1.189170	-1.183348	-0.334196
B	0.580932	-0.761234	-1.987728
B	1.512794	2.090672	0.129788
B	1.799848	0.730105	-1.810652
B	2.602099	-1.279602	-0.757778
B	2.959398	0.862220	0.298057
B	2.344876	-1.311873	1.143980
B	0.067328	-0.797202	1.812026
B	1.296803	0.669258	2.038094
N	0.339733	0.704447	-2.103661
N	-0.211187	-1.745734	-1.320357
N	-0.515435	-1.735864	0.899485

N	-0.188753	0.662744	1.971542
N	2.466974	1.616914	-0.888642
N	2.075130	-0.712074	-1.972153
N	3.304735	-0.530117	0.318296
N	1.909521	-2.272250	0.101490
N	1.514227	-0.782488	2.192509
N	2.177211	1.579595	1.342896
B	0.486432	-2.186098	-0.091758
N	0.085778	2.190852	-0.051688
H	-6.102643	-0.871992	-0.474480
H	-5.082030	1.144019	0.731692
Ni	-2.130523	0.546180	-0.306183
C	-5.222049	-0.979783	0.166572
C	-4.472053	0.348517	0.294952
H	-5.557693	-1.332244	1.146859
H	-3.605779	0.234877	0.980834
H	-4.167727	0.720449	-0.703655
H	-4.572883	-1.746028	-0.266571

Table S31. The Cartesian coordinates of CO on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.427451	1.720169	0.308103
B	-0.209282	-1.978202	0.081578
B	0.476920	1.316552	-1.775633
B	0.105137	-1.215507	-1.623428
B	2.161043	-1.721780	-0.372145
B	2.079231	0.231032	-1.745266
B	3.033870	-0.206858	0.415210
B	1.573428	1.217313	1.672315
B	1.994409	1.908887	-0.057308
N	-1.160439	-1.438277	-0.907551
N	-0.070690	-1.636332	1.477045
N	0.950172	0.142771	2.386959
N	0.858306	2.199396	0.842442
N	0.710376	-0.071589	-2.271221
N	0.909648	-2.221376	-0.852689
N	2.947544	-0.647837	-1.009674
N	2.499218	-1.445882	1.045320
N	2.841339	1.135758	0.893456
N	1.880675	1.666503	-1.470871
B	1.301676	-1.168162	1.803420
N	-0.658742	1.925269	-1.144668
N	-1.195219	0.695799	0.997820
B	-0.347304	-0.185246	1.731371
Ni	-2.424484	-0.371043	-0.181202
C	-4.003477	0.770396	0.907748
C	-4.552841	0.263145	-0.058876
H	-3.584800	1.254006	1.764462
H	-5.182871	-0.109147	-0.838070
H	-2.761459	-0.216990	-1.577588
H	-1.541095	1.539671	-1.464053

Table S32. The Cartesian coordinates of TS1 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.439845	1.670394	0.430760
B	-0.181641	-1.975483	0.013163
B	0.427718	1.398200	-1.704586
B	0.095218	-1.129278	-1.683617
B	2.177850	-1.688431	-0.494325
B	2.047171	0.334302	-1.767357
B	3.049176	-0.206818	0.351895
B	1.602991	1.130687	1.716033
B	1.974294	1.914784	0.015249
N	-1.148660	-1.325757	-0.903728
N	-0.013959	-1.726435	1.415914
N	1.011069	0.013615	2.387820
N	0.858319	2.142797	0.951469
N	0.674096	0.042497	-2.291246
N	0.905993	-2.162772	-0.968702
N	2.934937	-0.575219	-1.094394
N	2.540439	-1.484863	0.925407
N	2.854574	1.104183	0.902907
N	1.833120	1.746048	-1.407572
B	1.359631	-1.259167	1.730990
N	-0.702407	1.941120	-1.012173
N	-1.178442	0.612233	1.089293
B	-0.310357	-0.289234	1.757123
Ni	-2.455122	-0.349364	-0.171043
C	-3.915392	0.749561	0.863184
C	-4.516028	0.222248	-0.075923
H	-3.567320	1.277814	1.725885
H	-5.290168	-0.107483	-0.736194
H	-3.220344	-0.567297	-1.380039
H	-1.584803	1.556397	-1.335617

Table S33. The Cartesian coordinates of IM1 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.047392	-2.076495	-0.047774
B	-0.309336	-1.310437	1.633565
B	0.378871	-0.300623	-1.718484
B	-2.384122	-1.497729	0.318687
B	-1.385968	-1.036878	-1.818558
B	-1.319045	1.363254	-1.660409
B	-3.002747	0.142011	-0.467557
B	-1.687202	2.078173	0.076436
B	-0.326281	1.237861	1.824536
B	-2.068447	0.405389	1.731623
N	-0.098342	-1.685993	-1.453071
N	1.347298	0.485800	-0.988909
N	0.906013	1.662146	1.220507
N	-0.778510	-0.101501	2.290828
N	-2.630618	-1.151628	-1.105093
N	-0.836999	0.220972	-2.383374

N	-2.603066	1.450473	-0.915367
N	-0.492161	2.217175	-0.791362
N	-1.650385	1.802101	1.484455
N	-3.027490	-0.325653	0.948178
B	0.697614	1.571139	-0.231039
N	-1.233735	-2.176431	0.826081
N	0.950111	-1.667654	0.957372
H	3.830263	1.609440	-1.323693
H	1.725346	1.153968	1.536716
Ni	2.285062	-0.756367	0.029296
C	3.827394	0.275469	0.320006
H	4.312401	-0.122811	1.221118
C	4.356634	1.213736	-0.458752
H	5.351556	1.615463	-0.258797

Table S34. The Cartesian coordinates of TS2 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.015387	-2.079653	0.378090
B	0.115174	-0.899858	1.792953
B	-0.016806	-0.787966	-1.773295
B	-2.213607	-1.294679	1.089606
B	-1.742097	-1.464850	-1.255827
B	-1.720260	0.877040	-1.797636
B	-3.033064	0.097817	0.051809
B	-1.678060	2.055348	-0.289961
B	0.090571	1.637424	1.235141
B	-1.596284	0.896506	1.792137
N	-0.393269	-2.037856	-1.030981
N	1.068178	0.111269	-1.511647
N	1.106448	1.940783	0.253468
N	-0.192867	0.493858	2.122542
N	-2.794529	-1.331042	-0.274588
N	-1.380727	-0.436054	-2.255842
N	-2.787465	1.219369	-0.817667
N	-0.740479	1.920520	-1.424620
N	-1.287398	2.167776	1.094665
N	-2.708427	0.037798	1.507597
B	0.563460	1.373913	-1.030601
N	-0.980187	-1.878433	1.490149
N	1.182401	-1.529789	1.024054
H	4.101603	1.199541	-1.161428
H	2.242675	1.443105	0.541650
Ni	2.292304	-0.730707	-0.261041
C	3.365350	0.773212	0.785493
H	3.528531	0.501976	1.826953
C	4.328058	0.871647	-0.147031
H	5.372291	0.643397	0.069228

Table S35. The Cartesian coordinates of IM2 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.038067	-1.662990	-1.269484
B	0.412147	-1.816435	0.525769
B	-0.397585	0.679378	-1.928261
B	-1.988556	-1.895609	0.073463
B	-1.993987	-0.354658	-1.762513
B	-2.059937	1.726354	-0.537210
B	-2.979657	-0.283036	0.429819
B	-1.693008	1.550062	1.329110
B	0.345941	0.365200	1.773821
B	-1.223586	-0.710042	2.012482
N	-0.626080	-0.746109	-2.188049
N	0.719074	1.354892	-1.296520
N	1.171254	1.227017	0.961654
N	0.194834	-1.100268	1.782579
N	-2.829131	-1.060963	-0.826801
N	-1.819007	1.119632	-1.820300
N	-2.894322	1.150031	0.550422
N	-1.037124	2.392272	0.299622
N	-1.005037	0.730012	2.293462
N	-2.378930	-1.270420	1.364578
B	0.291923	1.889101	0.003203
N	-0.711911	-2.442728	-0.238222
N	1.308731	-1.506629	-0.578697
H	4.268598	1.250266	0.911964
H	3.374503	-0.942930	1.659745
Ni	2.112276	0.269481	-0.487441
C	3.909626	-0.839680	0.719450
H	4.049038	-1.745188	0.138411
C	4.389485	0.353525	0.309096
H	4.964219	0.445509	-0.610145

Table S36. The Cartesian coordinates of IM3 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.420275	1.927783	-1.183768
B	0.226272	2.105786	0.661130
B	0.167904	-0.519729	-1.890759
B	2.531973	1.545728	0.018255
B	1.988104	0.131098	-1.819116
B	1.693814	-1.963784	-0.665814
B	3.122121	-0.260490	0.262674
B	1.509827	-1.773579	1.225380
B	-0.191419	-0.160195	1.815090
B	1.613040	0.514510	1.958371
N	0.708949	0.846748	-2.105983
N	-0.991759	-1.033789	-1.222370
N	-1.232566	-0.813722	1.069814
N	0.308079	1.234399	1.821941
N	3.062545	0.577604	-0.965499
N	1.479348	-1.249031	-1.896721

N	2.716429	-1.633860	0.365343
N	0.620851	-2.427602	0.242231
N	1.079025	-0.833906	2.232566
N	2.839330	0.806753	1.263946
B	-0.569572	-1.628442	0.038620
N	1.418818	2.399518	-0.181386
N	-0.754521	2.288078	-0.399908
H	-4.673735	-1.161581	0.682055
H	-3.447744	0.656171	1.870510
Ni	-2.473449	-0.290460	-0.379362
C	-3.867551	0.812006	0.881943
H	-3.870701	1.830831	0.502682
C	-4.542781	-0.180493	0.228869
H	-5.103772	0.018202	-0.678952
H	-2.850304	0.386351	-1.599976
H	-1.678579	1.892069	-0.487202

Table S37. The Cartesian coordinates of TS3 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.294983	1.954252	-1.097396
B	0.142900	2.061806	0.756999
B	0.145555	-0.476390	-1.901414
B	2.452744	1.632178	0.034865
B	1.931441	0.260699	-1.841887
B	1.764034	-1.889938	-0.766072
B	3.131483	-0.153333	0.196468
B	1.614228	-1.776678	1.132883
B	-0.146259	-0.260329	1.820983
B	1.629781	0.487803	1.955350
N	0.611035	0.923064	-2.067393
N	-0.978546	-1.065965	-1.226810
N	-1.162219	-0.924970	1.052228
N	0.292909	1.155375	1.882198
N	3.002940	0.726763	-0.997616
N	1.487846	-1.139315	-1.965408
N	2.793484	-1.546873	0.253851
N	0.737445	-2.440714	0.144895
N	1.161971	-0.893062	2.179968
N	2.823960	0.861741	1.242876
B	-0.496051	-1.694666	-0.000838
N	1.296747	2.439803	-0.106259
N	-0.874925	2.232490	-0.272318
H	-5.096532	-0.296558	-0.596883
H	-4.065523	-0.620094	1.665044
Ni	-2.459708	-0.394073	-0.287378
C	-3.876580	0.278609	1.084452
H	-3.431159	1.111827	1.621670
C	-4.438797	0.454336	-0.167202
H	-4.495903	1.440793	-0.616987
H	-3.044500	0.195159	-1.483400
H	-1.775019	1.779854	-0.337542

Table S38. The Cartesian coordinates of IM4 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.224869	2.047686	-0.936033
B	0.051079	1.955682	0.917180
B	0.148196	-0.306889	-1.940864
B	2.381469	1.685840	0.178138
B	1.912111	0.482262	-1.825463
B	1.817314	-1.758231	-0.952083
B	3.121920	-0.078336	0.174204
B	1.668348	-1.834186	0.951062
B	-0.167641	-0.480447	1.782092
B	1.586143	0.337486	1.970639
N	0.571488	1.119891	-1.994207
N	-0.958348	-0.963824	-1.312673
N	-1.153772	-1.190547	1.026350
N	0.221392	0.950446	1.947334
N	2.965804	0.904372	-0.934449
N	1.513649	-0.914172	-2.078037
N	2.837220	-1.482539	0.097734
N	0.811504	-2.424842	-0.101260
N	1.181844	-1.072864	2.073135
N	2.774093	0.821338	1.309520
B	-0.448401	-1.713826	-0.148701
N	1.197618	2.462446	0.109452
N	-0.961619	2.210231	-0.106144
H	-5.311270	0.147495	-0.501201
H	-4.132129	-0.259690	1.605739
Ni	-2.425613	-0.558062	-0.151511
C	-3.657574	0.433470	0.909177
H	-3.266274	1.318297	1.407898
C	-4.327620	0.616081	-0.427626
H	-4.361079	1.652818	-0.769557
H	-3.739955	0.100957	-1.272348
H	-1.844107	1.743800	-0.225670

Table S39. The Cartesian coordinates of TS4 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	0.090608	1.998186	-0.934230
B	-0.113186	1.865112	0.943917
B	0.188379	-0.330090	-1.977932
B	2.245940	1.761515	0.239784
B	1.900220	0.579620	-1.799942
B	1.932261	-1.673615	-0.961958
B	3.105535	0.058984	0.222606
B	1.745817	-1.796136	0.934073
B	-0.169255	-0.579009	1.770523
B	1.517062	0.344383	2.002511
N	0.527785	1.136138	-2.003242
N	-0.878198	-1.053353	-1.389893
N	-1.100375	-1.292141	0.949923
N	0.112516	0.870764	1.972612

N	2.904598	1.051684	-0.870510
N	1.606332	-0.830225	-2.079378
N	2.911498	-1.356869	0.118360
N	0.947320	-2.411055	-0.142899
N	1.200506	-1.091864	2.071794
N	2.678393	0.915383	1.369205
B	-0.358050	-1.778666	-0.243273
N	1.003020	2.443636	0.154915
N	-1.118537	2.058082	-0.107421
H	-5.254903	-0.040795	-0.595934
H	-4.154250	-0.619666	1.506528
Ni	-2.308122	-0.487418	-0.177380
C	-3.707824	0.197442	0.939459
H	-3.415824	1.034242	1.572642
C	-4.340193	0.519449	-0.391914
H	-4.495320	1.586855	-0.568259
H	-3.667119	0.218888	-1.277029
H	-2.087745	1.834153	-0.241246

Table S40. The Cartesian coordinates of IM5 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.106044	1.880107	-0.849412
B	-0.304947	1.630961	1.052985
B	0.227156	-0.303176	-2.034942
B	2.030654	1.865585	0.352974
B	1.846121	0.768091	-1.770218
B	2.056859	-1.506172	-1.033543
B	3.056175	0.260844	0.256327
B	1.867695	-1.747274	0.849588
B	-0.150596	-0.794259	1.753248
B	1.453342	0.281533	2.055453
N	0.432056	1.204274	-1.973862
N	-0.787204	-1.095485	-1.482591
N	-1.014779	-1.467887	0.868238
N	0.010241	0.678731	2.061615
N	2.766765	1.295147	-0.783629
N	1.692228	-0.642527	-2.125557
N	2.997631	-1.154809	0.073619
N	1.123384	-2.349386	-0.267042
N	1.274766	-1.171903	2.032547
N	2.536133	1.014164	1.440519
B	-0.252532	-1.830761	-0.344867
N	0.686987	2.392360	0.281259
N	-1.371464	1.556406	-0.043790
H	-5.261012	-0.219275	-0.558301
H	-3.962663	-0.990083	1.356170
Ni	-2.127648	-0.358026	-0.228949
C	-3.656770	-0.038747	0.920753
H	-3.472040	0.723113	1.676460
C	-4.387262	0.397285	-0.331781
H	-4.664508	1.454972	-0.324008
H	-3.749237	0.295934	-1.262106
H	-2.098808	2.267855	-0.018717

Table S41. The Cartesian coordinates of TS5 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.170246	1.630761	-1.229791
B	-0.313820	1.821136	0.644130
B	0.223375	-0.755504	-1.878150
B	1.996464	1.914017	-0.117009
B	1.805874	0.343783	-1.910146
B	2.065675	-1.702366	-0.662364
B	3.050432	0.338547	0.152163
B	1.911502	-1.493333	1.230593
B	-0.102911	-0.352684	1.896342
B	1.479369	0.764821	1.924428
N	0.381706	0.696851	-2.177435
N	-0.776425	-1.435552	-1.122284
N	-0.984369	-1.236855	1.204486
N	0.035290	1.133783	1.861169
N	2.733881	1.089847	-1.096581
N	1.667760	-1.126182	-1.922682
N	3.010576	-1.086962	0.310002
N	1.162111	-2.364613	0.301762
N	1.320532	-0.663654	2.249490
N	2.540307	1.337834	1.131560
B	-0.210555	-1.896865	0.150210
N	0.667014	2.419554	-0.288413
N	-1.363782	1.526972	-0.357967
H	-5.705284	0.034230	0.175811
H	-3.560516	0.030612	1.673067
Ni	-2.014821	-0.369953	-0.210119
C	-3.658638	0.556770	0.720535
H	-3.898528	1.603332	0.950023
C	-4.690603	-0.049661	-0.234330
H	-4.689031	0.459939	-1.204791
H	-4.525979	-1.121832	-0.412475
H	-2.548210	1.211016	0.130698

Table S42. The Cartesian coordinates of IM6 on B₁₁N₁₂Ni cluster.

Atom	X	Y	Z
B	-0.040880	1.549063	-1.350736
B	-0.234521	1.910619	0.443206
B	0.304642	-0.879154	-1.810394
B	2.113009	1.865618	-0.239004
B	1.918834	0.140993	-1.891012
B	2.075890	-1.805196	-0.471907
B	3.107265	0.273180	0.192448
B	1.879858	-1.425277	1.390652
B	-0.087604	-0.136721	1.884316
B	1.515490	0.907830	1.875432
N	0.517369	0.514828	-2.216827
N	-0.757442	-1.486682	-1.029529
N	-0.995208	-1.049416	1.217550
N	0.091747	1.314920	1.737301

N	2.849544	0.920484	-1.119776
N	1.726402	-1.327927	-1.785599
N	3.011202	-1.137029	0.470400
N	1.123359	-2.356243	0.519821
N	1.294241	-0.491647	2.318345
N	2.613938	1.366951	1.068836
B	-0.219303	-1.862588	0.281507
N	0.821466	2.410927	-0.487989
N	-1.245155	1.511020	-0.529917
H	-5.766549	-0.461099	-0.643163
H	-4.909465	-0.008269	1.717034
Ni	-1.993523	-0.226195	-0.226273
C	-4.531450	0.536984	0.847970
H	-5.059564	1.491636	0.772832
C	-4.705801	-0.282734	-0.440185
H	-4.310301	0.241050	-1.321608
H	-4.249729	-1.282510	-0.373102
H	-3.485876	0.804001	1.076088



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