

Electronic Supplementary Information

A Comparative Study of Bi, Sb, and BiSb for Electrochemical Nitrogen Reduction Leading to a New Catalyst Design Strategy

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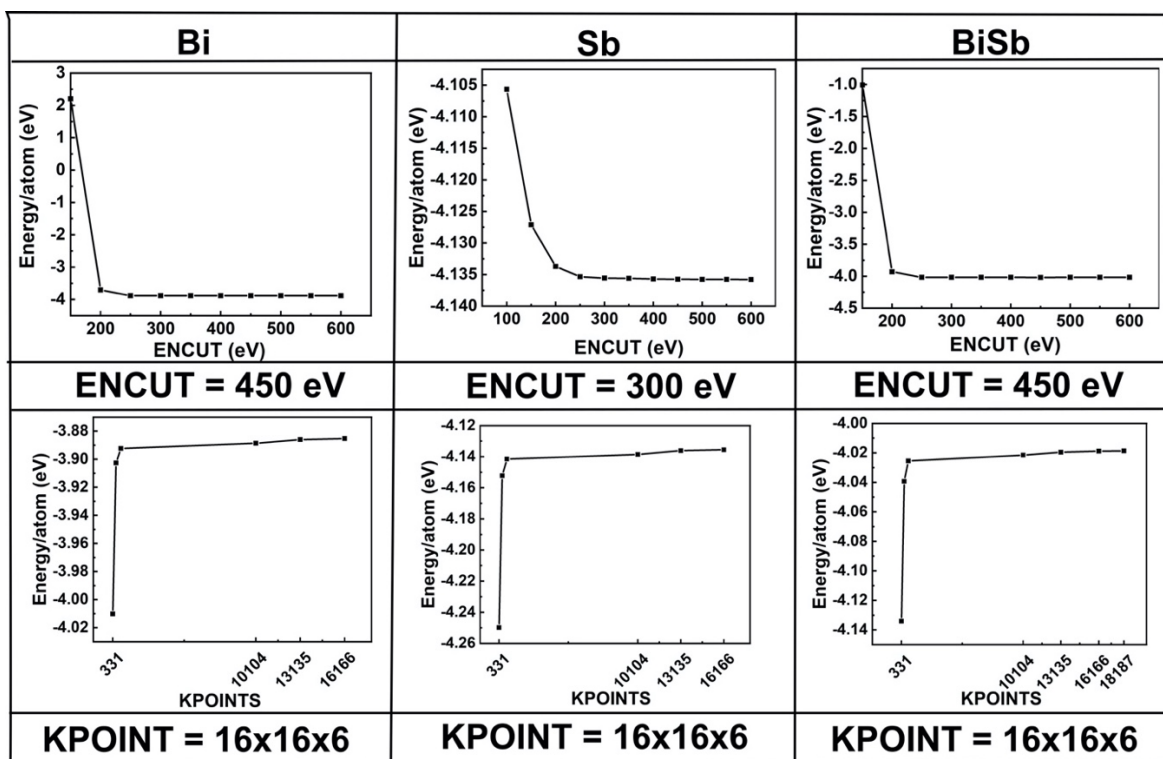


Figure S1. Converged ENCUT and KPOINT for the bulk system.

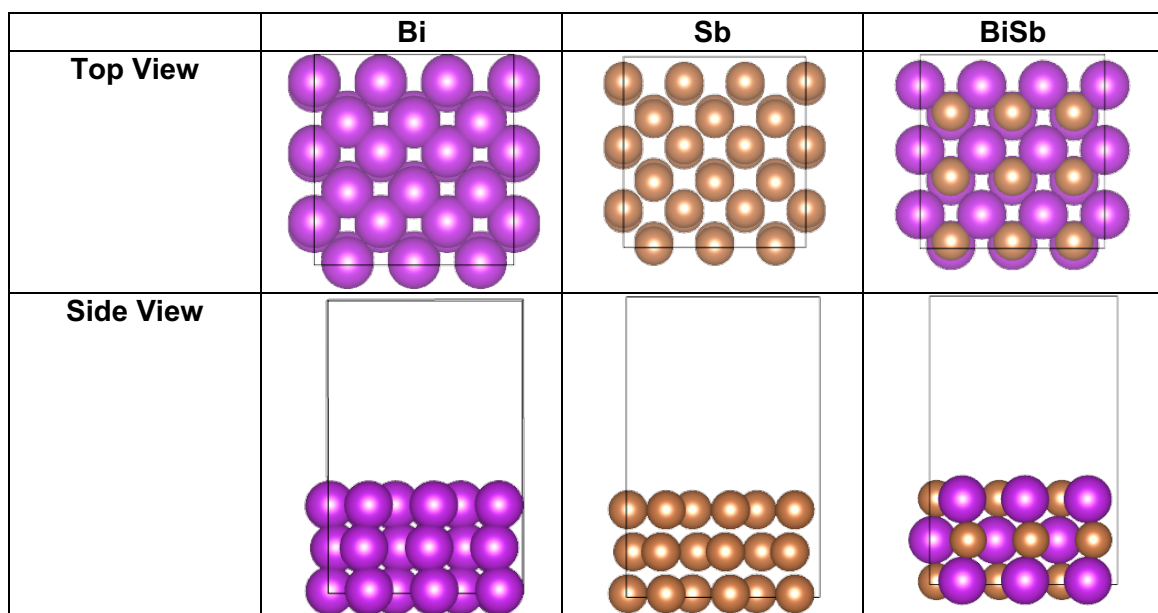


Figure S2. Optimized structure of the slab (012).

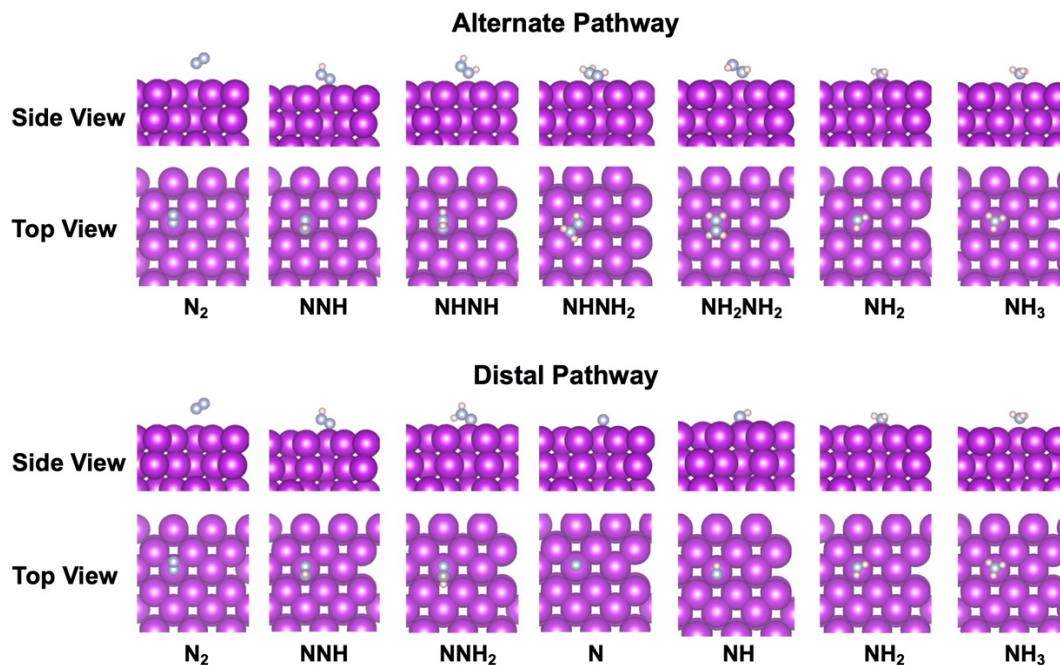


Figure S3. Intermediate structures in alternate and distal pathways for Bi (Bi: violet, N: gray, and H: beige).

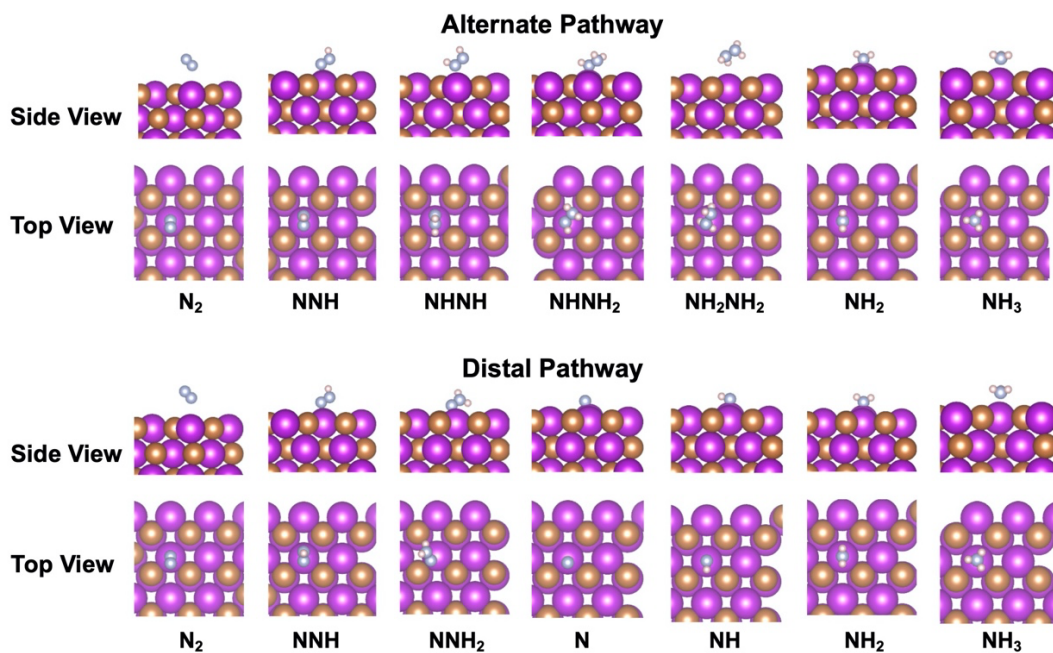


Figure S4. Intermediate structures in alternate and distal pathways for Bi in BiSb (Bi: violet, Sb: golden, N: gray, and H: beige).

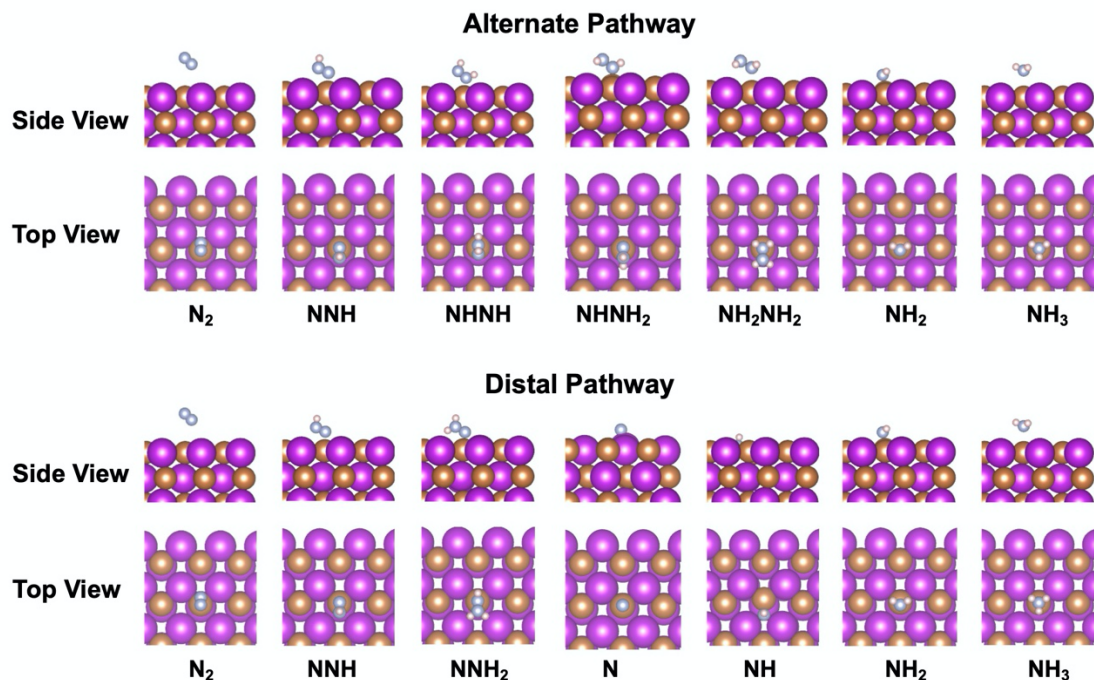


Figure S5. Intermediate structures in alternate and distal pathways for Sb in BiSb (Bi: violet, Sb: golden, N: gray, and H: beige).

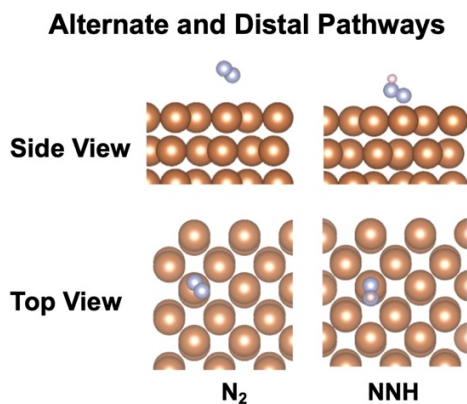


Figure S6. Intermediate structures for Sb. Since we have already established that the PDS is the formation of NNH for Bi, Bi in BiSb, and Sb in BiSb, we have calculated only the PDS step for Sb and avoided further calculations. Thus, only the structures of N_2 and NNH are shown, which are common for alternate and distal pathways (Sb: golden, N: gray, and H: beige).

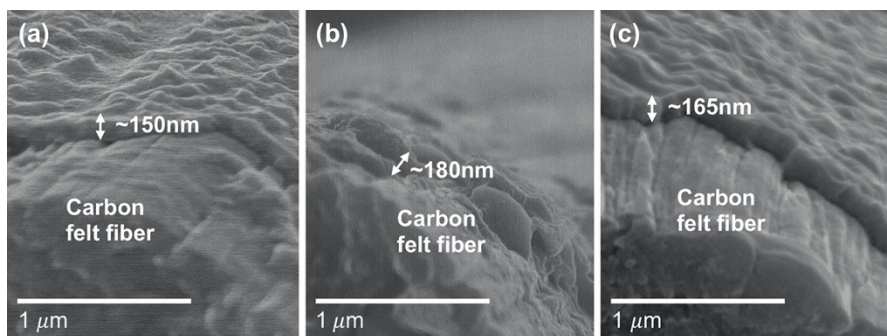


Figure S7. Side-view SEM images showing (a) Bi, (b) Sb, and (c) BiSb layers deposited on a single fiber of the carbon felt substrate.

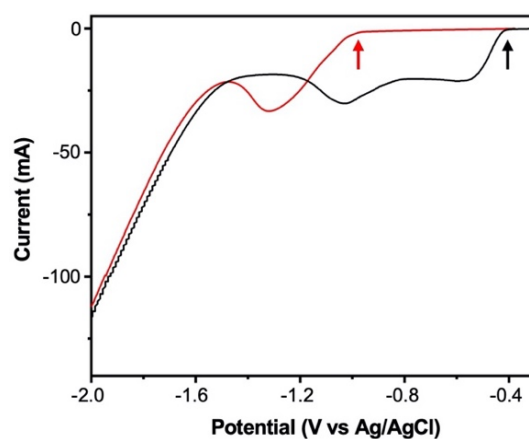


Figure S8. LSVs obtained using a carbon felt electrode in a tartrate plating solution containing 20 mM Bi (black) and 20 mM Sb (red) with a scan rate of 10 mV/s. The onset potentials for Bi deposition and Sb deposition are represented with a black arrow and a red arrow, respectively.

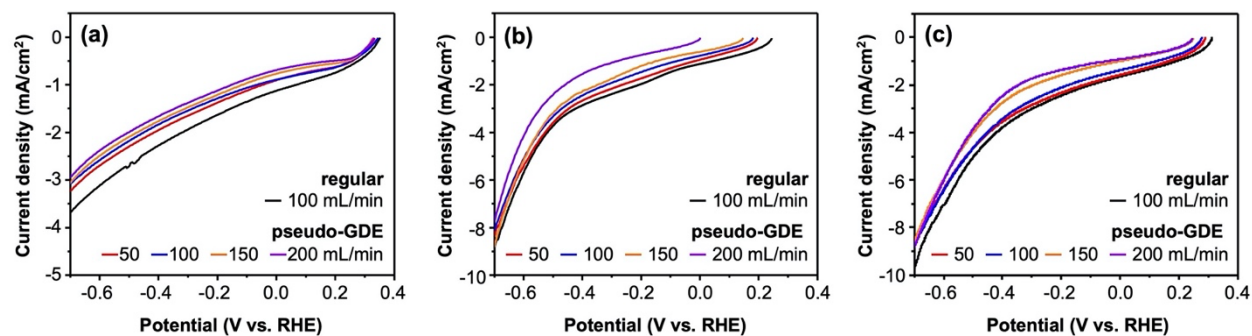


Figure S9. LSVs of (a) Bi, (b) Sb, and (c) BiSb as a pseudo-GDE obtained in 0.5 M borate (pH 9.3) with various N₂ flow rates. The LSVs obtained using each electrode as a regular electrode with the N₂ flow rate of 100 mL/min are also shown for comparison.

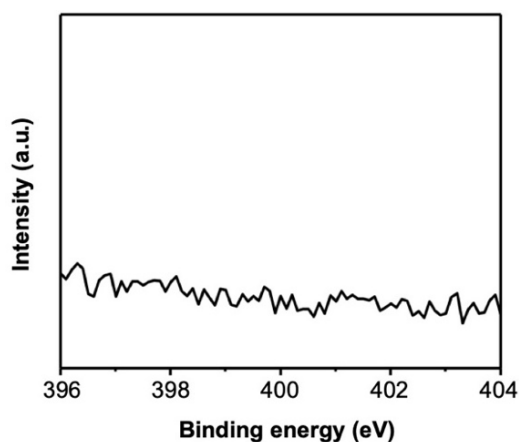


Figure S10. XPS spectrum of the N 1s region of a bare carbon felt substrate before any ENRR experiment.

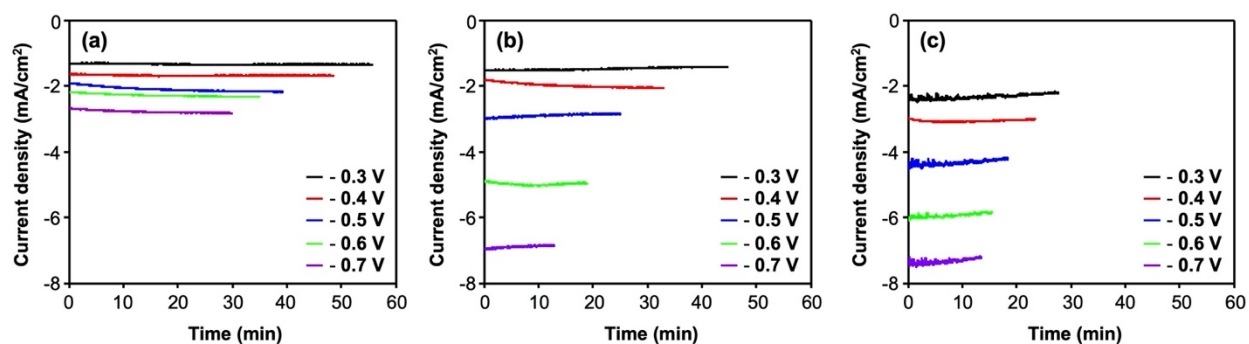


Figure S11. J-t plots of (a) Bi, (b) Sb, and (c) BiSb used as a psuedo-GDE obtained during the constant potential ENRR at various potentials with the N_2 flow rate of 100 mL/min in 0.5 M borate (pH 9.3).

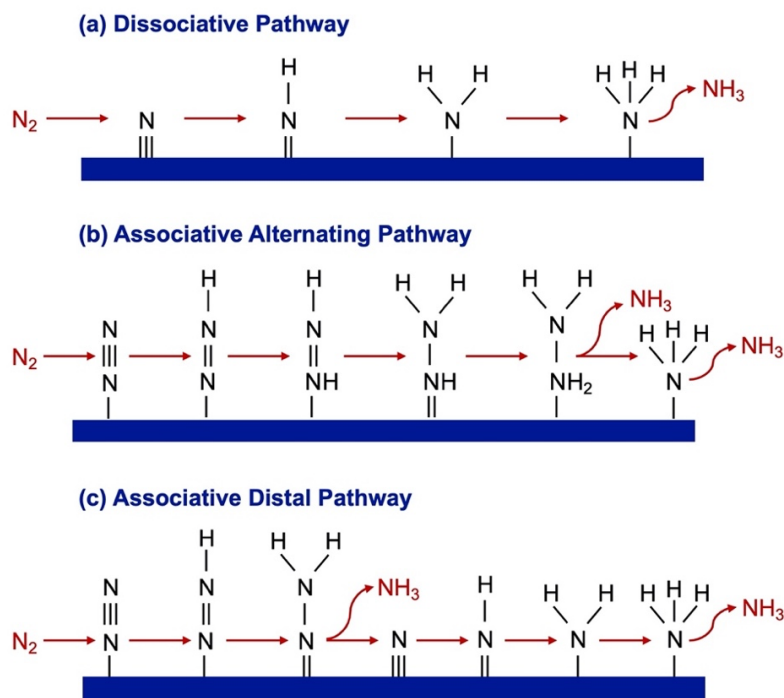


Figure S12. Schematic illustration of three possible ENRR pathways.^{S1}

Table S1. Optimized lattice constants of the bulk.^{S2}

Phase	Energy(eV)/atom	a (exp) (Å)	a (cal) (Å)	b (exp) (Å)	b (cal) (Å)	c (exp) (Å)	c (cal) (Å)
Bi	-3.886	4.610	4.585	4.610	4.585	11.975	12.186
Sb	-4.135	4.380	4.373	4.380	4.373	11.545	11.503
BiSb	-4.019	4.499	4.489	4.499	4.489	11.836	11.845

Table S2. Reaction mechanisms and corresponding Gibbs free energy changes for the alternate pathway.^{S3}

Step	Reaction and corresponding ΔG
1	$N_2 \rightarrow N_2^*$ $\Delta G = \Delta G_{N_2}^* - G_{slab} - \Delta G_{N_2} - T\Delta S$
2	$N_2^* + 6(H^+ + e^-) \rightarrow N_2H^* + 5(H^+ + e^-)$ $\Delta G = \Delta G_{NNH}^* - \Delta G_{N_2}^* - 1/2\Delta G_{H_2} - T\Delta S$
3	$N_2H^* + 5(H^+ + e^-) \rightarrow NHHNH^* + 4(H^+ + e^-)$ $\Delta G = \Delta G_{NHHNH}^* - \Delta G_{NNH}^* - 1/2\Delta G_{H_2} - T\Delta S$
4	$NHHNH^* + 4(H^+ + e^-) \rightarrow NHHNH_2^* + 3(H^+ + e^-)$ $\Delta G = \Delta G_{NHHNH_2}^* - \Delta G_{NHHNH}^* - 1/2\Delta G_{H_2} - T\Delta S$
5	$NHHNH_2^* + 3(H^+ + e^-) \rightarrow NH_2NH_2^* + 2(H^+ + e^-)$ $\Delta G = \Delta G_{NH_2NH_2}^* - \Delta G_{NHHNH_2}^* - 1/2\Delta G_{H_2} - T\Delta S$
6	$NH_2NH_2^* + 2(H^+ + e^-) \rightarrow NH_2^* + (H^+ + e^-) + NH_3$ $\Delta G = \Delta G_{NH_2}^* - \Delta G_{NH_2NH_2}^* - 1/2\Delta G_{H_2} + G_{NH_3} - T\Delta S$
7	$NH_2^* + (H^+ + e^-) \rightarrow NH_3^*$ $\Delta G = \Delta G_{NH_3}^* - \Delta G_{NH_2}^* - 1/2\Delta G_{H_2} - T\Delta S$

Table S3. Reaction mechanisms and corresponding Gibbs free energy changes for the distal pathway.^{S3}

Step	Reaction and corresponding ΔG
1	$N_2 \rightarrow N_2^*$ $\Delta G = \Delta G_{N_2}^* - G_{slab} - \Delta G_{N_2} - T\Delta S$
2	$N_2^* + 6(H^+ + e^-) \rightarrow N_2H^* + 5(H^+ + e^-)$ $\Delta G = \Delta G_{NNH}^* - \Delta G_{N_2}^* - 1/2\Delta G_{H_2} - T\Delta S$
3	$N_2H^* + 5(H^+ + e^-) \rightarrow NNH_2^* + 4(H^+ + e^-)$ $\Delta G = \Delta G_{NNH_2}^* - \Delta G_{NNH}^* - 1/2\Delta G_{H_2} - T\Delta S$
4	$NNH_2^* + 4(H^+ + e^-) \rightarrow N^* + NH_3 + 3(H^+ + e^-)$ $\Delta G = \Delta G_N^* - \Delta G_{NNH_2}^* - 1/2\Delta G_{H_2} + G_{NH_3} - T\Delta S$
5	$N^* + 3(H^+ + e^-) \rightarrow NH^* + 2(H^+ + e^-)$ $\Delta G = \Delta G_{NH}^* - \Delta G_N^* - 1/2\Delta G_{H_2} - T\Delta S$
6	$NH^* + 2(H^+ + e^-) \rightarrow NH_2^* + (H^+ + e^-)$ $\Delta G = \Delta G_{NH_2}^* - \Delta G_{NH}^* - 1/2\Delta G_{H_2} - T\Delta S$
7	$NH_2^* + (H^+ + e^-) \rightarrow NH_3^*$ $\Delta G = \Delta G_{NH_3}^* - \Delta G_{NH_2}^* - 1/2\Delta G_{H_2} - T\Delta S$

Table S4. The FEs for $^{15}\text{NH}_3$ production by Bi at various potentials when it is used as a regular electrode and as a pseudo GDE.

	-0.3 V_{RHE}	-0.4 V_{RHE}	-0.5 V_{RHE}	-0.6 V_{RHE}	-0.8 V_{RHE}
Regular	0%	0%	0.22%	0.4%	0.18%
Pseudo-DGE	0.25%	1.12%	1.45%	1.35%	0.9%

Table S5. ΔG values (in eV) for the formation of surface adsorbed intermediates in the alternate pathway on various metal sites. The PDS is the formation of adsorbed NNH.

Intermediate	Bi	Bi in BiSb	Sb in BiSb	Sb*
N ₂	0.098	0.020	0.021	0.111
NNH	1.912	2.020	1.968	1.964
NH-NH	-0.221	-0.329	-0.043	-
NH-NH ₂	-0.526	-0.382	-0.727	-
NH ₂ -NH ₂	-0.806	-0.839	-0.632	-
NH ₂	-0.799	-1.539	-1.072	-
NH ₃	-1.013	-1.189	-0.794	-

*Since we already established for the case of Bi and BiSb that the PDS is the formation of NNH, we have just calculated the PDS step for Sb and avoided further calculation.

Table S6. ΔG values (in eV) for the formation of surface adsorbed intermediates in the distal pathway on various metal sites. The PDS is the formation of adsorbed NNH.

Intermediate	Bi	Bi in BiSb	Sb in BiSb	Sb
N ₂	0.098	0.020	0.021	0.111
NNH	1.912	2.020	1.968	1.964
NNH ₂	0.085	-0.052	0.032	-
N	0.009	0.623	0.876	-
NH	-0.608	-1.702	-2.263	-
NH ₂	-1.950	-1.958	-1.191	-
NH ₃	-1.013	-1.189	-0.794	-

References

- S1. Shipman, M. A., Symes, M. D. Progress Towards the Electrosynthesis of Ammonia from Sustainable Resources. *Catalysis Today*, 2017, **286**, 57-58
- S2. <https://materialsproject.org/materials/mp-1227290/>.
- S3. Yang, Y., Li, J., Chen, K., Chen, Q.J. and Feng, Y., Catalytic Performance of Two-Dimensional Bismuth Tuned by Defect Engineering for Nitrogen Reduction Reaction. *J. Phys. Chem. C*, 2020, **124**, 19563-19570.

Sample input file used for the simulation

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54

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54 2

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0.4986070669819824	0.3476644265699420	0.3004650848696997
0.8333333129999971	0.3462312487432939	0.3025172225281310
0.9987193199437527	0.2068941115274043	0.0118489964530042
0.3333333429999996	0.2077578798960715	0.0116233320699450
0.6679473670562501	0.2068941115274043	0.0118489964530042
0.1674482899986458	0.3721973300732344	0.1553032397586094
0.4992183820013523	0.3721973300732344	0.1553032397586094
0.8333333129999971	0.3720153992816506	0.1577005438623900
0.0001684236925783	0.5422910702223689	0.3032293934502590
0.3333333429999996	0.5433707402133621	0.3079016441524587
0.6664982633074246	0.5422910702223689	0.3032293934502590
0.1660053054971868	0.6790443879519330	0.0130022713349618
0.5006613665028112	0.6790443879519330	0.0130022713349618
0.8333333129999971	0.6795224317436279	0.0122662450405002
0.9999593175777974	0.8498048496039559	0.1578826784458514
0.3333333429999996	0.8501087049646756	0.1587825720597351
0.6667073694222054	0.8498048496039559	0.1578826784458514
0.1670367417085998	0.0126984446850784	0.3026672279591054
0.4996299302913982	0.0126984446850784	0.3026672279591054
0.8333333129999971	0.0150523982674500	0.3026152315150838
0.1666027818665938	0.0381153618300871	0.1575013665972733

0.5000638901334042	0.0381153618300871	0.1575013665972733
0.8333333129999971	0.0381499732869202	0.1578185390296127
0.0004633056202721	0.8741710384716370	0.0128244944825511
0.3333333429999996	0.8719323164641750	0.0134607404314622
0.6662033813797237	0.8741710384716370	0.0128244944825511
0.0011275316220818	0.2095861503205612	0.3020557269337303
0.3333333429999996	0.2085593571758295	0.3016939626216342
0.6655391553779282	0.2095861503205612	0.3020557269337303
0.3333333429999996	0.5543578194109671	0.4199857004081906
0.3333337600000021	0.4798876036601101	0.4453597457178660
0.3333343859999971	0.4882318408634845	0.4933905844202684

Energy = -221.687 eV

4) NH-NH

1.0000000000000000

13.7550001143999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.5450000762999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.8722000122000004

Bi N H

54 2 2

Direct

0.1663397309730783	0.3456371919946193	0.0101756796768910
0.5003365975845568	0.3456170542161132	0.0101588162026047
0.8333181938873793	0.3468471244862741	0.0117022429719995
0.0002402476820578	0.5155676704677248	0.1566702225354248
0.3333253094669075	0.5151960980924386	0.1545102606211941
0.6664010023026208	0.5155826313962351	0.1566857312406640
0.1663329685763131	0.6801466999958308	0.3010670269649793
0.5003397272293881	0.6801618391895801	0.3010666563698123
0.8333476638531820	0.6790429337689616	0.3023259485525216
0.0005032413829582	0.5422607980140697	0.0120551333745880
0.3333425008289836	0.5417818111916830	0.0117701516364477
0.6661473834764848	0.5422705624785920	0.0120580665509848
0.1667070699860957	0.7033184042558673	0.1548692441133852
0.4999519623298454	0.7033436234219508	0.1548709096577099
0.8333257095213398	0.7037823449015335	0.1569256194338848
0.0002523499370426	0.8746344864401578	0.3014635074149297
0.3333289058814728	0.8739571112217064	0.3017463286604212
0.6664166518477757	0.8746329402299082	0.3014948001580890
0.1667503453105112	0.0131258832821928	0.0121055325633463
0.4999232819448736	0.0131199425332724	0.0121016128225833
0.8333278809247986	0.0130661247773105	0.0112791260931004
0.9999025193261915	0.1820415821668107	0.1561279434814793
0.3333228473174827	0.1821298525110535	0.1564020011721610
0.6667685290144192	0.1820438990786357	0.1561835223333858
0.1666500605148684	0.3458812685708708	0.3007589595991078
0.4999820795368279	0.3458756175851221	0.3007379539050561
0.8333672506692835	0.3456994733449719	0.3020801892900309
0.9993006662141255	0.2082213868003677	0.0111901721346399
0.3333407810236295	0.2081491798184203	0.0111467121139555
0.6673906531052936	0.2082209470084564	0.0112404250012759
0.1667215593990932	0.3703369198784401	0.1553647354803616

0.4999457943245389	0.3703372737118329	0.1553494717160433
0.8333242368772389	0.3706263813599406	0.1569387961437201
0.0004068479810684	0.5415664923568286	0.3013372741349798
0.3333442634168193	0.5410310235871734	0.3001695701345568
0.6662733503054881	0.5415816558639293	0.3013622891350352
0.1666033427827713	0.6807357993275076	0.0092490690493037
0.5000670598134320	0.6807405780203695	0.0092631693476335
0.8333351571783396	0.6796427270265752	0.0115566681741512
0.0001817124862882	0.8486383783551830	0.1563953897757528
0.3332788189669671	0.8484465670469845	0.1564483974931008
0.6664845322768329	0.8486627557930575	0.1564205721235155
0.1669799598277137	0.0122787186600846	0.3024249636515464
0.4996724577610792	0.0122744107097503	0.3024329192868080
0.8333346092072844	0.0122213102672433	0.3017221960501644
0.1666793515516076	0.0370405672282175	0.1571591218423620
0.4999854706559859	0.0370502329182258	0.1571661005982037
0.8333304355032496	0.0368130796817070	0.1564169259681307
0.0000770896704410	0.8751585499860042	0.0117110658741311
0.3333365072212402	0.8748907731680333	0.0118870014942303
0.6666010992445806	0.8751474285775060	0.0117182280257921
0.0000979326869981	0.2079537300274410	0.3009512868775985
0.3333234347447984	0.2080748073639924	0.3009562579086662
0.6665940234708714	0.2080014081670711	0.3009943264743242
0.3333533999810285	0.5511886410068811	0.4300509199375284
0.3333428955407314	0.4862119118843893	0.4674047699692210
0.3333262416328324	0.5089314331488950	0.5128059222349393
0.3333397378409089	0.6172487376358404	0.4492428504515331

Energy = -225.456 eV

5) NH-NH2

1.0000000000000000

13.7550001143999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.5450000762999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.8722000122000004

Bi N H

54 2 3

Direct

0.1677127186993843	0.3470397867560635	0.0129828406690677
0.5042071397816201	0.3463105338287704	0.0105867502388506
0.8365428870330476	0.3480796737259269	0.0136445385116986
0.0041017739978315	0.5204634279194593	0.1594232586045621
0.3369037920386546	0.5204566920485689	0.1476930616044001
0.6695560825171256	0.5202282639876259	0.1595563228903885
0.1694784410148245	0.6832333838303555	0.3049623383981128
0.5070724185003357	0.6846781150436030	0.3074181719386004
0.8371873776808911	0.6831001390106266	0.3030970266581505
0.0040757430501657	0.5440281632714417	0.0142492530932046
0.3374236513861604	0.5415362648958251	0.0083976542865543
0.6688893654989982	0.5444869377656829	0.0144913310711132
0.1707026754396423	0.7083474480264087	0.1602623021537042
0.5027365784203113	0.7076336723477468	0.1619627453718948
0.8366950818906886	0.7081108808757932	0.1577802581435677

0.0034136844191650	0.8785587339136995	0.3038581457052416
0.3366468643951492	0.8773787257099883	0.3050655331686869
0.6716161677344417	0.8793774198409494	0.3041309529764931
0.1709543987172069	0.0138680659720620	0.0135761588706487
0.5017392518932269	0.0140843171740741	0.0136631091181698
0.8364145721758689	0.0142900157267221	0.0138532132506413
0.0038078217862250	0.1875101416724831	0.1583109088980237
0.3366535407634359	0.1868999035993184	0.1580138183784427
0.6701672956498967	0.1868426457573023	0.1571257774998642
0.1740698476067379	0.3526382570458964	0.3037649383252372
0.5034551183943137	0.3497949842754977	0.3003253486785127
0.8376535891294097	0.3489211681185722	0.3035088161275610
0.0014649263965794	0.2087645375292766	0.0130461729874867
0.3357991365598352	0.2103136287907716	0.0122077959632421
0.6712670567902279	0.2089112142132947	0.0118781583287131
0.1712174662934416	0.3758645542150703	0.1572858536121373
0.5027378442344315	0.3752724154555764	0.1552497681762119
0.8370020304781605	0.3755550967872310	0.1588883753833557
0.0037986394199336	0.5451399573537401	0.3047179281887722
0.3393208824383578	0.5433296015189626	0.3073594567529412
0.6705412761625453	0.5449435980317006	0.3050313731016558
0.1688896371157043	0.6817767660652478	0.0143465919071275
0.5050447175954815	0.6827958175645961	0.0153810374422179
0.8367333148381064	0.6819556232315378	0.0130506188043000
0.0033864608637444	0.8532647445196417	0.1586003028582681
0.3370375818647631	0.8535694701822933	0.1601944201302246
0.6697705791445756	0.8529719373645221	0.1590924823992879
0.1701346007873781	0.0161162326618580	0.3032981464828168
0.5036001226126601	0.0156935985221978	0.3035467929284721
0.8379069423535839	0.0180940461598311	0.3035245610474391
0.1699307729120179	0.0419517926814592	0.1582259416533560
0.5034967708840199	0.0418402244818452	0.1583457964660866
0.8371913349086668	0.0417743240508344	0.1588821245926297
0.0035374654239249	0.8766648603483631	0.0135606601515192
0.3365265165259146	0.8742523579794153	0.0146863825475663
0.6691726931421726	0.8768697248826456	0.0139341560910466
0.0062446442054522	0.2133655740768816	0.3040643433265018
0.3377019605716498	0.2110952529568166	0.3028593645037247
0.6699838171146695	0.2117880084176988	0.3023701378097741
0.3440673711629003	0.5128772827662758	0.4114133775383024
0.2729283668024962	0.4461972935303322	0.4274444071255772
0.2184164138591669	0.4713107472457025	0.4543817944793958
0.3257521676741391	0.5741696951833717	0.4316628251421832
0.3061773862485921	0.3922873240904536	0.4488965134464991

Energy = -229.571 eV

6) NH₂-NH₂

1.0000000000000000

13.7550001143999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.5450000762999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.8722000122000004

Bi N H

54 2 4
Direct

0.1661354113225428	0.3461681912527652	0.0106358612555582
0.5005325443046473	0.3461682934693684	0.0106358569216738
0.8333338623753335	0.3471919339088743	0.0119030183803872
0.0003717313318390	0.5169731411982639	0.1571171220596739
0.3333337230038964	0.5170904152695357	0.1542465109595383
0.6662955884969648	0.5169730500578424	0.1571172956871862
0.1652478750880917	0.6831884930876981	0.3007352291298204
0.5014200070489210	0.6831884797945875	0.3007351855768405
0.8333340273867194	0.6812912526684087	0.3027636387687735
0.0005328906879498	0.5430850239701357	0.0124189950431131
0.3333328876967698	0.5418568624095244	0.0125482174256248
0.6661327317705386	0.5430851856629104	0.0124189232397072
0.1664522859663435	0.7047008827585373	0.1546351697445729
0.5002103572908752	0.7047007717793790	0.1546360248888803
0.8333330820203813	0.7050303281166705	0.1572471234161128
0.9999057970360852	0.8769844435197669	0.3023533714768334
0.3333326650511097	0.8760899846317258	0.3025127791266939
0.6667599947706222	0.8769842299956565	0.3023533744564375
0.1668631803507736	0.0137403208291502	0.0122386701004231
0.4998047287267511	0.0137406441326817	0.0122387239568624
0.8333340790535999	0.0139765403091729	0.0118018032532916
0.0001889314061145	0.1835625530178504	0.1571887278049715
0.3333335912110869	0.1833235731134408	0.1576647025572555
0.6664783484727579	0.1835626389271354	0.1571886942285090
0.1667463137970486	0.3479360139969785	0.3015689042216536
0.4999217237042828	0.3479359679571488	0.3015690341470076
0.8333339606925705	0.3481028270976978	0.3023732829790475
0.9992344572085869	0.2085580089811501	0.0122265769822576
0.3333328560340618	0.2087110784008317	0.0126382201747290
0.6674313068672646	0.2085581627248416	0.0122267125127564
0.1670714351770002	0.3719249710660577	0.1555416483920524
0.4995949026461517	0.3719250649286110	0.1555417029648893
0.8333330224624049	0.3720857510213094	0.1570445601908688
0.0003176241718350	0.5437574024048288	0.3019303857827396
0.3333328440915224	0.5449797107011918	0.3020538576538812
0.6663480586152133	0.5437573235229110	0.3019303247587501
0.1663434488337217	0.6815155309064664	0.0089889580268689
0.5003245345673548	0.6815154869548721	0.0089889270874650
0.8333339198065772	0.6805191430264586	0.0118438072979572
0.9999925853837865	0.8501118646423294	0.1571133288748001
0.3333335988352815	0.8496098691180975	0.1571295111929558
0.6666747626215255	0.8501118198574673	0.1571132810784945
0.1668627321928184	0.0144001244498639	0.3027140092067171
0.4998052836554479	0.0144003002103830	0.3027140348346080
0.8333340668110694	0.0149497094590529	0.3022267767909668
0.1666638654162682	0.0381898041466258	0.1573903183546079
0.5000022928133916	0.0381897893841909	0.1573902911472302
0.8333331044193812	0.0385942860077577	0.1569841426858360
0.9999856475364339	0.8760324438456877	0.0124353859962767

0.3333326196143602	0.8753061613116841	0.0125230729723640
0.6666802118731638	0.8760323233445959	0.0124353455313795
0.9999117886339661	0.2102013777763077	0.3022738653157688
0.3333327677491411	0.2100375737168108	0.3026757768069857
0.6667536559617560	0.2102013537706782	0.3022738530321263
0.3333332750889113	0.5501651716835170	0.4276281413855401
0.3333335394819343	0.4677150012364635	0.4657813183621329
0.2740228422623758	0.5883698519319580	0.4405727041018466
0.3926441266089071	0.5883699159716187	0.4405727510501478
0.3920799229061274	0.4300708383915364	0.4511649546334340
0.2745867445876016	0.4300707831709332	0.4511648930140879

Energy = -233.954 eV

7) NH2

1.0000000000000000

13.7550001143999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.5450000762999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.8722000122000004

Bi N H

54 1 2

Direct

0.1650983715912844	0.3440455991974076	0.0096830118660449
0.5015063183806490	0.3438411995578790	0.0095965703156793
0.8333245431340828	0.3459787872176889	0.0125670861293372
0.0004819653180519	0.5174511375950104	0.1577804172127060
0.3335497901704585	0.5177092172339357	0.1495345130496943
0.6660221694643624	0.5170292372118155	0.1577966238555675
0.1646008106142958	0.6820405125174887	0.3051493485851609
0.5034116848846750	0.6825856483610551	0.3038095642676595
0.8334485132322698	0.6804663660313395	0.3017284106630669
0.0012046371844150	0.5419240149056748	0.0127150876280879
0.3332704936866620	0.5372196109077265	0.0109279833561757
0.6657811147003940	0.5419981713312723	0.0128130749239332
0.1667280237220865	0.7052747313030778	0.1606349741541706
0.4994562982360833	0.7049078054006515	0.1588269168254328
0.8332871286965684	0.7051943063521477	0.1568273193792322
0.9999093877684331	0.8757910447029005	0.3030023879458952
0.3335464972144919	0.8737970379368889	0.3038072295157335
0.6676920983848191	0.8766648392515890	0.3029266183686943
0.1678693282525785	0.0115192622395384	0.0127327190750677
0.4988357434101829	0.0115025477442359	0.0127606724715719
0.8334990151756756	0.0119729167071299	0.0126844931663044
0.0001175077923889	0.1835133415916346	0.1569453681779578
0.3333182279692011	0.1831694061568498	0.1570363015354630
0.6665831068319861	0.1834575893721677	0.1569197404058968
0.1678436047500398	0.3480594390718039	0.2999126729882988
0.4988178797085681	0.3477189604789004	0.2997768219633343
0.8334129275073110	0.3466114779469365	0.3025859011673830
0.9982894032520733	0.2066531447491826	0.0118786363364407
0.3332645174673559	0.2076277843104535	0.0115000263718059
0.6683893209911673	0.2065814061297004	0.0118401716121639
0.1675370321186662	0.3726655487405637	0.1546483349966223

0.4991151787713690	0.3722426313849354	0.1545870535031568
0.8334651439900114	0.3724408884046824	0.1578165327114576
0.0007777990290947	0.5430367696371547	0.3029408724163147
0.3350305551032804	0.5425693382348413	0.3170699606168128
0.6667187751417032	0.5426349165457651	0.3029185643915255
0.1654821371980759	0.6795994541714094	0.0141972122346630
0.5010759236945077	0.6796937144644275	0.0128268708975980
0.8333955785661828	0.6796602826722875	0.0120838358361866
0.9997223728712257	0.8503682967331727	0.1578699217677482
0.3332321543500925	0.8502901267918404	0.1588563081006313
0.6665542864332750	0.8500931853278857	0.1576799936573678
0.1671818230095639	0.0126794297116675	0.3025240289331848
0.4997070021510694	0.0128833799386499	0.3025986156600027
0.8338411870790878	0.0152890598745827	0.3023942027907225
0.1665498831501893	0.0382952432291717	0.1574269203632355
0.5001821540592815	0.0382861621789488	0.1574871983894752
0.8334159413588225	0.0381149469339235	0.1578155250303155
0.0006218832645999	0.8742426535626322	0.0127813812239950
0.3333780631754379	0.8717085527080215	0.0134958054195735
0.6662796447960559	0.8743034281158941	0.0127280053759335
0.0010797401250997	0.2098640528537317	0.3019960886802409
0.3332213081344477	0.2086776913149109	0.3014097620796079
0.6659363458962417	0.2096605147723736	0.3019490327013585
0.3291835121965292	0.5535359149411789	0.4187829770163347
0.3960219734923953	0.5756870423200766	0.4336121660730896
0.3214226633510577	0.4881785569212127	0.4358642808188335

Energy = -218.650 eV

8) NH₃

1.0000000000000000

13.7550001143999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.5450000762999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.8722000122000004

Bi N H

54 1 3

Direct

0.1663797123775694	0.3458953763969888	0.0100901164303693
0.5002605238931181	0.3458841835573168	0.0100956334777607
0.8333430542529570	0.3468526053614127	0.0115564825050996
0.0003754303357155	0.5164820938367924	0.1564060738485225
0.3333233210329993	0.5163998236837841	0.1553332934652616
0.6662927434421704	0.5164715618257034	0.1563548878768870
0.1660608126367364	0.6816422129305053	0.2995016182598746
0.5004996979970429	0.6816540153611967	0.2995059212290485
0.8333118409341580	0.6797876213175371	0.3023767973519256
0.0001441601801275	0.5425688974373131	0.0116436307157457
0.3332867502327375	0.5419029274927141	0.0120960073122376
0.6664609665630579	0.5425706972609419	0.0116141515289030
0.1664995133933829	0.7043041562267192	0.1539059237135234
0.5001479395151947	0.7042926597437429	0.1539328174546313
0.8333260128563893	0.7047456821977605	0.1571134494209829
0.9997429605194696	0.8760755668372084	0.3021226079700483

0.3333159970158235	0.8754897660456322	0.3024148162362081
0.6668720104621713	0.8760622445246327	0.3021530056445414
0.1666783153771974	0.0134767493808496	0.0122314491387101
0.4999404562571215	0.0134658743190172	0.0122275745404323
0.8333106615206489	0.0133875244172259	0.0111311700901950
0.0002198172800050	0.1831018906850375	0.1567144988211879
0.3333194767379837	0.1827429697554521	0.1567986758337909
0.6664283853032913	0.1831298202886842	0.1566832749588656
0.1667029930308175	0.3471613995701333	0.3005929890819132
0.4999627464124998	0.3471847161317640	0.3005937463920816
0.8333018864649517	0.3472449612502189	0.3016556462553623
0.9994371192561360	0.2083913112819857	0.0116659517501105
0.3332879166830693	0.2083534023254288	0.0116043348584967
0.6672196790478537	0.2084026323823380	0.0116465639289984
0.1670010684064067	0.3713500251480326	0.1551679965564858
0.4996474482916113	0.3713608044225580	0.1551757951167900
0.8333401080575271	0.3716852807218132	0.1565317270564819
0.0006063147161228	0.5425978894605237	0.3012316425797223
0.3332654733261009	0.5429887868757817	0.3015893864361630
0.6659360309199798	0.5426390613093446	0.3011949848767443
0.1664838239467841	0.6805989382066073	0.0080427575538025
0.5001133721869522	0.6805960385598411	0.0080918689477016
0.8333254401471777	0.6803655258033672	0.0117604148520698
0.0000804717019065	0.8497164617507806	0.1569022834995266
0.3333273592169803	0.8492538120221482	0.1568404993053392
0.6665712494620522	0.8497135428643006	0.1569243917413488
0.1667386999958396	0.0133782128364146	0.3026122428745026
0.4998974886701930	0.0133726844420963	0.3026116341853111
0.8332795579531620	0.0141106822010073	0.3012789901073916
0.1666291838641314	0.0376779886957124	0.1572847884202986
0.5000037369905570	0.0376900225862684	0.1572701642202006
0.8333158341006808	0.0382733684150764	0.1561499774085746
0.0000110632087171	0.8754684200500762	0.0120810085022711
0.3332929947816083	0.8752299160658907	0.0123005608684181
0.6666132178522943	0.8754644041943465	0.0121127995598087
0.9999718040318442	0.2094201681871652	0.3017274532554026
0.3333389630343078	0.2092016111428450	0.3015325925857795
0.6666299047634467	0.2094015102375835	0.3017033743485058
0.3335897602772988	0.5474114402984824	0.4343074726274878
0.3987553022657195	0.5732649734733215	0.4487461013646907
0.3218060795553797	0.4864826072703750	0.4563426363860899
0.2803088252628072	0.5923877949321934	0.4471838816713998

Energy = -223.211 eV

9) NNH2

1.0000000000000000

13.7550001143999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.5450000762999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.8722000122000004

Bi N H

54 2 2

Direct

0.1651225195932540	0.3449667935798928	0.0105305235623376
0.5015441374067464	0.3449667935798928	0.0105305235623376
0.8333333129999971	0.3465423184386509	0.0128517934982284
0.0005929487299170	0.5167613928744217	0.1584685520005635
0.3333333429999996	0.5167041659359342	0.1483083796921321
0.6660737512700834	0.5167613928744217	0.1584685520005635
0.1640343657192318	0.6822790113689834	0.3071445652480165
0.5026323052807697	0.6822790113689834	0.3071445652480165
0.8333333129999971	0.6804132238889480	0.3026560191351493
0.0012060688593181	0.5427455011493691	0.0136358308607001
0.3333333429999996	0.5393378363821739	0.0096503552473024
0.6654606211406815	0.5427455011493691	0.0136358308607001
0.1667910114629905	0.7038486985860928	0.1602605517802402
0.4998756305370122	0.7038486985860928	0.1602605517802402
0.8333333129999971	0.7043961862866936	0.1570960968273454
0.0001192204155416	0.8759374336379508	0.3027095729531695
0.3333333429999996	0.8742409649762592	0.3036175155515863
0.6665474665844613	0.8759374336379508	0.3027095729531695
0.1677448455110664	0.0122118181467883	0.0124938219442612
0.4989218554889376	0.0122118181467883	0.0124938219442612
0.8333333129999971	0.0126654296508377	0.0126078254142783
0.0000947165904037	0.1830672520172030	0.1574258236088966
0.3333333429999996	0.1829708632707536	0.1581590861947646
0.6665719904096079	0.1830672520172030	0.1574258236088966
0.1669568245095547	0.3474416012187262	0.3014786175619690
0.4997098464904468	0.3474416012187262	0.3014786175619690
0.8333333129999971	0.3465130602465578	0.3032406388630875
0.9983284811739424	0.2071958293045384	0.0124140609787915
0.3333333429999996	0.2083604656910865	0.0131634111066461
0.6683382658260513	0.2071958293045384	0.0124140609787915
0.1673242124924599	0.3716036988140345	0.1551863787066523
0.4993424585075417	0.3716036988140345	0.1551863787066523
0.8333333129999971	0.3719354701739093	0.1582465485054101
0.0001948900558801	0.5426591976453068	0.3036712359073519
0.3333333429999996	0.5426992911689297	0.3056423462723288
0.6664717779441247	0.5426591976453068	0.3036712359073519
0.1656753950936718	0.6812446218716488	0.0138737887392821
0.5009912759063297	0.6812446218716488	0.0138737887392821
0.8333333129999971	0.6797615397338390	0.0118367596810813
0.0000860900970991	0.8494602286038457	0.1576200379331993
0.3333333429999996	0.8490386196618758	0.1588887548084443
0.6665805369028988	0.8494602286038457	0.1576200379331993
0.1672237168306623	0.0132249723668636	0.3028804004196388
0.4994429701693406	0.0132249723668636	0.3028804004196388
0.8333333129999971	0.0140573211641808	0.3028887081202143
0.1666203314334993	0.0377685005715591	0.1576128765321485
0.5000463395665022	0.0377685005715591	0.1576128765321485
0.8333333129999971	0.0376130603419682	0.1578988213999253
0.0003790678027826	0.8749295859119357	0.0126444378737176
0.3333333429999996	0.8726814762107153	0.0135780957882474
0.6662876181972095	0.8749295859119357	0.0126444378737176

0.0002060061848965	0.2091364383747703	0.3026615708088798
0.3333333429999996	0.2094252120513005	0.3034051608067259
0.6664606708150984	0.2091364383747703	0.3026615708088798
0.3333333429999996	0.5543832774509880	0.4111939376073792
0.3333333429999996	0.4779319389495029	0.4403584159114402
0.3333333429999996	0.4787264980224535	0.4873132024710500
0.3333333429999996	0.4137937842146826	0.4197825062575262

Energy = -225.153 eV

10) N

1.0000000000000000

13.7550001143999996 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.5450000762999991 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.8722000122000004

Bi N

54 1

Direct

0.1651537720578276	0.3442995420026662	0.0108783806983013
0.5015128849421728	0.3442995420026662	0.0108783806983013
0.8333333129999971	0.3467330736354413	0.0130059746418212
0.0003643018330379	0.5182712280936386	0.1587651840827462
0.3333333429999996	0.5186369689456356	0.1478262983288730
0.6663023981669625	0.5182712280936386	0.1587651840827462
0.1634872481733467	0.6824211447983402	0.3076742348477950
0.5031794228266548	0.6824211447983402	0.3076742348477950
0.8333333129999971	0.6809096627958411	0.3012357726519923
0.0011457252956575	0.5422740279787774	0.0136233280362745
0.3333333429999996	0.5384102815206404	0.0094069340836924
0.6655209647043421	0.5422740279787774	0.0136233280362745
0.1672112589823840	0.7063980561823939	0.1632692043277757
0.4994553830176187	0.7063980561823939	0.1632692043277757
0.8333333129999971	0.7064101032918444	0.1563488910349307
0.0001850227919817	0.8750957358029439	0.3031666011418679
0.3333333429999996	0.8746957930171604	0.3049948324625333
0.6664816642080211	0.8750957358029439	0.3031666011418679
0.1680459967486314	0.0117288055240792	0.0131448572334136
0.4986207042513726	0.0117288055240792	0.0131448572334136
0.8333333129999971	0.0118620423675608	0.0135112977353771
0.9999868499412017	0.1846178780579706	0.1571291347934718
0.3333333429999996	0.1847755652052072	0.1573056449375869
0.6666798570588028	0.1846178780579706	0.1571291347934718
0.1679021584652247	0.3475748353614492	0.3009317885717309
0.4987645125347768	0.3475748353614492	0.3009317885717309
0.8333333129999971	0.3466523714382674	0.3028596781183026
0.9980907783630002	0.2070883100087997	0.0119477595808917
0.3333333429999996	0.2080779403097210	0.0113915299859926
0.6685759686369934	0.2070883100087997	0.0119477595808917
0.1673849577709206	0.3735177593348311	0.1557398017277265
0.4992817132290810	0.3735177593348311	0.1557398017277265
0.8333333129999971	0.3731977957332049	0.1583846886942979
0.0002043365309632	0.5432160471765002	0.3043924596334264
0.3333333429999996	0.5374304489535362	0.3144535417851131

0.6664623314690417	0.5432160471765002	0.3043924596334264
0.1653944230691593	0.6800883951135148	0.0175802410566348
0.5012722479308422	0.6800883951135148	0.0175802410566348
0.8333333129999971	0.6800794260432284	0.0119525031755501
0.0000288916766706	0.8514027264092405	0.1578858627252728
0.3333333429999996	0.8517325077851723	0.1601722798329206
0.6666377353233273	0.8514027264092405	0.1578858627252728
0.1667417839205001	0.0130402256646320	0.3027859399603159
0.4999249030795028	0.0130402256646320	0.3027859399603159
0.8333333129999971	0.0141035160185226	0.3029796000488716
0.1666136036723316	0.0396811218689521	0.1577058113807581
0.5000530673276700	0.0396811218689521	0.1577058113807581
0.8333333129999971	0.0388302946828105	0.1587328138437201
0.0006598512867058	0.8744838947132791	0.0126696510445896
0.3333333429999996	0.8717438817152043	0.0142513322678823
0.6660068347132935	0.8744838947132791	0.0126696510445896
0.0005745142342590	0.2094866453233521	0.3023283924643252
0.3333333429999996	0.2084140115645639	0.3018783378311340
0.6660921627657359	0.2094866453233521	0.3023283924643252
0.3333333429999996	0.5111374244181448	0.4102282246373434

Energy = -209.041 eV

11) NH

1.0000000000000000

13.7550001143999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.5450000762999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.8722000122000004

Bi N H

54 1 1

Direct

0.1651537720578276	0.3442995420026662	0.0108783806983013
0.5015128849421728	0.3442995420026662	0.0108783806983013
0.8333333129999971	0.3467330736354413	0.0130059746418212
0.0003643018330379	0.5182712280936386	0.1587651840827462
0.3333333429999996	0.5186369689456356	0.1478262983288730
0.6663023981669625	0.5182712280936386	0.1587651840827462
0.1634872481733467	0.6824211447983402	0.3076742348477950
0.5031794228266548	0.6824211447983402	0.3076742348477950
0.8333333129999971	0.6809096627958411	0.3012357726519923
0.0011457252956575	0.5422740279787774	0.0136233280362745
0.3333333429999996	0.5384102815206404	0.0094069340836924
0.6655209647043421	0.5422740279787774	0.0136233280362745
0.1672112589823840	0.7063980561823939	0.1632692043277757
0.4994553830176187	0.7063980561823939	0.1632692043277757
0.8333333129999971	0.7064101032918444	0.1563488910349307
0.0001850227919817	0.8750957358029439	0.3031666011418679
0.3333333429999996	0.8746957930171604	0.3049948324625333
0.6664816642080211	0.8750957358029439	0.3031666011418679
0.1680459967486314	0.0117288055240792	0.0131448572334136
0.4986207042513726	0.0117288055240792	0.0131448572334136
0.8333333129999971	0.0118620423675608	0.0135112977353771
0.9999868499412017	0.1846178780579706	0.1571291347934718

0.3333333429999996	0.1847755652052072	0.1573056449375869
0.6666798570588028	0.1846178780579706	0.1571291347934718
0.1679021584652247	0.3475748353614492	0.3009317885717309
0.4987645125347768	0.3475748353614492	0.3009317885717309
0.8333333129999971	0.3466523714382674	0.3028596781183026
0.9980907783630002	0.2070883100087997	0.0119477595808917
0.3333333429999996	0.2080779403097210	0.0113915299859926
0.6685759686369934	0.2070883100087997	0.0119477595808917
0.1673849577709206	0.3735177593348311	0.1557398017277265
0.4992817132290810	0.3735177593348311	0.1557398017277265
0.8333333129999971	0.3731977957332049	0.1583846886942979
0.0002043365309632	0.5432160471765002	0.3043924596334264
0.3333333429999996	0.5374304489535362	0.3144535417851131
0.6664623314690417	0.5432160471765002	0.3043924596334264
0.1653944230691593	0.6800883951135148	0.0175802410566348
0.5012722479308422	0.6800883951135148	0.0175802410566348
0.8333333129999971	0.6800794260432284	0.0119525031755501
0.0000288916766706	0.8514027264092405	0.1578858627252728
0.3333333429999996	0.8517325077851723	0.1601722798329206
0.6666377353233273	0.8514027264092405	0.1578858627252728
0.1667417839205001	0.0130402256646320	0.3027859399603159
0.4999249030795028	0.0130402256646320	0.3027859399603159
0.8333333129999971	0.0141035160185226	0.3029796000488716
0.1666136036723316	0.0396811218689521	0.1577058113807581
0.5000530673276700	0.0396811218689521	0.1577058113807581
0.8333333129999971	0.0388302946828105	0.1587328138437201
0.0006598512867058	0.8744838947132791	0.0126696510445896
0.3333333429999996	0.8717438817152043	0.0142513322678823
0.6660068347132935	0.8744838947132791	0.0126696510445896
0.0005745142342590	0.2094866453233521	0.3023283924643252
0.3333333429999996	0.2084140115645639	0.3018783378311340
0.6660921627657359	0.2094866453233521	0.3023283924643252
0.3333333429999996	0.5111374244181448	0.4102282246373434
0.3333336709999983	0.5743055257275387	0.4323330752874455

Energy = -213.101 eV

2. BiSb_Bi

1) surface

1.0000000000000000

13.4676008223999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.1693000792999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.7192001342999994

Bi Sb

27 27

Direct

0.0000000000000000 0.5080053251605747 0.0137022924938748

0.3333333429999996 0.5080053251605747 0.0137022924938748

0.6666666870000029 0.5080053251605747 0.0137022924938748

0.1666666719999981 0.6831440783415275 0.1548537175990461

0.5000000000000000 0.6831440783415275 0.1548537175990461

0.8333333129999971 0.6831440783415275 0.1548537175990461

0.0000000000000000 0.8411400565704881 0.2959844909941225

0.3333333429999996	0.8411400565704881	0.2959844909941225
0.6666666870000029	0.8411400565704881	0.2959844909941225
0.0000000000000000	0.1747355218338527	0.0133182317074301
0.3333333429999996	0.1747355218338527	0.0133182317074301
0.6666666870000029	0.1747355218338527	0.0133182317074301
0.1666666719999981	0.3495081827678419	0.1546785086460076
0.5000000000000000	0.3495081827678419	0.1546785086460076
0.8333333129999971	0.3495081827678419	0.1546785086460076
0.0000000000000000	0.5075553268075197	0.2959653157118609
0.3333333429999996	0.5075553268075197	0.2959653157118609
0.6666666870000029	0.5075553268075197	0.2959653157118609
0.1666666719999981	0.0164075279806823	0.1545201455979566
0.5000000000000000	0.0164075279806823	0.1545201455979566
0.8333333129999971	0.0164075279806823	0.1545201455979566
0.0000000000000000	0.8412800989154334	0.0134665357585249
0.3333333429999996	0.8412800989154334	0.0134665357585249
0.6666666870000029	0.8412800989154334	0.0134665357585249
0.0000000000000000	0.1742812338960178	0.2957376382217589
0.3333333429999996	0.1742812338960178	0.2957376382217589
0.6666666870000029	0.1742812338960178	0.2957376382217589
0.1666666719999981	0.3706312149915050	0.0108934463039247
0.5000000000000000	0.3706312149915050	0.0108934463039247
0.8333333129999971	0.3706312149915050	0.0108934463039247
0.0000000000000000	0.5386850992243026	0.1548618896364005
0.3333333429999996	0.5386850992243026	0.1548618896364005
0.6666666870000029	0.5386850992243026	0.1548618896364005
0.1666666719999981	0.7038089786386195	0.2985523312371114
0.5000000000000000	0.7038089786386195	0.2985523312371114
0.8333333129999971	0.7038089786386195	0.2985523312371114
0.1666666719999981	0.0373454246968876	0.0106861078464675
0.5000000000000000	0.0373454246968876	0.0106861078464675
0.8333333129999971	0.0373454246968876	0.0106861078464675
0.0000000000000000	0.2049845875426612	0.1545678219801019
0.3333333429999996	0.2049845875426612	0.1545678219801019
0.6666666870000029	0.2049845875426612	0.1545678219801019
0.1666666719999981	0.3701570948581718	0.2984937206028420
0.5000000000000000	0.3701570948581718	0.2984937206028420
0.8333333129999971	0.3701570948581718	0.2984937206028420
0.1666666719999981	0.7039215567784609	0.0110851911110856
0.5000000000000000	0.7039215567784609	0.0110851911110856
0.8333333129999971	0.7039215567784609	0.0110851911110856
0.1666666719999981	0.0370197363465863	0.2982412900135643
0.5000000000000000	0.0370197363465863	0.2982412900135643
0.8333333129999971	0.0370197363465863	0.2982412900135643
0.0000000000000000	0.8719890446488705	0.1546613155379220
0.3333333429999996	0.8719890446488705	0.1546613155379220
0.6666666870000029	0.8719890446488705	0.1546613155379220

Energy = -210.820 eV

2) N2

1.0000000000000000

13.4979000092000003 0.0000000000000000 0.0000000000000000

0.0000000000000000	14.1709003447999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7392005919999995

Bi Sb N
27 27 2

Direct

0.0000126120232622	0.5069646143517303	0.0095933437684010
0.3333333429999996	0.5064766808553287	0.0087515743251103
0.6666540749767407	0.5069646143517303	0.0095933437684010
0.1667239528449187	0.6819351916490533	0.1238605869010243
0.4999427191550794	0.6819351916490533	0.1238605869010243
0.8333333129999971	0.6820424459494134	0.1238816474911815
0.0000674059719401	0.8397463605479487	0.2389586839250057
0.3333333429999996	0.8397866033695962	0.2389473341684294
0.6665992810280699	0.8397463605479487	0.2389586839250057
0.9999831928210199	0.1734865827047969	0.0099335097561735
0.3333333429999996	0.1735155400544954	0.0099961249338278
0.6666834941789830	0.1734865827047969	0.0099335097561735
0.1665949699569396	0.3483919977760408	0.1237514439151610
0.5000717020430585	0.3483919977760408	0.1237514439151610
0.8333333129999971	0.3483166311817669	0.1244189610270752
0.9999756560230963	0.5071079563415282	0.2389543108575296
0.3333333429999996	0.5070962133899144	0.2377526759938036
0.6666910309769065	0.5071079563415282	0.2389543108575296
0.1666649664267865	0.0148201215433517	0.1243075410609364
0.5000017055732116	0.0148201215433517	0.1243075410609364
0.8333333129999971	0.0147725424172904	0.1242319996257351
0.0000007405150768	0.8400641170297263	0.0095040411983476
0.3333333429999996	0.8400710329843264	0.0094803821731233
0.6666659464849261	0.8400641170297263	0.0095040411983476
0.0000364261598662	0.1734238626149249	0.2393599446441286
0.3333333429999996	0.1734657197467016	0.2393867491579300
0.6666302608401367	0.1734238626149249	0.2393599446441286
0.1664743374626241	0.3697094966465642	0.0067123846003909
0.5001923345373740	0.3697094966465642	0.0067123846003909
0.8333333129999971	0.3700211076113362	0.0076045430237528
0.9999941110435699	0.5377900605724335	0.1243197983348239
0.3333333429999996	0.5376198205027194	0.1234007912400941
0.6666725759564400	0.5377900605724335	0.1243197983348239
0.1667075876353579	0.7027210531579229	0.2405188104731906
0.4999590843646402	0.7027210531579229	0.2405188104731906
0.8333333129999971	0.7028307727532734	0.2404947661459289
0.1667039243681074	0.0363647821763280	0.0076831225400440
0.4999627476318906	0.0363647821763280	0.0076831225400440
0.8333333129999971	0.0363984679820959	0.0075939271128931
0.9999702891187283	0.2040555149035796	0.1246240397530016
0.3333333429999996	0.2041241833293839	0.1246202141073312
0.6666963978812745	0.2040555149035796	0.1246240397530016
0.1666523615147995	0.3699927960280220	0.2402511503048075
0.5000143104851986	0.3699927960280220	0.2402511503048075
0.8333333129999971	0.3700304164432140	0.2409676658849307
0.1666645995163165	0.7030994967756072	0.0070190855904855

0.5000020724836816	0.7030994967756072	0.0070190855904855
0.8333333129999971	0.7030423031680471	0.0069783563617065
0.1667084335069191	0.0363672654522773	0.2411218741199832
0.4999582384930790	0.0363672654522773	0.2411218741199832
0.8333333129999971	0.0363946521655052	0.2410067677230145
0.0000330910955384	0.8704462041795651	0.1243137797545089
0.3333333429999996	0.8704617555614931	0.1243154072532420
0.6666335959044645	0.8704462041795651	0.1243137797545089
0.3333333429999996	0.5129783190642172	0.3800533583249006
0.3333336410000030	0.4581010475671761	0.4099386339300182

Energy = -227.435 eV

3) NNH

1.0000000000000000

13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H

27 27 2 1

Direct

0.0008080423970114	0.5064179206550392	0.0135852015303755
0.3333333429999996	0.5103578116926641	0.0125617842853885
0.6658586446029986	0.5064179206550392	0.0135852015303755
0.1678830167051402	0.6796218459779837	0.1532511343841279
0.4987836552948650	0.6796218459779837	0.1532511343841279
0.8333333129999971	0.6802876764620720	0.1547874744277280
0.0006977737185991	0.8385497090184870	0.2956581627258004
0.3333333429999996	0.8391589366473013	0.2954101673349001
0.6659689132814108	0.8385497090184870	0.2956581627258004
0.0005123537713061	0.1742720237040345	0.0144451421329492
0.3333333429999996	0.1753811646710091	0.0146981061443512
0.6661543332286968	0.1742720237040345	0.0144451421329492
0.1667843581372068	0.3486686278012456	0.1559640407869125
0.4998823138627912	0.3486686278012456	0.1559640407869125
0.8333333129999971	0.3478085862739491	0.1543898877375369
0.0001509051329762	0.5055987513772777	0.2967213740488859
0.3333333429999996	0.5053841702800241	0.3033199880443576
0.6665157818670266	0.5055987513772777	0.2967213740488859
0.1666980708473744	0.0143851688809704	0.1548429073300213
0.4999686011526236	0.0143851688809704	0.1548429073300213
0.8333333129999971	0.0143201462821025	0.1551452022352038
0.9991562248503385	0.8408627098522743	0.0135020024449446
0.3333333429999996	0.8402727971779527	0.0130560050662751
0.6675104621496644	0.8408627098522743	0.0135020024449446
0.9998009484538741	0.1723100248359160	0.2965515818401840
0.3333333429999996	0.1732969996526634	0.2967922918100498
0.6668657385461287	0.1723100248359160	0.2965515818401840
0.1662199061457557	0.3698870755087142	0.0111269050279290
0.5004467658542424	0.3698870755087142	0.0111269050279290
0.8333333129999971	0.3695048016867801	0.0107148366277059
0.0004098665633236	0.5360136211063491	0.1551231317686970
0.3333333429999996	0.5345361455686373	0.1508833155412503

0.6662568204366792	0.5360136211063491	0.1551231317686970
0.1677191655250923	0.7009057186805876	0.2967971167989134
0.4989475064749058	0.7009057186805876	0.2967971167989134
0.8333333129999971	0.7020294311993425	0.2982635400768245
0.1673320463300243	0.0370169539149074	0.0113748957929616
0.4993346256699738	0.0370169539149074	0.0113748957929616
0.8333333129999971	0.0371208934365015	0.0114889468983606
0.0001723865238219	0.2036014140004809	0.1554370784329961
0.3333333429999996	0.2041184470140820	0.1558722508898569
0.6664943004761810	0.2036014140004809	0.1554370784329961
0.1647602083788087	0.3672685680744010	0.2995947870589006
0.5019064636211894	0.3672685680744010	0.2995947870589006
0.8333333129999971	0.3684763737812276	0.2980448745403805
0.1658925094200967	0.7037509077583692	0.0094916868373431
0.5007741625798943	0.7037509077583692	0.0094916868373431
0.8333333129999971	0.7028487966958323	0.0110141260106928
0.1668525170709003	0.0354594343659613	0.2986261446251177
0.4998141549290978	0.0354594343659613	0.2986261446251177
0.8333333129999971	0.0344577559705996	0.2985751680398323
0.0001428733626625	0.8697926028003593	0.1546078593234483
0.3333333429999996	0.8698733483142647	0.1545840644268424
0.6665238136373333	0.8697926028003593	0.1546078593234483
0.3333333129999971	0.4860448420478534	0.4180972499909856
0.3333337899999975	0.5596281481070378	0.4464665231331040
0.3333344159999996	0.5481070124114993	0.4946429489572068

Energy = -228.921 eV

4) NH-NH

1.0000000000000000

13.4676008223999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.1693000792999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.7192001342999994

Bi Sb N H

27 27 2 2

Direct

0.0003928056572349	0.5053764512066294	0.0141666480454745
0.3333330150000009	0.5070026385690980	0.0137290587078098
0.6662741913427652	0.5053764512066294	0.0141666480454745
0.1667705354952176	0.6817873035461233	0.1533728476176606
0.4998964645047792	0.6817873035461233	0.1533728476176606
0.8333330150000009	0.6814004897800956	0.1545184172785738
0.0001272987940055	0.8397822486750997	0.2951099179253163
0.3333330150000009	0.8396894725895905	0.2952103316161043
0.6665386802059885	0.8397822486750997	0.2951099179253163
0.0001401154687599	0.1731825511659864	0.0139269937844233
0.3333330150000009	0.1738577082685353	0.0139773788333031
0.6665269065312458	0.1731825511659864	0.0139269937844233
0.1665449628481568	0.3486943647092531	0.1545430926496039
0.5001210681518415	0.3486943647092531	0.1545430926496039
0.8333330150000009	0.3483045102152502	0.1549095900680442
0.9999819042179894	0.5065198043242560	0.2961728349443788
0.3333330150000009	0.5086311375108465	0.2954061615957215

0.6666840757820083	0.5065198043242560	0.2961728349443788
0.1667857161007760	0.0149954988774610	0.1545592941356233
0.4998813128992268	0.0149954988774610	0.1545592941356233
0.8333330150000009	0.0151039865827372	0.1544713815104615
0.9994672330036991	0.8400993301016371	0.0128463846036624
0.3333330150000009	0.8396709139048681	0.0128903431475820
0.6671987979963063	0.8400993301016371	0.0128463846036624
0.0000928149319392	0.1729660814809719	0.2959358662843030
0.3333330150000009	0.1733044073732302	0.2960184942923121
0.6665741700680670	0.1729660814809719	0.2959358662843030
0.1663760473993889	0.3678221695732731	0.0105380406681164
0.5002909676006055	0.3678221695732731	0.0105380406681164
0.8333330150000009	0.3686342297374452	0.0109456658233356
0.0003505492473224	0.5371709915966676	0.1550751713748326
0.3333330150000009	0.5379016972158936	0.1518103288169783
0.6663164407526807	0.5371709915966676	0.1550751713748326
0.1668384798477334	0.7024553131758964	0.2974873774653233
0.4998285351522682	0.7024553131758964	0.2974873774653233
0.8333330150000009	0.7027815667498629	0.2983096639041491
0.1669445023947347	0.0361106703958711	0.0109102959039262
0.4997224816052679	0.0361106703958711	0.0109102959039262
0.8333330150000009	0.0359273287684090	0.0107286320219302
0.0000441496738475	0.2038779553331977	0.1548766260457839
0.3333330150000009	0.2043240540499554	0.1550051919540749
0.6666228523261566	0.2038779553331977	0.1548766260457839
0.1666062759443676	0.3692950345790393	0.2999909577399364
0.5000607390556340	0.3692950345790393	0.2999909577399364
0.8333330150000009	0.3691632993049865	0.2990038580573611
0.1660750093523404	0.7029050635390846	0.0094414598410850
0.5005919756476658	0.7029050635390846	0.0094414598410850
0.8333330150000009	0.7023880899163402	0.0106399562149733
0.1667527089670600	0.0358326430985940	0.2987253660137412
0.4999142910329439	0.0358326430985940	0.2987253660137412
0.8333330150000009	0.0358154330112228	0.2986065228555717
0.0000043433861023	0.8705460634473141	0.1540522082296150
0.3333330150000009	0.8703650793825304	0.1543028641801385
0.6666626816139001	0.8705460634473141	0.1540522082296150
0.3333333129999971	0.4899329858034278	0.4177808637560503
0.3333333129999971	0.5550576283367121	0.4567205963724774
0.3333333129999971	0.5292620883145602	0.5017934926525172
0.3333333129999971	0.4209240499617337	0.4348804747949657

Energy = -232.807 eV

5) NH-NH2

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H
27 27 2 3

Direct

0.0004342097839682	0.5042443788420101	0.0147572669092781
--------------------	--------------------	--------------------

0.3324687813736631	0.5089758035547050	0.0129348511035587
0.6648768816990867	0.5048133633667433	0.0155778571437253
0.1669939571821715	0.6773596090370333	0.1535021484495402
0.4974868654242712	0.6774260129545411	0.1537004621193105
0.8324042555494628	0.6779891065193624	0.1561990408881542
0.9994222612304924	0.8369218627287012	0.2962042691550621
0.3325297596269579	0.8372629497284052	0.2956085713680849
0.6644050143471176	0.8365649353366393	0.2963269617135253
0.9996470489325020	0.1726922768696753	0.0154105052576412
0.3324425915779017	0.1739829762229519	0.0158339617577781
0.6651057009185735	0.1725298832026709	0.0153655474451710
0.1660897498727323	0.3468880108846619	0.1572991938393997
0.4987996519033615	0.3466988210135042	0.1585768144774349
0.8320818096601172	0.3458120813412577	0.1552720983844296
0.9997740300914870	0.5030639686450300	0.2982882662530670
0.3286547511235867	0.5052764603005002	0.3091236000422271
0.6653036720960017	0.5035789822564283	0.2989556401650972
0.1657506424623136	0.0124559216521263	0.1556197062960933
0.4991648904513468	0.0122777832196164	0.1556067098811411
0.8323088790411504	0.0125496005857073	0.1561507225536758
0.9980378498344749	0.8393791454525612	0.0142069432822751
0.3327723897930071	0.8385060844938721	0.0134427115548093
0.6672125675432312	0.8394359847465438	0.0142311007010676
0.9983691169558426	0.1698572234426337	0.2973329888498455
0.3323564996372994	0.1709665977529937	0.2978818999180746
0.6654523458203556	0.1709763221024261	0.2976550993432454
0.1650452099749202	0.3675394180745784	0.0120905156900690
0.4999119466441044	0.3678642333769417	0.0143257787217266
0.8322887460453074	0.3677992193049207	0.0117710058324647
0.9996237499604064	0.5337186181177103	0.1565451846049939
0.3323050174285882	0.5323429288559467	0.1496667120385240
0.6650853255424991	0.5340394683338232	0.1569927196525214
0.1665703577589213	0.6992407633302307	0.2967572902058251
0.4977415811172889	0.6982295056631216	0.2973448876655027
0.8320864778365475	0.7003188241720082	0.2993660036544767
0.1666344609989423	0.0354954460127459	0.0122413316028940
0.4982842640406133	0.0352301509054556	0.0123228573315970
0.8323919499992130	0.0354925056709519	0.0124670608888735
0.9992576768788268	0.2019591586761820	0.1563527868725672
0.3324028846241589	0.2022148433002897	0.1571165719932281
0.6653842342890286	0.2014390717790135	0.1564935049761758
0.1630760295930642	0.3639022942616990	0.3007350190835325
0.4996102642610794	0.3667833302155543	0.3023888466220228
0.8322654287358020	0.3665875236178096	0.2988971667989375
0.1648439001809834	0.7024685548649288	0.0097726646175929
0.5005971404970140	0.7023252440912700	0.0099211626740825
0.8325790528928039	0.7009691649799805	0.0123309958204771
0.1658136978135829	0.0331606086102525	0.2994969763597766
0.4991397998047873	0.0333508003822729	0.2994824004522343
0.8318289749962631	0.0322865550083975	0.2994109779741905
0.9992283441374781	0.8679966125265182	0.1552873127694525

0.3324224978784827	0.8679438755369233	0.1550116758698010
0.6658148922152591	0.8677614681121000	0.1552957990598358
0.3055792144982661	0.5117103139897239	0.4145801861448604
0.3659528019334530	0.5820099892955213	0.4420480367259145
0.4158891447617705	0.5560964159831059	0.4730710866453336
0.3274998640529461	0.4466829479248133	0.4304792005598301
0.3215633186749116	0.6311505687718437	0.4626564942379048

Energy = -236.763 eV

6) NH₂-NH₂

1.0000000000000000

13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H

27 27 2 4

Direct

0.0005313766923436	0.5055992551173389	0.0098166572192895
0.3341896839682690	0.5056922946337252	0.0084790501251604
0.6677385167680967	0.5055736772161126	0.0098075770867254
0.1674152391255816	0.6804858062386998	0.1511702711052223
0.5008781471517167	0.6806095369008034	0.1510135025364576
0.8341373882345664	0.6806539561488449	0.1513256994858452
0.0004771227137468	0.8392261538342325	0.2926494867925058
0.3339112044264212	0.8394463429760606	0.2927084184750797
0.6673003810722236	0.8393119852619151	0.2925784231030093
0.0008711897866363	0.1722726607368585	0.0100235467453800
0.3342556041951568	0.1724287998798886	0.0101237645487657
0.6676342317537376	0.1721868351993407	0.0099806977750418
0.1673134143387713	0.3472536216028459	0.1507780449190932
0.5008491221307523	0.3471502676059615	0.1505301410185140
0.8339238226652910	0.3474679840245045	0.1513169605518456
0.0006725756687018	0.5059921095420066	0.2922905823338411
0.3346664587464119	0.5060681016796806	0.2906429704240310
0.6675155146936476	0.5059523189265107	0.2923157141291881
0.1673828082701689	0.0139209532996389	0.1512905209710169
0.5007158614280058	0.0137179156905063	0.1514779284754297
0.8341299866170857	0.0137400896732274	0.1512201320479321
0.0005882855086838	0.8389061608492483	0.0101674926317443
0.3339324577685758	0.8389316693048698	0.0103479916478548
0.6673433887375211	0.8389638136165303	0.0100534410152093
0.0008177835034786	0.1728595438637299	0.2924204534192540
0.3340153585415209	0.1727944777547918	0.2925149360495780
0.6674952261639788	0.1726851180229403	0.2924056889450597
0.1671419996174208	0.3685162365021952	0.0069091824561767
0.5009776114641014	0.3684879278333710	0.0066750061711645
0.8340506520012880	0.3681852817961229	0.0075599799160386
0.0006661720336822	0.5360755032214684	0.1510971533781245
0.3342064055251228	0.5361489002434325	0.1494864105193656
0.6675390270178738	0.5360919047873978	0.1510982406570989
0.1672930499667586	0.7020526446640005	0.2952738881359949
0.5004874489970632	0.7020805365040701	0.2950598784752856

0.8338570739825713	0.7019305773674631	0.2950911899193613
0.1676559370484654	0.0351257593115122	0.0075261014573229
0.5008127296192129	0.0350664281344066	0.0077077636966223
0.8342841454188843	0.0348863259507439	0.0074182064021713
0.0005312549392471	0.2028844905789953	0.1511767552681746
0.3339783991783492	0.2028300784784207	0.1512661026064350
0.6674958902658830	0.2027081285475845	0.1511323588827764
0.1675396863535781	0.3689805542279103	0.2945490807399409
0.5009090864490560	0.3685154519679088	0.2943585665011312
0.8339966544141575	0.3686114496592054	0.2951040729992158
0.1672321416934253	0.7016191123547415	0.0076229875096345
0.5006044602027444	0.7016918837923285	0.0074596983205524
0.8338609249963937	0.7016937239592238	0.0075840675164756
0.1674015603288979	0.0354743163584601	0.2949742449161405
0.5007824150794704	0.0355266215176613	0.2952083191611763
0.8342522626477660	0.0354480004042159	0.2949497471204410
0.0008213165891817	0.8693188485707566	0.1513270367163315
0.3339243372566827	0.8693711447810060	0.1514980308026850
0.6673756980769454	0.8693232110663303	0.1513293236074915
0.3134396637157479	0.4829266505534022	0.4696487612692408
0.3544808008516895	0.5624239293201683	0.5016319873253607
0.3071418089053424	0.5787382187685495	0.5367440405018655
0.3707424343530334	0.4460735583483952	0.4504566370665373
0.3602734911098224	0.6206828321814939	0.4739194519723640
0.2659390462290361	0.5020335716462085	0.4348583254332681

Energy = -241.164 eV

7) NH₂

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	1	2

Direct

0.0014971058807092	0.5060341508191257	0.0148158806322130
0.3333330150000009	0.5114670053675709	0.0134074663518788
0.6651698741192931	0.5060341508191257	0.0148158806322130
0.1677970690553394	0.6797184430356111	0.1528047588343426
0.4988699449446585	0.6797184430356111	0.1528047588343426
0.8333330150000009	0.6795614310283469	0.1555748540110287
0.0001269238675974	0.8391411654808536	0.2952165101301460
0.3333330150000009	0.8398931390885878	0.2946084957128576
0.6665390761324019	0.8391411654808536	0.2952165101301460
0.0005447560927152	0.1747707888042882	0.0148085961071729
0.3333330150000009	0.1763258720286771	0.0155220020549294
0.6661221939072846	0.1747707888042882	0.0148085961071729
0.1669133701257905	0.3487106713819372	0.1582847650927945
0.4997526458742101	0.3487106713819372	0.1582847650927945
0.8333330150000009	0.3475879044057919	0.1550545542628328
0.0009055560034810	0.5049376766181766	0.2980715655510622
0.3333330150000009	0.5090671459959921	0.3139496640077226

0.6657604489965223	0.5049376766181766	0.2980715655510622
0.1665663866993512	0.0142772680728314	0.1549777401895582
0.5001006133006456	0.0142772680728314	0.1549777401895582
0.8333330150000009	0.0148713137493530	0.1557162675245607
0.9982680401666784	0.8412692932716794	0.0133063078931315
0.3333330150000009	0.8402140383906911	0.0126239264952162
0.6683979908333200	0.8412692932716794	0.0133063078931315
0.0001293642182176	0.1729292140514502	0.2968495543706524
0.3333330150000009	0.1730529566444332	0.2975987576680410
0.6665376287817821	0.1729292140514502	0.2968495543706524
0.1661145413399439	0.3692522065783805	0.0131842057794671
0.5005524876600518	0.3692522065783805	0.0131842057794671
0.8333330150000009	0.3695987411635215	0.0116297732823014
0.0007071352108596	0.5356223156546278	0.1563725829123044
0.3333330150000009	0.5351543902382048	0.1492755296668520
0.6659598627891370	0.5356223156546278	0.1563725829123044
0.1673738799502971	0.7017315811691063	0.2961284421736750
0.4992931350496974	0.7017315811691063	0.2961284421736750
0.8333330150000009	0.7019516697741182	0.2985477356916633
0.1675862803274768	0.0376242526995938	0.0117401078493558
0.4990807036725187	0.0376242526995938	0.0117401078493558
0.8333330150000009	0.0376143617163507	0.0120889439376342
0.0002420812756796	0.2035220820884973	0.1557724103412710
0.3333330150000009	0.2042511106301248	0.1569578488441010
0.6664249347243256	0.2035220820884973	0.1557724103412710
0.1650370160331533	0.3669352859204551	0.3016591890605156
0.5016300279668471	0.3669352859204551	0.3016591890605156
0.8333330150000009	0.3684158693555375	0.2986290600301018
0.1651277281811687	0.7043557813547352	0.0090108292160593
0.5015392258188314	0.7043557813547352	0.0090108292160593
0.8333330150000009	0.7025156593643658	0.0115452371207212
0.1667387897167885	0.0353475914308703	0.2988250668430510
0.4999281942832141	0.0353475914308703	0.2988250668430510
0.8333330150000009	0.0346844345008321	0.2988454275844177
0.9998908954368630	0.8699702986687612	0.1543195411878671
0.3333330150000009	0.8699149953664786	0.1540755293850253
0.6667760885631324	0.8699702986687612	0.1543195411878671
0.3333333129999971	0.5141216521865033	0.4132216489237663
0.3333333129999971	0.4564496077176656	0.4408875778258121
0.3333333129999971	0.5762414510849254	0.4364498692893335

Energy = -225.796 eV

8) NH₃

1.0000000000000000

13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H

27 27 1 3

Direct

0.0004822967606231	0.5053321103924517	0.0133581684812754
0.3332901141709073	0.5066505831673851	0.0141501168506935

0.6661539959205527	0.5052860358577718	0.0133732478880830
0.1668820454916755	0.6810608848255910	0.1537000524743846
0.4997232930509767	0.6810220972828631	0.1536628145036545
0.8332915167051453	0.6807318187548503	0.1544693639142238
0.9997422459796894	0.8395029519457466	0.2955283832950713
0.3332949029448713	0.8397701925125318	0.2953356602570381
0.6668860018388614	0.8395119043793784	0.2955482725450551
0.9999181833828388	0.1728869910907704	0.0140653658732361
0.3333145502515009	0.1733487788631152	0.0140570319180711
0.6667392481632817	0.1728939929311437	0.0140618538763277
0.1664603700133256	0.3483308777355774	0.1539223161459873
0.5001207078707708	0.3483402788657060	0.1538490358274132
0.8333001598854679	0.3479884306881615	0.1548105717806649
0.0000753343846611	0.5059041091162442	0.2955440698952927
0.3332181131104051	0.5074439483000788	0.2965552813453343
0.6664924034115458	0.5059183952483011	0.2956033442564774
0.1665871710482634	0.0146872549740777	0.1546338053610299
0.5000162046655063	0.0147112578075408	0.1546192574772860
0.8333040129096787	0.0146235148351721	0.1547554197358281
0.9996377680086752	0.8397727134258943	0.0133982979576217
0.3332698845210587	0.8395304185293710	0.0132716644465916
0.6669081539682011	0.8398057910275298	0.0134360578934434
0.0000170590138282	0.1728327713393938	0.2960729757251670
0.3333428059302577	0.1732088094723849	0.2960318287483759
0.6665632148956888	0.1728060070949553	0.2960686672049562
0.1664763016337290	0.3679764452044623	0.0095634446054049
0.5000481540628883	0.3680069330915288	0.0094642472998672
0.8333085793336323	0.3685009795041765	0.0108257934199685
0.0002919426947869	0.5364796795593421	0.1543848107544790
0.3332627592229684	0.5370412278445258	0.1531385880811342
0.6662791085204063	0.5364457970267509	0.1544266751517753
0.1667266279045094	0.7024412311557882	0.2980100575756524
0.4998293864839951	0.7024651623265328	0.2980593507293747
0.8333105511660079	0.7021243407544091	0.2984279008020607
0.1667648785821640	0.0357772608766282	0.0109689008313651
0.4998075919928979	0.0357719588804599	0.0109308342383940
0.8333313616411715	0.0354820606687696	0.0110436535173690
0.9999485623272406	0.2035393109751169	0.1549791174663113
0.3333057266329575	0.2039776352023779	0.1548974004438719
0.6666116161706270	0.2035921267641285	0.1549628197375341
0.1662242083477850	0.3685942688150377	0.2984155585770196
0.5003036785450732	0.3686121037793271	0.2983697683322148
0.8332762393590656	0.3689034597790908	0.2988427597438914
0.1662656074382980	0.7024990153210382	0.0099957854043566
0.5002512357986788	0.7024646709578590	0.0099891959502898
0.8332474330256900	0.7021668542190511	0.0108348590500427
0.1667693300985889	0.0356961405918668	0.2987634396320829
0.4998588120287479	0.0356326813948513	0.2987679856786301
0.8332997559266033	0.0356109258331188	0.2988043518525245
0.9999328168310626	0.8701016742918384	0.1544822788209146
0.3333212398027285	0.8702192105974120	0.1543859861969210

0.6666309028298585	0.8701355589170703	0.1545096961847889
0.3336588626881252	0.5177275349679960	0.4258132900469960
0.3674909426384048	0.4589082566748530	0.4431578530912645
0.3714999752664312	0.5757517948051998	0.4409809313191673
0.2629636327066294	0.5207239527554250	0.4427717747857471

Energy = -230.575 eV

9) NNH2

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	2	2

Direct

0.0057850609902488	0.5051475788772564	0.0156610948252549
0.3392211800251914	0.5085185182541210	0.0108419411090566
0.6709573662311499	0.5055701462417943	0.0160441418683774
0.1731954600649601	0.6805594507308896	0.1538992713327048
0.5044550413322568	0.6811062379319495	0.1543199145041214
0.8382829676957115	0.6810156924916839	0.1571820609784425
0.0044919766796028	0.8399054295462349	0.2980901122427611
0.3390473030107515	0.8404799278935968	0.2975935728545451
0.6712502723758860	0.8402593628726791	0.2973518149486623
0.0055709033039051	0.1731923317824950	0.0155491746098448
0.3386480132021177	0.1741590619757147	0.0161278904728448
0.6714469237721730	0.1733055633942158	0.0157776149403190
0.1725421352171637	0.3500390654486409	0.1573838680933619
0.5057911452985380	0.3491318190699246	0.1580926574042323
0.8392961601147277	0.3484620810615908	0.1567544353266541
0.0044389906695059	0.5072424042849661	0.2979881923143566
0.3399277223378832	0.5092375636779352	0.2981578190552980
0.6711322580137420	0.5064034652968772	0.2987574631142564
0.1719443635247444	0.0155020418107625	0.1568105694351658
0.5051068841462012	0.0155155816205763	0.1567747474687877
0.8387751004080570	0.0155037100722382	0.1567791753343855
0.0037209041612414	0.8405968077932542	0.0160874892786751
0.3384266231591155	0.8396480685703196	0.0157101750118613
0.6731507520683309	0.8412059287205054	0.0152954692677199
0.0056636305574571	0.1737488962241898	0.2977191997302739
0.3379179583619987	0.1747511366113841	0.2981959348623917
0.6717345682234424	0.1732898465252930	0.2979520079844988
0.1718815896406909	0.3668695639919832	0.0146077002649463
0.5070870728747749	0.3680454151058257	0.0130365240133514
0.8394426801135495	0.3689555840160565	0.0129603927327793
0.0055862151973471	0.5368657351244295	0.1567027887967569
0.3389415484698759	0.5362044317222470	0.1469873342294861
0.6711630441424816	0.5367670504188169	0.1573126309741824
0.1726633449644055	0.7026726557364071	0.2997400963224166
0.5047817638405334	0.7024780852877868	0.2990480688388502
0.8379564975770819	0.7030925999973121	0.3011313302980625
0.1726543006615131	0.0361466635800696	0.0128228125360508

0.5047606079759106	0.0360678527449281	0.0130326387516391
0.8385464173547490	0.0361069077674685	0.0129387940742589
0.0062339809898688	0.2046018760063362	0.1565337783400622
0.3386262370785218	0.2051286415368807	0.1573536486761924
0.6725261256900197	0.2039903072649096	0.1568517757021155
0.1724212918336363	0.3711363730506250	0.3072592317996197
0.5067629898684274	0.3684141646118064	0.3030826972887652
0.8394749775786963	0.3695626110313484	0.3008605125478141
0.1705256030058209	0.7029198044963749	0.0112440149918385
0.5065847025122778	0.7038800282270756	0.0110873948472019
0.8384516672884317	0.7024932645714088	0.0133976394234523
0.1721764890249347	0.0362105739666347	0.3006914812026906
0.5046435490847898	0.0367849582864821	0.3008720703242105
0.8390745154315979	0.0362981217985165	0.3006632511387295
0.0055164972973856	0.8707605263062348	0.1570619569173886
0.3385132630747165	0.8709282443048565	0.1568843733159468
0.6719739468204935	0.8710205887311133	0.1563748402943617
0.2852447161119827	0.4721559380923850	0.3987169890753677
0.2456344031399738	0.5404267537538701	0.4288513490424180
0.2045097373309943	0.5256509514327590	0.4675018562334898
0.2389059910785036	0.6084807222559050	0.4116084456366522

Energy = -232.557 eV

10) N

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N

27 27 1

Direct

0.0011263866177913	0.5063200788397992	0.0145672696888042
0.3335166501492139	0.5113812121845385	0.0104305194579482
0.6659687898386579	0.5062755088579465	0.0144588080071273
0.1683701009491685	0.6791335224670263	0.1528853788754461
0.4987559164029065	0.6791364006751763	0.1527792129699037
0.8335614151804762	0.6800920482028943	0.1555237301652497
0.0010842477814350	0.8389247961472748	0.2956669390730369
0.3335764981721496	0.8391955951362675	0.2951807808137232
0.6660025612515312	0.8389329833036498	0.2955919965297653
0.0009708445237209	0.1745262182627343	0.0147430079365947
0.3335489092077921	0.1763110250358721	0.0157032438475682
0.6661796012128605	0.1745404715022687	0.0148343632122234
0.1672029419825449	0.3490388461161089	0.1585243364595286
0.4998924094385657	0.3490203080297078	0.1584273439959603
0.8335530411252776	0.3475976858435388	0.1547972523658316
0.0001663225612276	0.5056704708262600	0.2980930388830885
0.3335468219291116	0.5063491523495287	0.3115777595613594
0.6668920545349764	0.5056845822342169	0.2979898287901719
0.1669354841515869	0.0142739109508625	0.1552187051503893
0.5001830856327274	0.0142932428695062	0.1552602008180415
0.8335692755297117	0.0148680320535846	0.1557806967845892

0.9986714046007847	0.8416112048988609	0.0135849222667233
0.3335144604258105	0.8405831780947111	0.0130306028012726
0.6684857243783995	0.8416209358796678	0.0135159149623192
0.0006901466229365	0.1725525038968101	0.2968890720506607
0.3335776472634961	0.1736498736858394	0.2979147018881179
0.6664648335071703	0.1725577031728918	0.2969373511152540
0.1656313090389716	0.3693701281531858	0.0138016136042438
0.5014253088423999	0.3693465967941805	0.0136834353617203
0.8335657524925395	0.3693947533822595	0.0113473676092610
0.0006385644889235	0.5357734184603515	0.1561161170654586
0.3335568627983747	0.5340284890997324	0.1461099963435117
0.6665057989130290	0.5357650851505724	0.1559976330359305
0.1676130173582706	0.7009531564290370	0.2965084330475563
0.4995272793817662	0.7009491980419966	0.2964038452847149
0.8335432241025202	0.7024291395310627	0.2986488811641834
0.1680116403484107	0.0374959046517915	0.0118498758711922
0.4991231926650457	0.0375216883369376	0.0119354101389675
0.8335774601984696	0.0375286190537238	0.0120833979944024
0.0005238110506838	0.2035925592655232	0.1557277408191098
0.3335443876157100	0.2043835141991934	0.1571728011948750
0.6665945045144852	0.2035765501923379	0.1557892742371223
0.1630231423742359	0.3666100200451154	0.3028017439246469
0.5040703804716316	0.3666210272539772	0.3027231474751773
0.8335332595746294	0.3684537444461284	0.2983522869063719
0.1654202833527449	0.7046266201203508	0.0093108166176066
0.5016866298076437	0.7046461637971149	0.0092518156546078
0.8335917711271676	0.7029440697584377	0.0116404521759534
0.1675310731626638	0.0352752008526380	0.2990610932420878
0.4996168368905458	0.0352911023815849	0.2990919572935979
0.8335865795315840	0.0347972703508574	0.2989687654986710
0.0002148502984056	0.8699691292673606	0.1547048929191632
0.3335605563725252	0.8697702971876708	0.1546067791476915
0.6669022763213803	0.8700071243664027	0.1546366520124423
0.3336038439332256	0.4744260209129294	0.4093847328890732

Energy = -215.076 eV

11) NH

1.0000000000000000

13.4676008223999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.1693000792999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.7192001342999994

Bi Sb N H

27 27 1 1

Direct

0.0011928329627935	0.5063651869285195	0.0149629838203396
0.3333330150000009	0.5118559322549530	0.0117822500269327
0.6654741640372066	0.5063651869285195	0.0149629838203396
0.1682116506973443	0.6791025622055216	0.1529580889488926
0.4984553493026525	0.6791025622055216	0.1529580889488926
0.8333330150000009	0.6796528525735894	0.1555387857259802
0.0008652685748061	0.8389213288003674	0.2952855479737906
0.3333330150000009	0.8393737493714681	0.2948724575473491

0.6658007104251880	0.8389213288003674	0.2952855479737906
0.0006078480993992	0.1747784125413787	0.0145948171874011
0.3333330150000009	0.1762918581829354	0.0152955436305930
0.6660591739005994	0.1747784125413787	0.0145948171874011
0.1670263229149711	0.3488510267220022	0.1590255237119038
0.4996397080850272	0.3488510267220022	0.1590255237119038
0.8333330150000009	0.3477086694313769	0.1548653053547611
0.0004112957511921	0.5050650496669391	0.2987193640192345
0.3333330150000009	0.5100844188455085	0.3141270391514581
0.6662546842488055	0.5050650496669391	0.2987193640192345
0.1665282540133219	0.0141286960618743	0.1549280494476761
0.5001387749866808	0.0141286960618743	0.1549280494476761
0.8333330150000009	0.0147747735323662	0.1558417613263714
0.9984032618060823	0.8413536480251338	0.0132343111489348
0.3333330150000009	0.8404043227455773	0.0125569721699250
0.6682627691939231	0.8413536480251338	0.0132343111489348
0.0005954011985025	0.1731088704492834	0.2966701153899294
0.3333330150000009	0.1732783260514239	0.2972956122522277
0.6660715838015037	0.1731088704492834	0.2966701153899294
0.1659159853248227	0.3696065325829494	0.0144717972884649
0.5007510296751789	0.3696065325829494	0.0144717972884649
0.8333330150000009	0.3696023505389263	0.0116071949140064
0.0005710693510537	0.5355758155751928	0.1566091426884597
0.3333330150000009	0.5340453516245489	0.1474239678680149
0.6660959206489494	0.5355758155751928	0.1566091426884597
0.1677592419451344	0.7009121833762393	0.2960947333409720
0.4989077730548672	0.7009121833762393	0.2960947333409720
0.8333330150000009	0.7025055393237594	0.2983822511759300
0.1676167618505531	0.0375646146511173	0.0117392217591714
0.4990502221494495	0.0375646146511173	0.0117392217591714
0.8333330150000009	0.0377074325798716	0.0121623531436228
0.0001503747506320	0.2036043584867713	0.1556077761163337
0.3333330150000009	0.2041870108551080	0.1568332151340641
0.6665166272493721	0.2036043584867713	0.1556077761163337
0.1642537846635719	0.3671382098007427	0.3029138809468961
0.5024132303364297	0.3671382098007427	0.3029138809468961
0.8333330150000009	0.3680748490122951	0.2983529089321095
0.1652491198382933	0.7045705118027286	0.0090881727160053
0.5014178651617129	0.7045705118027286	0.0090881727160053
0.8333330150000009	0.7026509222365505	0.0114892549083123
0.1669486638122635	0.0353529807767927	0.2987256876359154
0.4997183361877404	0.0353529807767927	0.2987256876359154
0.8333330150000009	0.0351194103143868	0.2987862953425946
0.9999503827998382	0.8697999683894153	0.1543272407768583
0.3333330150000009	0.8697810817076856	0.1542367314267850
0.6667166422001642	0.8697999683894153	0.1543272407768583
0.3333333129999971	0.5144786712315295	0.4137781867612063
0.3333336410000030	0.4445133459002619	0.4281828003733992

Energy = -220.274 eV

2. BiSb_Sb

1) surface

```

1.0000000000000000
13.4676008223999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 14.1693000792999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.7192001342999994
Bi Sb
27 27
Direct
0.0000000000000000 0.5080053251605747 0.0137022924938748
0.3333333429999996 0.5080053251605747 0.0137022924938748
0.6666666870000029 0.5080053251605747 0.0137022924938748
0.1666666719999981 0.6831440783415275 0.1548537175990461
0.5000000000000000 0.6831440783415275 0.1548537175990461
0.8333333129999971 0.6831440783415275 0.1548537175990461
0.0000000000000000 0.8411400565704881 0.2959844909941225
0.3333333429999996 0.8411400565704881 0.2959844909941225
0.6666666870000029 0.8411400565704881 0.2959844909941225
0.0000000000000000 0.1747355218338527 0.0133182317074301
0.3333333429999996 0.1747355218338527 0.0133182317074301
0.6666666870000029 0.1747355218338527 0.0133182317074301
0.1666666719999981 0.3495081827678419 0.1546785086460076
0.5000000000000000 0.3495081827678419 0.1546785086460076
0.8333333129999971 0.3495081827678419 0.1546785086460076
0.0000000000000000 0.5075553268075197 0.2959653157118609
0.3333333429999996 0.5075553268075197 0.2959653157118609
0.6666666870000029 0.5075553268075197 0.2959653157118609
0.1666666719999981 0.0164075279806823 0.1545201455979566
0.5000000000000000 0.0164075279806823 0.1545201455979566
0.8333333129999971 0.0164075279806823 0.1545201455979566
0.0000000000000000 0.8412800989154334 0.0134665357585249
0.3333333429999996 0.8412800989154334 0.0134665357585249
0.6666666870000029 0.8412800989154334 0.0134665357585249
0.0000000000000000 0.1742812338960178 0.2957376382217589
0.3333333429999996 0.1742812338960178 0.2957376382217589
0.6666666870000029 0.1742812338960178 0.2957376382217589
0.1666666719999981 0.3706312149915050 0.0108934463039247
0.5000000000000000 0.3706312149915050 0.0108934463039247
0.8333333129999971 0.3706312149915050 0.0108934463039247
0.0000000000000000 0.5386850992243026 0.1548618896364005
0.3333333429999996 0.5386850992243026 0.1548618896364005
0.6666666870000029 0.5386850992243026 0.1548618896364005
0.1666666719999981 0.7038089786386195 0.2985523312371114
0.5000000000000000 0.7038089786386195 0.2985523312371114
0.8333333129999971 0.7038089786386195 0.2985523312371114
0.1666666719999981 0.0373454246968876 0.0106861078464675
0.5000000000000000 0.0373454246968876 0.0106861078464675
0.8333333129999971 0.0373454246968876 0.0106861078464675
0.0000000000000000 0.2049845875426612 0.1545678219801019
0.3333333429999996 0.2049845875426612 0.1545678219801019
0.6666666870000029 0.2049845875426612 0.1545678219801019
0.1666666719999981 0.3701570948581718 0.2984937206028420
0.5000000000000000 0.3701570948581718 0.2984937206028420

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0.8333333129999971	0.3701570948581718	0.2984937206028420
0.1666666719999981	0.7039215567784609	0.0110851911110856
0.5000000000000000	0.7039215567784609	0.0110851911110856
0.8333333129999971	0.7039215567784609	0.0110851911110856
0.1666666719999981	0.0370197363465863	0.2982412900135643
0.5000000000000000	0.0370197363465863	0.2982412900135643
0.8333333129999971	0.0370197363465863	0.2982412900135643
0.0000000000000000	0.8719890446488705	0.1546613155379220
0.3333333429999996	0.8719890446488705	0.1546613155379220
0.6666666870000029	0.8719890446488705	0.1546613155379220

Energy = -210.820 eV

2) N2

1.0000000000000000		
13.4979000092000003	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1709003447999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7392005919999995

Bi Sb N

27 27 2

Direct

0.0000000000000000	0.5064841329857614	0.0091279383454932
0.3333723479222570	0.5061069358516832	0.0084799654179903
0.6666276820777455	0.5061069358516832	0.0084799654179903
0.1667130943501007	0.6814158176410814	0.1233863878874573
0.5000000000000000	0.6815225649644745	0.1234108119829358
0.8332868906498945	0.6814158176410814	0.1233863878874573
0.0000000000000000	0.8395946685689353	0.2386070049743694
0.3333922188212242	0.8396138510932545	0.2387751729525078
0.6666078111787783	0.8396138510932545	0.2387751729525078
0.0000000000000000	0.1731215937339243	0.0096602278757913
0.3333399342170367	0.1731121945850091	0.0096532090434636
0.6666600957829658	0.1731121945850091	0.0096532090434636
0.1666746413661500	0.3480922471129020	0.1237114285635315
0.5000000000000000	0.3481193611166944	0.1231532580180001
0.8333253436338381	0.3480922471129020	0.1237114285635315
0.0000000000000000	0.5067996240562991	0.2385905367241321
0.3336010564747767	0.5064349382554241	0.2378666087878116
0.6663989735252258	0.5064349382554241	0.2378666087878116
0.1666982574073614	0.0146157796182464	0.1239075558930693
0.5000000000000000	0.0144041592369604	0.1241139521944348
0.8333017275926338	0.0146157796182464	0.1239075558930693
0.0000000000000000	0.8400017921963112	0.0091291122600694
0.3333697920135208	0.8398888149346959	0.0093109940890486
0.6666302379864746	0.8398888149346959	0.0093109940890486
0.0000000000000000	0.1730609902605806	0.2389588402748899
0.3332670189580824	0.1730952453367394	0.2389442012662428
0.6667330110419272	0.1730952453367394	0.2389442012662428
0.1665178955929463	0.3693355915275447	0.0067450433978422
0.5000000000000000	0.3690739422504166	0.0059880566269612
0.8334820894070489	0.3693355915275447	0.0067450433978422
0.0000000000000000	0.5371482761636486	0.1238916189233521
0.3334400703139409	0.5370958930918093	0.1232443714187639

0.6665599596860616	0.5370958930918093	0.1232443714187639
0.1667403391557016	0.7025918685978354	0.2400899422482539
0.5000000000000000	0.7025247029682475	0.2401597257649044
0.8332596458442936	0.7025918685978354	0.2400899422482539
0.1666638097585036	0.0360884234106607	0.0072096121845675
0.5000000000000000	0.0360163656851782	0.0075216994439842
0.8333361752414916	0.0360884234106607	0.0072096121845675
0.0000000000000000	0.2038067372678896	0.1242861294912601
0.3333388038258533	0.2038038404048308	0.1242507558745345
0.6666612261741491	0.2038038404048308	0.1242507558745345
0.1667004262765843	0.3696518528536217	0.2402034937929827
0.5000000000000000	0.3691055792452715	0.2395172942832602
0.8332995587234109	0.3696518528536217	0.2402034937929827
0.1666658175665461	0.7029617322504649	0.0065075974344637
0.5000000000000000	0.7028625552731356	0.0065923395047776
0.8333341674334491	0.7029617322504649	0.0065075974344637
0.1666339013608749	0.0359945176608676	0.2407172859122895
0.5000000000000000	0.0361188713599176	0.2408599586842470
0.8333660836391203	0.0359945176608676	0.2407172859122895
0.0000000000000000	0.8703450163728093	0.1239647294599848
0.3332706869360820	0.8702204335790995	0.1241547362459912
0.6667293430639276	0.8702204335790995	0.1241547362459912
0.5000000000000000	0.4237766016186981	0.3884618140632980
0.5000003580000012	0.3657449590633846	0.4166228822822475

Energy = -227.434 eV

3) NNH

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	2	1

Direct

0.0000000000000000	0.5101319720395381	0.0143613507969391
0.3317655057972431	0.5099752864755587	0.0150557645545675
0.6682345242027523	0.5099752864755587	0.0150557645545675
0.1670205335888113	0.6840770828732374	0.1559376167992852
0.5000000000000000	0.6836927652418936	0.1572382883794958
0.8329794514111910	0.6840770828732374	0.1559376167992852
0.0000000000000000	0.8452201975510647	0.2971869388661119
0.3334269289575928	0.8433640043849380	0.2968137332369309
0.6665731010424096	0.8433640043849380	0.2968137332369309
0.0000000000000000	0.1756091957378132	0.0137376013645820
0.3321494648330585	0.1743709234817175	0.0120870220143416
0.6678505651669440	0.1743709234817175	0.0120870220143416
0.1673070687541625	0.3511586379364928	0.1565153466355937
0.5000000000000000	0.3500726256090800	0.1468921672204218
0.8326929162458399	0.3511586379364928	0.1565153466355937
0.0000000000000000	0.5108157519328103	0.2972640326349634
0.3295961749645002	0.5137125643127831	0.2994084495113043
0.6704038550355023	0.5137125643127831	0.2994084495113043

0.1669683048564536	0.0179456475371751	0.1549177764245826
0.5000000000000000	0.0174973860555525	0.1552814270042120
0.8330316801435345	0.0179456475371751	0.1549177764245826
0.0000000000000000	0.8416254505404481	0.0145544465657181
0.3344970270749457	0.8410535044395715	0.0141843584131891
0.6655030029250639	0.8410535044395715	0.0141843584131891
0.0000000000000000	0.1769064584907127	0.2966915290527723
0.3353528735288478	0.1777430554841715	0.2955192095209469
0.6646471564711547	0.1777430554841715	0.2955192095209469
0.1672873220615756	0.3726386692705361	0.0132339069427090
0.5000000000000000	0.3701324311247234	0.0091112366887103
0.8327126629384054	0.3726386692705361	0.0132339069427090
0.0000000000000000	0.5398556920768556	0.1555377266452425
0.3335348426170839	0.5390858268424097	0.1579721027576539
0.6664651873829186	0.5390858268424097	0.1579721027576539
0.1660917628568797	0.7072367586040968	0.2997570591313732
0.5000000000000000	0.7053801967373801	0.3006833041900805
0.8339082221431156	0.7072367586040968	0.2997570591313732
0.1654645532896311	0.0373647428888049	0.0110830229418397
0.5000000000000000	0.0384916474048325	0.0109430293476649
0.8345354317103642	0.0373647428888049	0.0110830229418397
0.0000000000000000	0.2069499185591610	0.1555700216068630
0.3336764205554630	0.2062188773212981	0.1536692611652413
0.6663236094445395	0.2062188773212981	0.1536692611652413
0.1666664181754669	0.3734952217514333	0.3002651380175863
0.5000000000000000	0.3750762429543428	0.3006491525340351
0.8333335668245212	0.3734952217514333	0.3002651380175863
0.1670483526260256	0.7046931099768372	0.0121109490619418
0.5000000000000000	0.7018771059954574	0.0131394487921952
0.8329516323739696	0.7046931099768372	0.0121109490619418
0.1676771708670302	0.0407790883311634	0.2989351548740160
0.5000000000000000	0.0389858384351456	0.2984938187695292
0.8323228141329650	0.0407790883311634	0.2989351548740160
0.0000000000000000	0.8734331064307312	0.1560321972488907
0.3332729840094046	0.8731317661938789	0.1552597730165104
0.6667270459905978	0.8731317661938789	0.1552597730165104
0.5000000000000000	0.3791928394887947	0.4064588750281573
0.5000004770000004	0.3008849446782733	0.4304214301282698
0.5000010730000000	0.3085726067031160	0.4786478950957616

Energy = -228.996 eV

4) NH-NH

1.0000000000000000

13.4676008223999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.1693000792999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.7192001342999994

Bi Sb N H

27 27 2 2

Direct

0.0000000000000000 0.5090984341241125 0.0131469637790147

0.3321177958953712 0.5111424466795782 0.0118350563964142

0.6678822041046288 0.5111424466795782 0.0118350563964142

0.1672150159448691	0.6817249365276865	0.1547587916731459
0.5000000000000000	0.6806848590831578	0.1551999033981062
0.8327849840551309	0.6817249365276865	0.1547587916731459
0.0000000000000000	0.8414595341863063	0.2963636692622416
0.3339543729068168	0.8415689913735775	0.2965559056892957
0.6660456270931903	0.8415689913735775	0.2965559056892957
0.0000000000000000	0.1755983111337613	0.0136481712243679
0.3322912928972528	0.1744986360225411	0.0125550775693029
0.6677086171027398	0.1744986360225411	0.0125550775693029
0.1674122472446271	0.3497065067901985	0.1558077582067767
0.5000000000000000	0.3490529217683900	0.1512074738265881
0.8325877677553777	0.3497065067901985	0.1558077582067767
0.0000000000000000	0.5093122259146696	0.2973315738384699
0.3306779247073948	0.5116143155978676	0.2989327306679783
0.6693220452926028	0.5116143155978676	0.2989327306679783
0.1667257746779285	0.0158747045474854	0.1547108440141542
0.5000000000000000	0.0155923988375193	0.1550402155081088
0.8332741953220690	0.0158747045474854	0.1547108440141542
0.0000000000000000	0.8417478922922967	0.0137265819852388
0.3340059169000824	0.8416505490391231	0.0136662777933623
0.6659940530999222	0.8416505490391231	0.0136662777933623
0.0000000000000000	0.1752717292427164	0.2966220617576099
0.3337004071713068	0.1750178552868746	0.2962755905096799
0.6662996218286921	0.1750178552868746	0.2962755905096799
0.1673130596625754	0.3725473097651246	0.0128261193286860
0.5000000000000000	0.3706879971427313	0.0139164482213587
0.8326859423374273	0.3725473097651246	0.0128261193286860
0.0000000000000000	0.5376459816787005	0.1550703134437939
0.3331669482519075	0.5361044796153749	0.1542565560299565
0.6668330517480925	0.5361044796153749	0.1542565560299565
0.1671754540049264	0.7045389331659706	0.2986297143964904
0.5000000000000000	0.7033616579826116	0.2991172133931386
0.8328244869950652	0.7045389331659706	0.2986297143964904
0.1656529318430700	0.0373654732783066	0.0111171065469833
0.5000000000000000	0.0383525736793828	0.0110318621265435
0.8343470531569324	0.0373654732783066	0.0111171065469833
0.0000000000000000	0.2053664268466662	0.1552728160568790
0.3335619358923410	0.2045257685147703	0.1541828129690117
0.6664381241076569	0.2045257685147703	0.1541828129690117
0.1668208361574628	0.3722828872801216	0.2992838699441904
0.5000000000000000	0.3720752598023509	0.3019910163898203
0.8331791638425372	0.3722828872801216	0.2992838699441904
0.1669923535320592	0.7046744073730693	0.0113445849739975
0.5000000000000000	0.7032310575603447	0.0119829329769487
0.8330076754679396	0.7046744073730693	0.0113445849739975
0.1666549387279375	0.0380704378185968	0.2985388313596786
0.5000000000000000	0.0375199602524745	0.2982646565856300
0.8333450462720648	0.0380704378185968	0.2985388313596786
0.0000000000000000	0.8711856747673465	0.1550878912293854
0.3332482073884080	0.8710676244999007	0.1550330047494839
0.6667517626115824	0.8710676244999007	0.1550330047494839

0.5000000000000000	0.3878368913367893	0.4071343624850030
0.5000000000000000	0.3183240988546530	0.4444731213145019
0.5000000000000000	0.3422534613393537	0.4896460785965715
0.5000000000000000	0.4560576558212972	0.4246701079635002

Energy = -232.561 eV

5) NH-NH2

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H

27 27 2 3

Direct

0.0000000000000000	0.5108224174894360	0.0138119799395113
0.3314996491024900	0.5110347841965250	0.0150985956885776
0.6685003508975100	0.5110347841965250	0.0150985956885776
0.1668128431553839	0.6850917661823317	0.1555968692876917
0.5000000000000000	0.6845733019747797	0.1571466730906721
0.8331871568446161	0.6850917661823317	0.1555968692876917
0.0000000000000000	0.8456407498509364	0.2964788162299357
0.3334069666284591	0.8438550608784681	0.2966324796584345
0.6665930333715409	0.8438550608784681	0.2966324796584345
0.0000000000000000	0.1763622145439854	0.0134985053283856
0.3317214382453599	0.1748216527152309	0.0110069733668539
0.6682784717546397	0.1748216527152309	0.0110069733668539
0.1672818473793427	0.3515641656653585	0.1559069453135962
0.5000000000000000	0.3505535423657307	0.1476795618822848
0.8327181676206621	0.3515641656653585	0.1559069453135962
0.0000000000000000	0.5113083804402905	0.2961062088150754
0.3294691267112313	0.5136306169294187	0.2982934414334935
0.6705308432887591	0.5136306169294187	0.2982934414334935
0.1666984427789089	0.0185085906497449	0.1547593782679968
0.5000000000000000	0.0182089118246509	0.1550228117166554
0.8333015272210886	0.0185085906497449	0.1547593782679968
0.0000000000000000	0.8424636835246559	0.0141028830137770
0.3345215321329036	0.8417904883717782	0.0140769331301200
0.6654784378670939	0.8417904883717782	0.0140769331301200
0.0000000000000000	0.1775291071117877	0.2965278422267374
0.3339223886151643	0.1782266368768859	0.2946073636928688
0.6660776403848345	0.1782266368768859	0.2946073636928688
0.1674824952925036	0.3734042972661413	0.0125866976917024
0.5000000000000000	0.3698440442445872	0.0116865075037040
0.8325165067074991	0.3734042972661413	0.0125866976917024
0.0000000000000000	0.5407820648731700	0.1547573737483887
0.3333289692520864	0.5403215342051908	0.1574256265771012
0.6666710307479136	0.5403215342051908	0.1574256265771012
0.1661804834647498	0.7074282918865080	0.2995283525717554
0.5000000000000000	0.7058319291242299	0.3006250249369771
0.8338194575352489	0.7074282918865080	0.2995283525717554
0.1651254535892477	0.0377997521410620	0.0109676359269457
0.5000000000000000	0.0392883675440245	0.0109493093287867

0.8348745314107617	0.0377997521410620	0.0109676359269457
0.0000000000000000	0.2072549358647464	0.1552619739421388
0.3335053717260337	0.2066055906973290	0.1525032642073469
0.6664946882739713	0.2066055906973290	0.1525032642073469
0.1665484368251384	0.3739933405951703	0.2994875290204249
0.5000000000000000	0.3752252146565169	0.3100415063994220
0.8334515631748616	0.3739933405951703	0.2994875290204249
0.1670516080141979	0.7054656330806566	0.0118344461790159
0.5000000000000000	0.7025328738207719	0.0131369511050465
0.8329484209857938	0.7054656330806566	0.0118344461790159
0.1670227259155155	0.0408240323994917	0.2986671731277966
0.5000000000000000	0.0404599097325544	0.2982731920087005
0.8329772590844868	0.0408240323994917	0.2986671731277966
0.0000000000000000	0.8738515712885899	0.1555366012803816
0.3332198522467991	0.8739937889171898	0.1551327452256857
0.6667801177531985	0.8739937889171898	0.1551327452256857
0.5000000000000000	0.3763541501499859	0.4060708423145272
0.5000000000000000	0.2978622373862123	0.4452370621895625
0.5000000000000000	0.4385300591342869	0.4294054132225753
0.5616626763188961	0.2567107568725149	0.4386344265209914
0.4383373236811039	0.2567107568725149	0.4386344265209914

Energy = -236.875 eV

6) NH₂-NH₂

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	2	4

Direct

0.0000000000000000	0.5107876558363813	0.0122361492874603
0.3329826580240365	0.5119941038568143	0.0097378774985444
0.6670173419759635	0.5119941038568143	0.0097378774985444
0.1669122129485245	0.6852215565661126	0.1536607999656781
0.5000000000000000	0.6842010754696659	0.1539348256604782
0.8330877870514755	0.6852215565661126	0.1536607999656781
0.0000000000000000	0.8441974502149208	0.2950434353213893
0.3335568030397056	0.8444438208569522	0.2953291566071030
0.6664431969602944	0.8444438208569522	0.2953291566071030
0.0000000000000000	0.1774367791387377	0.0124779094428646
0.3328671690893685	0.1772751514504947	0.0120475329955099
0.6671327409106311	0.1772751514504947	0.0120475329955099
0.1669730050872360	0.3521219916216864	0.1540584612047269
0.5000000000000000	0.3523115736042115	0.1530331023981049
0.8330270099127688	0.3521219916216864	0.1540584612047269
0.0000000000000000	0.5115357535052070	0.2955786341489670
0.3323176180056961	0.5132483619626598	0.2942110738562036
0.6676823519943014	0.5132483619626598	0.2942110738562036
0.1667003517577896	0.0187330966870149	0.1540659570160940
0.5000000000000000	0.0184882681604108	0.1544426162765404
0.8332996182422079	0.0187330966870149	0.1540659570160940

0.0000000000000000	0.8441895973614209	0.0123103587972437
0.3335570007634132	0.8441152237368001	0.0125377989710955
0.6664429692365843	0.8441152237368001	0.0125377989710955
0.0000000000000000	0.1780644032106480	0.2954055809501455
0.3329321640015905	0.1777670078767670	0.2952792410077336
0.6670678649984083	0.1777670078767670	0.2952792410077336
0.1669592804383839	0.3739096381568601	0.0108125297934833
0.5000000000000000	0.3737534903988973	0.0119952887825079
0.8330397215616188	0.3739096381568601	0.0108125297934833
0.0000000000000000	0.5409198867381093	0.1538549920243710
0.3329816386960616	0.5398733152283697	0.1516247650935583
0.6670183613039384	0.5398733152283697	0.1516247650935583
0.1669250659124373	0.7072467454478897	0.2977119220394684
0.5000000000000000	0.7069197807439309	0.2980464578570903
0.8330748750875614	0.7072467454478897	0.2977119220394684
0.1663858327555303	0.0398920901904063	0.0104736703759869
0.5000000000000000	0.0402868709906272	0.0111070352621851
0.8336141522444720	0.0398920901904063	0.0104736703759869
0.0000000000000000	0.2076131826016478	0.1539074441330968
0.3335818792686993	0.2075201737037915	0.1533058756219248
0.6664181807313057	0.2075201737037915	0.1533058756219248
0.1671033734308551	0.3747360577094199	0.2977009419843384
0.5000000000000000	0.3752151454313974	0.2980303256486465
0.8328966265691449	0.3747360577094199	0.2977009419843384
0.1667486210168008	0.7069446872380070	0.0101627151441832
0.5000000000000000	0.7065297088558040	0.0107761368950960
0.8332514079831981	0.7069446872380070	0.0101627151441832
0.1663306592359817	0.0405386690938130	0.2979558267981801
0.5000000000000000	0.0410050960944233	0.2985104629000404
0.8336693257640206	0.0405386690938130	0.2979558267981801
0.0000000000000000	0.8741132785525565	0.1536935332796645
0.3332722050290471	0.8740024199291412	0.1539508524493414
0.6667277649709433	0.8740024199291412	0.1539508524493414
0.5000000000000000	0.3739849184365056	0.4258730230289416
0.5000000000000000	0.2849737867530848	0.4598282165079084
0.4394218518593718	0.4113722563678053	0.4409199419318313
0.5599504150233088	0.2481960747699290	0.4430764483436320
0.4400495849766912	0.2481960747699290	0.4430764483436320
0.5605781181406186	0.4113722563678053	0.4409199419318313

Energy = -241.086 eV

7) NH2

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	1	2

Direct

0.0000000000000000	0.5108823196110066	0.0141100140321129
0.3314254753219288	0.5105721941384829	0.0159803366443683
0.6685745246780712	0.5105721941384829	0.0159803366443683

0.1670613739195090	0.6844285988600447	0.1561895132337696
0.5000000000000000	0.6841530931526449	0.1575992593312918
0.8329386260804910	0.6844285988600447	0.1561895132337696
0.0000000000000000	0.8454024172333092	0.2968540560641699
0.3333129168827114	0.8442254709669754	0.2967189243358206
0.6666870831172886	0.8442254709669754	0.2967189243358206
0.0000000000000000	0.1758855196140559	0.0134737812872814
0.3317799800099692	0.1742616642599444	0.0109236076303887
0.6682199299900304	0.1742616642599444	0.0109236076303887
0.1673837113526560	0.3516708607760819	0.1565956567881557
0.5000000000000000	0.3498895657915781	0.1478330623797888
0.8326163036473488	0.3516708607760819	0.1565956567881557
0.0000000000000000	0.5115567910544740	0.2969614015240580
0.3302628115664277	0.5137574700259009	0.3001082797317949
0.6697371584335698	0.5137574700259009	0.3001082797317949
0.1666696399067575	0.0182301756563703	0.1546157006745759
0.5000000000000000	0.0182980595550006	0.1548772887220053
0.8333303300932400	0.0182301756563703	0.1546157006745759
0.0000000000000000	0.8417135116930936	0.0145517749561108
0.3346079717393806	0.8414355521895729	0.0142730267471265
0.6653919982606169	0.8414355521895729	0.0142730267471265
0.0000000000000000	0.1776509854313275	0.2963829117011727
0.3346828705701199	0.1784247654461524	0.2941982138906383
0.6653171584298789	0.1784247654461524	0.2941982138906383
0.1672482678300682	0.3732043780115788	0.0135657757872991
0.5000000000000000	0.3694804129410372	0.0121120903135292
0.8327507341699345	0.3732043780115788	0.0135657757872991
0.0000000000000000	0.5403406581175076	0.1552800402900658
0.3335667044381623	0.5394915033686232	0.1585058731836710
0.6664332955618377	0.5394915033686232	0.1585058731836710
0.1664314538457390	0.7073864827221570	0.3000103707870920
0.5000000000000000	0.7063286209969206	0.3009178475626513
0.8335684871542597	0.7073864827221570	0.3000103707870920
0.1651404050051539	0.0373303490587347	0.0106803368924986
0.5000000000000000	0.0387796167362495	0.0101837828503832
0.8348595799948484	0.0373303490587347	0.0106803368924986
0.0000000000000000	0.2074415415926580	0.1553894379779237
0.3332625311111670	0.2063781081153593	0.1525810168582566
0.6667375288888380	0.2063781081153593	0.1525810168582566
0.1668460695474465	0.3743887476106948	0.3004747966431012
0.5000000000000000	0.3725923384316019	0.3100302821829644
0.8331539304525535	0.3743887476106948	0.3004747966431012
0.1672325806804977	0.7048941872121262	0.0123684611658490
0.5000000000000000	0.7021648771893254	0.0134448281530908
0.8327674483195011	0.7048941872121262	0.0123684611658490
0.1672998595963193	0.0411491773992623	0.2983021062232751
0.5000000000000000	0.0399862846670374	0.2978400083816268
0.8327001254036830	0.0411491773992623	0.2983021062232751
0.0000000000000000	0.8733831614218275	0.1559450496027068
0.3333711590909658	0.8739314085914884	0.1552341465238740
0.6666288109090317	0.8739314085914884	0.1552341465238740

0.5000000000000000	0.3523665965246607	0.4064456389355726
0.5609728105280141	0.3842594262128074	0.4255871111341918
0.4390271894719859	0.3842594262128074	0.4255871111341918

Energy = -226.054 eV

8) NH₃

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H

27 27 1 3

Direct

0.0000000000000000	0.5099934414911615	0.0114118246556529
0.3333743697716045	0.5107350468297867	0.0092869654820547
0.6666256302283955	0.5107350468297867	0.0092869654820547
0.1665544859651718	0.6845636422710015	0.1526060234618569
0.5000000000000000	0.6844232581741068	0.1525429693707920
0.8334455140348282	0.6845636422710015	0.1526060234618569
0.0000000000000000	0.8431980628758282	0.2940158842154688
0.3333897130042516	0.8432918187312239	0.2943349733932337
0.6666102869957484	0.8432918187312239	0.2943349733932337
0.0000000000000000	0.1766988250877830	0.0115851017996818
0.3333524258804914	0.1766070138362394	0.0116788371505478
0.6666474841195082	0.1766070138362394	0.0116788371505478
0.1668492554189100	0.3513551522248193	0.1526855586407834
0.5000000000000000	0.3520251803627730	0.1524978813977924
0.8331507595810947	0.3513551522248193	0.1526855586407834
0.0000000000000000	0.5101237432933772	0.2943536659073303
0.3334689863127593	0.5105615649760509	0.2925172514209606
0.6665309836872382	0.5105615649760509	0.2925172514209606
0.1666841607672751	0.0182212919441795	0.1530120728605482
0.5000000000000000	0.0179762563736361	0.1534055768831593
0.8333158092327224	0.0182212919441795	0.1530120728605482
0.0000000000000000	0.8438363191948284	0.0115355749561914
0.3332029987160823	0.8437074365957571	0.0119100508397736
0.6667969712839152	0.8437074365957571	0.0119100508397736
0.0000000000000000	0.1767846657728356	0.2941390713981349
0.3332229032992373	0.1767303008886927	0.2942114529328848
0.6667771257007544	0.1767303008886927	0.2942114529328848
0.1668352561924209	0.3730032155811926	0.0090638184091603
0.5000000000000000	0.3736096908298734	0.0085537316947182
0.8331637458075818	0.3730032155811926	0.0090638184091603
0.0000000000000000	0.5398680980058970	0.1528819975237568
0.3332461849210091	0.5399130116402091	0.1510429391873700
0.6667538150789909	0.5399130116402091	0.1510429391873700
0.1667196306568997	0.7058943076529545	0.2965925193834238
0.5000000000000000	0.7059095836204676	0.2966483691653821
0.8332803103430990	0.7058943076529545	0.2965925193834238
0.1666747719838142	0.0395027520318791	0.0091839572501797
0.5000000000000000	0.0393062894515523	0.0097797751245139
0.8333252130161881	0.0395027520318791	0.0091839572501797

0.0000000000000000	0.2069599763607570	0.1527712718725596
0.3337293783228290	0.2072152702773522	0.1528191767506755
0.6662706816771760	0.2072152702773522	0.1528191767506755
0.1669929922248130	0.3731095915701488	0.2963577504992045
0.5000000000000000	0.3725294355550091	0.2955409121563193
0.8330070077751870	0.3731095915701488	0.2963577504992045
0.1665212708294277	0.7063671330905592	0.0089785656715833
0.5000000000000000	0.7064092447844033	0.0091770065868033
0.8334787581705712	0.7063671330905592	0.0089785656715833
0.1665355240347424	0.0394169919821721	0.2967875341976125
0.5000000000000000	0.0396941996830549	0.2974163332713715
0.8334644609652599	0.0394169919821721	0.2967875341976125
0.0000000000000000	0.8737600363161349	0.1527698379616211
0.3332120597697070	0.8735786093728848	0.1531562158565904
0.6667879102302834	0.8735786093728848	0.1531562158565904
0.5000000000000000	0.3726582701039263	0.4438460298299063
0.5611539315008685	0.4078747746539264	0.4595994064541884
0.4388460984991340	0.4078747746539264	0.4595994064541884
0.5000000000000000	0.3074970523605245	0.4640060535435495

Energy = -230.384 eV

9) NNH2

1.0000000000000000		
13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi	Sb	N	H
27	27	2	2

Direct

0.0000000000000000	0.5101722354813418	0.0141935296151487
0.3310948230215018	0.5114183699328407	0.0163938124614873
0.6689051769784982	0.5114183699328407	0.0163938124614873
0.1670928445276303	0.6834753693126459	0.1557106719978805
0.5000000000000000	0.6828342707190913	0.1576144397735888
0.8329071554723697	0.6834753693126459	0.1557106719978805
0.0000000000000000	0.8435933431815954	0.2973027964274948
0.3337305469652350	0.8429034930130399	0.2971324178776271
0.6662694530347579	0.8429034930130399	0.2971324178776271
0.0000000000000000	0.1760597692091395	0.0142555656721370
0.3316721170452865	0.1743352629544646	0.0117436171855587
0.6683277929547131	0.1743352629544646	0.0117436171855587
0.1674410171521927	0.3510928767007115	0.1570262366728628
0.5000000000000000	0.3496248066360081	0.1446435762672209
0.8325589978478050	0.3510928767007115	0.1570262366728628
0.0000000000000000	0.5105024151441313	0.2974752099771365
0.3294404111641072	0.5128346170581111	0.3019724131820922
0.6705595588358904	0.5128346170581111	0.3019724131820922
0.1667490419874795	0.0174013636617687	0.1549852495671189
0.5000000000000000	0.0170710859594436	0.1558310027271119
0.8332509280125180	0.0174013636617687	0.1549852495671189
0.0000000000000000	0.8418234776256242	0.0145515873088158
0.3345532869341028	0.8413885005256319	0.0142687301147291

0.6654466830658947	0.8413885005256319	0.0142687301147291
0.0000000000000000	0.1758407153674142	0.2973498836760413
0.3334303299679533	0.1768451020676025	0.2951585087524364
0.6665696990320455	0.1768451020676025	0.2951585087524364
0.1675603888323494	0.3731113978860776	0.0138042724815364
0.5000000000000000	0.3708266995982683	0.0086622291781424
0.8324386131676533	0.3731113978860776	0.0138042724815364
0.0000000000000000	0.5393330504230889	0.1554839694785457
0.3334035907575341	0.5382290925625099	0.1592770340481380
0.6665964092424659	0.5382290925625099	0.1592770340481380
0.1668186638203650	0.7060983628893993	0.2994837164814115
0.5000000000000000	0.7048524138850922	0.3007869114590562
0.8331812771796336	0.7060983628893993	0.2994837164814115
0.1649720809847253	0.0373344293010476	0.0111728784230039
0.5000000000000000	0.0384000438363614	0.0123361226586098
0.8350279040152770	0.0373344293010476	0.0111728784230039
0.0000000000000000	0.2067326693905542	0.1562177066100006
0.3335104949350480	0.2057296925580019	0.1528343957794576
0.6664895650649569	0.2057296925580019	0.1528343957794576
0.1665175030593034	0.3730101632214087	0.3009953687262623
0.5000000000000000	0.3743230797470360	0.3014563284446439
0.8334824969406966	0.3730101632214087	0.3009953687262623
0.1671391626512175	0.7049706814174286	0.0118110172290002
0.5000000000000000	0.7023030463761373	0.0133065366616449
0.8328608663487813	0.7049706814174286	0.0118110172290002
0.1668668240673767	0.0391191957573724	0.2990798056015578
0.5000000000000000	0.0398695700864309	0.3001504181831436
0.8331331609326256	0.0391191957573724	0.2990798056015578
0.0000000000000000	0.8725306383587110	0.1561798410855317
0.3332170181866516	0.8725725572886915	0.1555328363380681
0.6667829518133459	0.8725725572886915	0.1555328363380681
0.5000000000000000	0.3859688812062529	0.3995775933083934
0.5000000000000000	0.3059592858810944	0.4295599661594096
0.5000000000000000	0.3084522243389287	0.4765050038230285
0.5000000000000000	0.2404361133307091	0.4090029706647513

Energy = -232.498 eV

10) N

1.0000000000000000

13.4676008223999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.1693000792999992 0.0000000000000000

0.0000000000000000 0.0000000000000000 21.7192001342999994

Bi Sb N

27 27 1

Direct

0.0000000000000000 0.5101963009138615 0.0141892433117761

0.3308673260932125 0.5100580910395962 0.0165471415419418

0.6691326739067875 0.5100580910395962 0.0165471415419418

0.1668208846408845 0.6845494511424448 0.1555430936523905

0.5000000000000000 0.6841941398073956 0.1572972638446970

0.8331791153591155 0.6845494511424448 0.1555430936523905

0.0000000000000000 0.8439748682475638 0.2970660855091083

0.3342124987773687	0.8434482173110425	0.2969735019756641
0.6657875012226313	0.8434482173110425	0.2969735019756641
0.0000000000000000	0.1755792973154442	0.0135648153156822
0.3319325630006560	0.1739015753385118	0.0120210455473000
0.6680673469993437	0.1739015753385118	0.0120210455473000
0.1671670186826972	0.3512422183355000	0.1563542474981787
0.5000000000000000	0.3504745067677817	0.1450964185901711
0.8328329963173076	0.3512422183355000	0.1563542474981787
0.0000000000000000	0.5112461659890073	0.2967679570847608
0.3253376176663494	0.5150025153668949	0.3004513981081871
0.6746623523336481	0.5150025153668949	0.3004513981081871
0.1668108856598138	0.0178168804866417	0.1547019642908865
0.5000000000000000	0.0176198393546798	0.1551368011457228
0.8331890843401837	0.0178168804866417	0.1547019642908865
0.0000000000000000	0.8417407999053381	0.0144157932771591
0.3345510346252354	0.8410843327771502	0.0141346761142955
0.6654489353747621	0.8410843327771502	0.0141346761142955
0.0000000000000000	0.1765746217163766	0.2966233979155533
0.3340998317944965	0.1773063016837355	0.2956370846166863
0.6659001972055023	0.1773063016837355	0.2956370846166863
0.1671585620638751	0.3723764328406745	0.0131100648251063
0.5000000000000000	0.3695180188694707	0.0089474043043722
0.8328404399361276	0.3723764328406745	0.0131100648251063
0.0000000000000000	0.5401577443673133	0.1551689327466335
0.3335178173623063	0.5396238538856366	0.1589052682304057
0.6664821826376937	0.5396238538856366	0.1589052682304057
0.1672769544938433	0.7064952370597553	0.2998010195325094
0.5000000000000000	0.7053285246657666	0.3006686744455891
0.8327229865061554	0.7064952370597553	0.2998010195325094
0.1651567676265557	0.0370743171508110	0.0107749591475752
0.5000000000000000	0.0382539067030052	0.0108091900603142
0.8348432173734466	0.0370743171508110	0.0107749591475752
0.0000000000000000	0.2068504356664747	0.1554652825570955
0.3335889112030586	0.2062467463422237	0.1535354225945369
0.6664111487969464	0.2062467463422237	0.1535354225945369
0.1656476749419937	0.3733384574014593	0.3003696364576030
0.5000000000000000	0.3759904752859171	0.3072656869886359
0.8343523250580063	0.3733384574014593	0.3003696364576030
0.1670469160891130	0.7047131749322730	0.0117937079050066
0.5000000000000000	0.7019407179156545	0.0129293888244675
0.8329531129108858	0.7047131749322730	0.0117937079050066
0.1671268860322286	0.0399453510080292	0.2987387465333171
0.5000000000000000	0.0393335158339525	0.2984673178527615
0.8328730989677737	0.0399453510080292	0.2987387465333171
0.0000000000000000	0.8728441860994138	0.1561396562061717
0.3331363490631460	0.8731286085516956	0.1553381688556286
0.6668636209368515	0.8731286085516956	0.1553381688556286
0.5000000000000000	0.3798463962674248	0.3996123631649127

Energy = -215.519 eV

11) NH

1.0000000000000000

13.4676008223999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.1693000792999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	21.7192001342999994

Bi Sb N H
27 27 1 1

Direct

0.0000000000000000	0.5115943801886260	0.0184039576590322
0.3320157341244681	0.5131753349388504	0.0163565994858601
0.6679842658755319	0.5131753349388504	0.0163565994858601
0.1660733585460576	0.6870822605584834	0.1582472105702593
0.5000000000000000	0.6869359475017447	0.1599247472603267
0.8339266414539424	0.6870822605584834	0.1582472105702593
0.0000000000000000	0.8556181979661304	0.2997628379449324
0.3330855992884452	0.8461800927401981	0.2992034635833747
0.6669144007115548	0.8461800927401981	0.2992034635833747
0.0000000000000000	0.1785516345659204	0.0174120824294945
0.3333217722570794	0.1785649076726514	0.0164910013609401
0.6666781377429203	0.1785649076726514	0.0164910013609401
0.1672364095380630	0.3527242018631753	0.1594297563626128
0.5000000000000000	0.3531134610166262	0.1507036190731554
0.8327636054619418	0.3527242018631753	0.1594297563626128
0.0000000000000000	0.5124622724725469	0.3009844360677505
0.3159070033032663	0.5246570921509246	0.3012781859453000
0.6840929666967313	0.5246570921509246	0.3012781859453000
0.1661405555362450	0.0202173063088580	0.1592505171137404
0.5000000000000000	0.0197085578620957	0.1561768733225719
0.8338594144637455	0.0202173063088580	0.1592505171137404
0.0000000000000000	0.8456731664858594	0.0164382557108027
0.3333453494222525	0.8449268913937757	0.0170257126766415
0.6666546205777450	0.8449268913937757	0.0170257126766415
0.0000000000000000	0.1752923280126808	0.3007094003019546
0.3445381698299101	0.1817097784000055	0.3004866871032732
0.6554618591700816	0.1817097784000055	0.3004866871032732
0.1671991242542887	0.3744555452723972	0.0160005656882944
0.5000000000000000	0.3774000510452566	0.0074449018427956
0.8327998777457069	0.3744555452723972	0.0160005656882944
0.0000000000000000	0.5417149867658537	0.1591082980148144
0.3330518320581461	0.5422550752116493	0.1591505008910801
0.6669481679418539	0.5422550752116493	0.1591505008910801
0.1637003321638844	0.7122583713741619	0.3018859853040397
0.5000000000000000	0.7088795685161244	0.3034169660651074
0.8362996088361143	0.7122583713741619	0.3018859853040397
0.1664004127638918	0.0412195067533574	0.0150665321480687
0.5000000000000000	0.0413952076412230	0.0122094131115134
0.8335995722361105	0.0412195067533574	0.0150665321480687
0.0000000000000000	0.2082105441804458	0.1590465944961608
0.3347516427991479	0.2084172400788944	0.1579957695110821
0.6652484172008570	0.2084172400788944	0.1579957695110821
0.1648919185169433	0.3739216623427097	0.3036219895193781
0.5000000000000000	0.4052141225855905	0.2904135336242391
0.8351080814830567	0.3739216623427097	0.3036219895193781

0.1661828771182599	0.7077454041117477	0.0145481286537361
0.5000000000000000	0.7070298435451221	0.0162129267888318
0.8338171518817390	0.7077454041117477	0.0145481286537361
0.1687788940834096	0.0412659136569928	0.3025157544719477
0.5000000000000000	0.0337447511095235	0.2991493977318314
0.8312210909165927	0.0412659136569928	0.3025157544719477
0.0000000000000000	0.8749018541274793	0.1581013377534362
0.3327253772661933	0.8757997144383296	0.1577510550307508
0.6672745927338042	0.8757997144383296	0.1577510550307508
0.5000000000000000	0.2774259965081285	0.3362191310664855
0.5000003580000012	0.2896960533686936	0.3831394948939959

Energy = -221.328 eV