

Electronic Supplementary Information:

**Can Boron Antisites of BNNT be an Efficient Metal-Free
Catalyst for Nitrogen Fixation? – A DFT Investigation**

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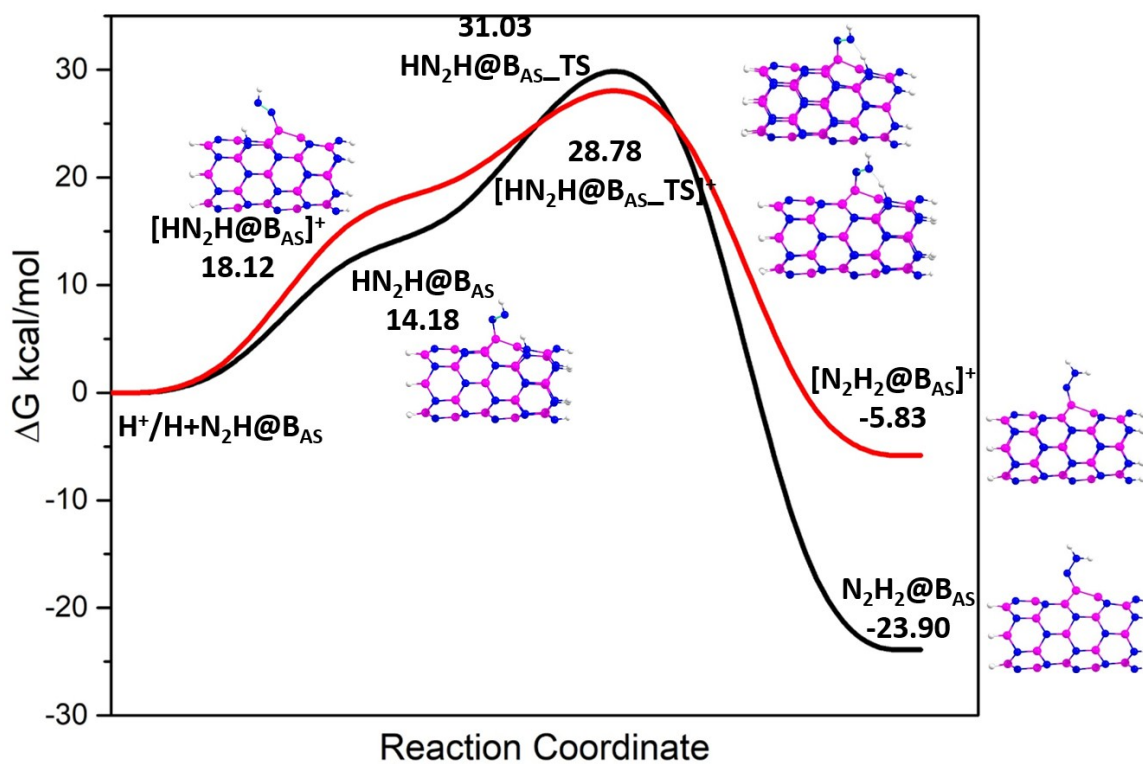


Fig. S1 Reaction profile for proton transfer and proton-electron coupled hydrogen transfer reactions at Step-2. Atom colour indication: H- white, N- blue and B- Pink.

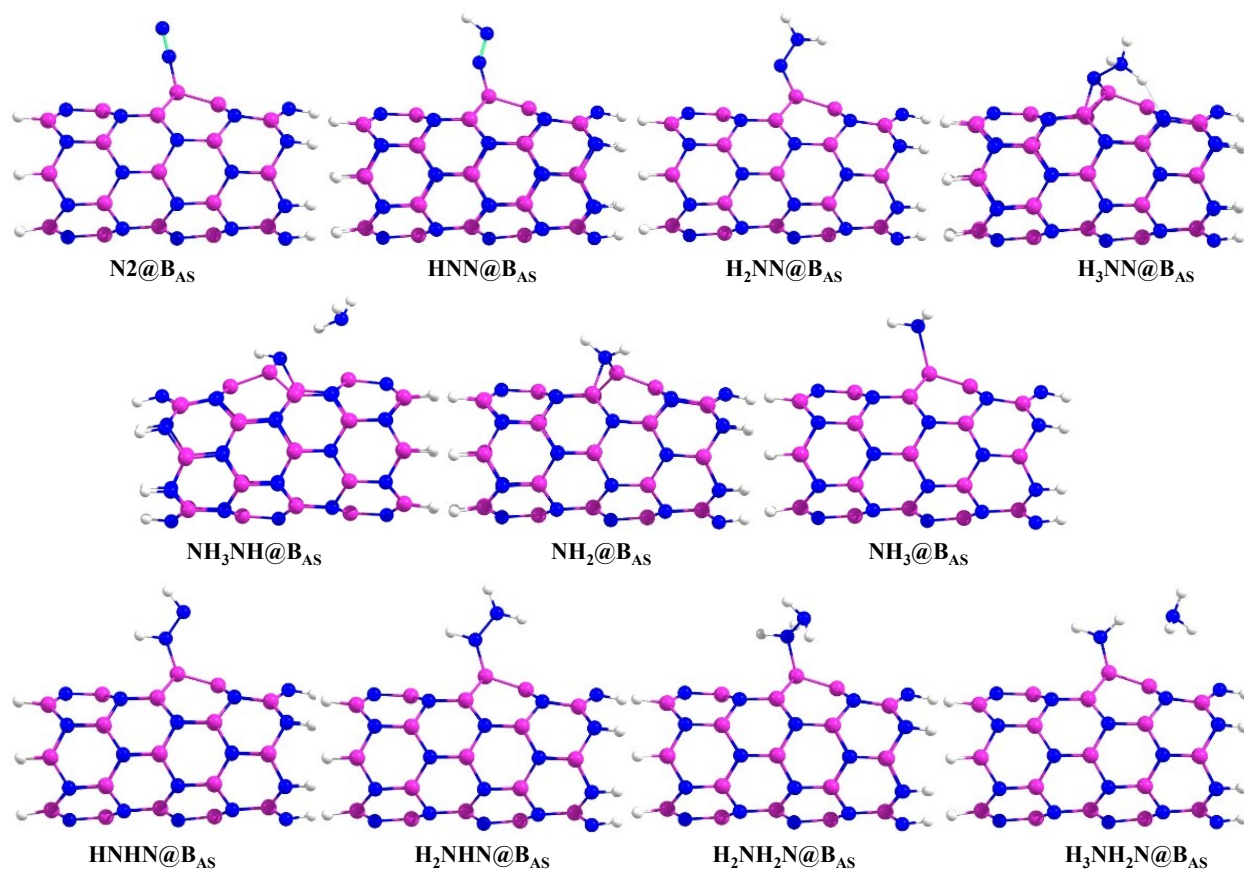


Fig. S2 Optimized geometries of all the intermediates involved in both distal and alternating pathways at $\omega\text{B97X-D/6-31G}^*$ level of theory. Atom colour indication: H- white, N- blue and B- Pink.

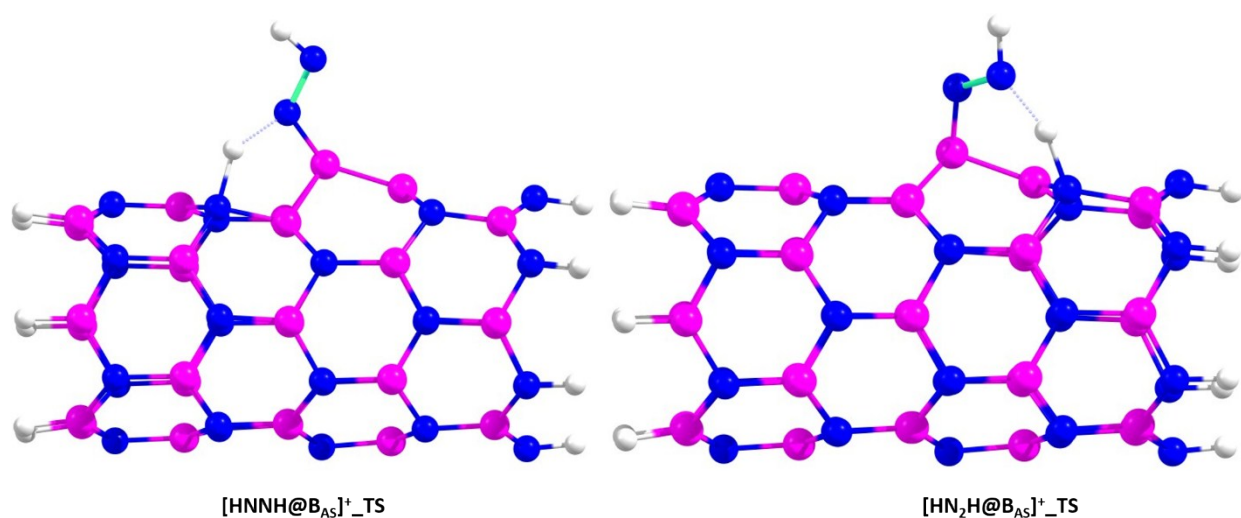


Fig. S3 Transition states involved in Step-3 of both pathways calculated at $\omega\text{B97X-D/6-31G}^*$ level of theory. Atom colour indication: H- white, N- blue and B- Pink.

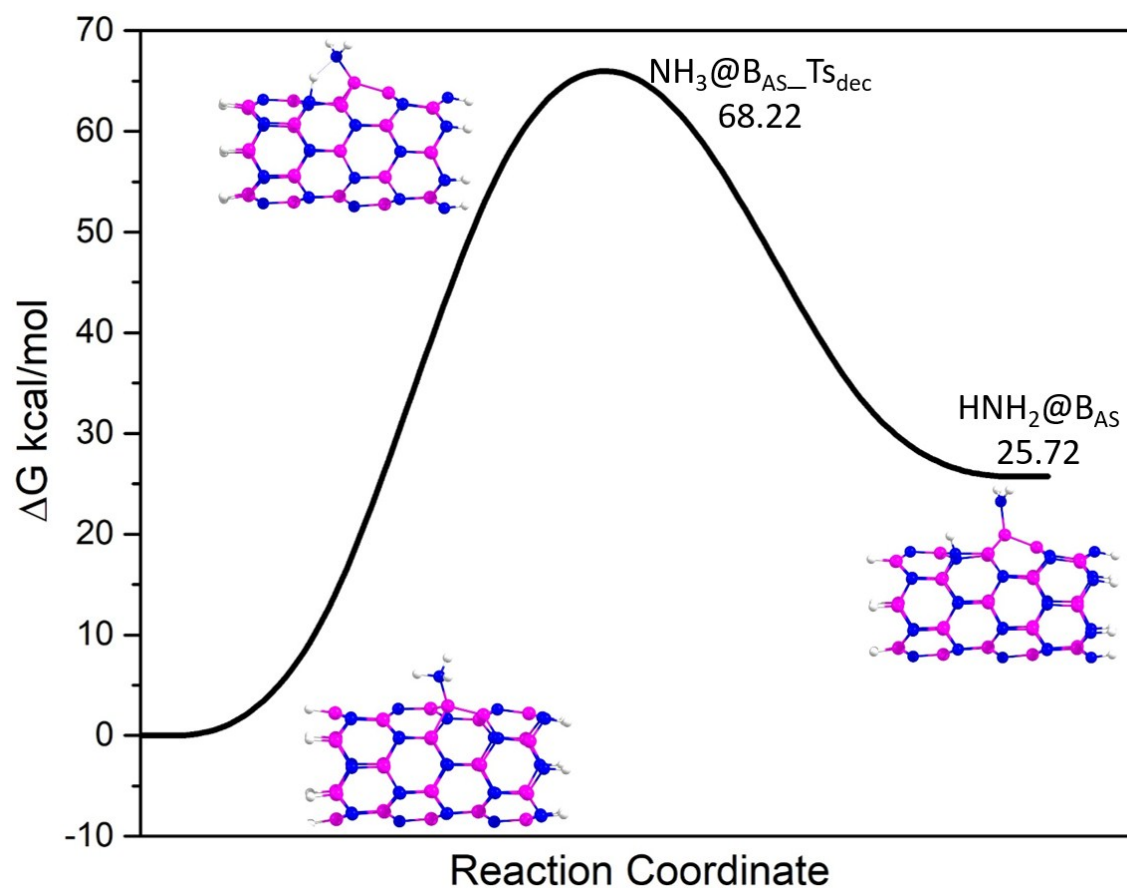


Fig. S4 Energy profile of ammonia decomposition reaction. Atom colour indication: H- white, N- blue and B- Pink.

Table S1 Nitrogen bond length in Å and bond order values in each elementary step of both the pathways calculated at ω B97X-D/6-31G* level of theory.

S. No	Structure	N-N bond	
		Bond length (Å)	Bond Order (NBO)
1	$N_{2S}@B_{AS}$	1.12	2.71
2	$N_{2En}@B_{AS}$	1.15	2.62
3	$HNN@B_{AS}$	1.20	2.11
4	$H_2NN@B_{AS}$	1.28	1.91
5	$H_3NN@B_{AS}$	1.46	1.29
6	$NH_3NH@B_{AS}$	3.42	0.18
7	$NH_2NH@B_{AS}$	1.26	1.89
8	$NH_2NH@B_{AS}$	1.35	1.45
9	$NH_2NH_2@B_{AS}$	1.44	1.28
10	$NH_3NH_2@B_{AS}$	3.05	0.22
11	$NH_3@B_{AS}$	-	-

Table S2 Variation of Mulliken atomic charge (the charge difference of the present step from the previous step) of various groups involved in distal as well as alternating pathways as derived from ω B97X-D/6-31G* level of calculations.

Distal Pathway			
Intermediate	Group1	Group2	Group3
B _{AS}	0.041	-0.041	
N ₂ @B _{AS}	-0.046	0.085	-0.039
HNN@B _{AS}	-0.079	0.167	-0.088
H ₂ NN@B _{AS}	-0.158	0.18	-0.022
H ₃ NN@B _{AS}	-0.19	0.028	0.162
NH ₃ NH@B _{AS}	-0.494	0.066	0.428
NH@B _{AS}	0.123	0.16	-0.283
NH ₂ @B _{AS}	-0.169	0.316	-0.147
NH ₃ @B _{AS}	-0.363	0.116	0.247
Alternating Pathway			
B _{AS}	0.041	-0.041	
N ₂ @B _{AS}	-0.046	0.085	-0.039
HNN@B _{AS}	-0.079	0.167	-0.088
NHNH@B _{AS}	-0.223	0.249	-0.026
NH ₂ NH@B _{AS}	-0.374	0.283	0.091
NH ₂ NH ₂ @B _{AS}	-0.335	0.09	0.245
NH ₃ NH ₂ @B _{AS}	-0.244	0.318	-0.074
NH ₃ @B _{AS}	-0.363	0.116	0.247

Table S3 Cartesian coordinates of optimized geometries at ω B97X-D/6-31G* level of theory.

B _{AS}				N _{AS}			
7	2.431580000	-2.185465000	1.245795000	7	-2.453096040	-0.052108294	-2.402499043
5	3.873980000	-2.111611000	1.195042000	5	-3.894115567	-0.027607652	-2.279492406
7	0.295234000	-1.204294000	2.100324000	7	-0.305588760	1.193839828	-2.111018864
5	1.732843000	-1.164732000	2.009385000	5	-1.722270811	1.112358597	-1.947817177
7	2.454129000	0.039480000	2.385557000	7	-2.396873958	2.111643759	-1.157796698
5	3.905280000	-0.027493000	2.361767000	5	-3.836379430	2.129883515	-1.143462646
7	0.305845000	1.299425000	2.037644000	7	-0.349711016	2.571379152	-0.001167338
5	1.781137000	1.264729000	1.964005000	7	-2.396832090	2.113172520	1.156198466
7	2.612063000	2.236775000	1.245023000	5	-3.836333878	2.131210120	1.141724611
5	4.044531000	2.025084000	1.200870000	7	-0.305592954	1.195829799	2.109956869
5	1.990286000	2.667794000	-0.000118000	5	-1.722273435	1.114306689	1.946881692
7	2.612035000	2.236674000	-1.245237000	7	-2.453100581	-0.049805234	2.402397949
5	4.044503000	2.024992000	-1.201108000	5	-3.894128876	-0.025342412	2.279450040
7	0.305788000	1.299296000	-2.037744000	7	-0.293271037	-1.308004152	2.148322675
5	1.781084000	1.264593000	-1.964138000	5	-1.737864378	-1.263610880	2.036485498
7	2.454061000	0.039311000	-2.385623000	7	-2.444735193	-2.267096619	1.252364583
5	3.905213000	-0.027662000	-2.361866000	5	-3.891601451	-2.155415581	1.179974548

7	0.295174000	-1.204430000	-2.100218000	7	-0.280693820	-2.600236849	0.001174782
5	1.732785000	-1.164869000	-2.009334000	5	-1.728250185	-2.500344991	0.001112231
7	2.431543000	-2.185550000	-1.245694000	7	-2.444705221	-2.268340958	-1.250383037
5	3.873945000	-2.111696000	-1.194991000	5	-3.891576908	-2.156626460	-1.178145701
7	0.286364000	-2.549413000	0.000097000	7	-0.293250883	-1.310028658	-2.147193580
5	1.723368000	-2.427761000	0.000070000	5	-1.737845053	-1.265569789	-2.035437785
7	-1.854035000	-2.166328000	1.247648000	7	1.847207474	-0.021005865	-2.462183749
5	-0.416903000	-2.077462000	1.182964000	5	0.410617183	-0.048734798	-2.350717473
7	-4.004689000	-1.250052000	2.146417000	7	3.979738378	1.259794798	-2.125316387
5	-2.560286000	-1.177334000	2.044137000	5	2.533211110	1.192674628	-2.035995363
7	-1.850749000	0.034248000	2.434826000	7	1.808432255	2.180613404	-1.240409062
5	-0.408059000	0.049401000	2.294824000	5	0.364096358	2.073231153	-1.177194902
7	-4.053719000	1.224162000	2.146809000	7	3.971289269	2.550587693	-0.001135276
5	-2.607622000	1.211928000	2.047835000	5	2.529070034	2.423880471	-0.001090183
7	-1.927411000	2.237010000	1.281392000	7	1.808427005	2.181806958	1.238453931
5	-0.479771000	2.279537000	1.297250000	5	0.364099853	2.074353130	1.175324684
7	-4.069656000	2.465108000	-0.000052000	7	3.979713210	1.261797215	2.124199966
7	-1.927463000	2.236976000	-1.281581000	7	1.847193985	-0.018717167	2.462182834
5	-0.479824000	2.279508000	-1.297464000	5	0.410602780	-0.046544942	2.350736243
7	-4.053785000	1.224013000	-2.146823000	7	4.021766651	-1.230424577	2.133435014
5	-2.607684000	1.211798000	-2.047889000	5	2.575883578	-1.209374938	2.046958365
7	-1.850817000	0.034080000	-2.434766000	7	1.874072200	-2.213226444	1.252696520
5	-0.408123000	0.049249000	-2.294798000	5	0.428503650	-2.144529320	1.195414618
7	-4.004749000	-1.250201000	-2.146197000	7	4.039141265	-2.508432756	0.001124787
5	-2.560343000	-1.177471000	-2.043962000	5	2.591257272	-2.427535144	0.001095465
7	-1.854069000	-2.166403000	-1.247418000	7	1.874074433	-2.214408748	-1.250700903
5	-0.416936000	-2.077536000	-1.182780000	5	0.428508250	-2.145659722	-1.193492566
7	-4.008487000	-2.496190000	0.000154000	7	4.021760586	-1.232432095	-2.132332462
5	-2.565917000	-2.394202000	0.000132000	5	2.575879365	-1.211298545	-2.045891681
7	4.542742000	-1.323082000	2.211512000	7	-4.530816087	1.260535567	-2.080985589
7	4.658562000	1.201309000	2.220124000	7	-4.482078037	2.753311206	-0.001224737
7	4.751524000	2.436770000	-0.000144000	7	-4.530764403	1.262700230	2.080064630
7	4.658505000	1.201145000	-2.220322000	7	-4.581450910	-1.293332634	2.126449816
7	4.542676000	-1.323242000	-2.211539000	7	-4.563684075	-2.678482103	0.001176273
7	4.549184000	-2.583687000	0.000033000	7	-4.581409555	-1.295507928	-2.125514849
5	-4.740018000	-0.025486000	2.403218000	5	4.685825074	2.129919509	-1.197031831
5	-4.776143000	2.054484000	1.201082000	5	4.685775463	2.131187206	1.195224251
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5	-4.713648000	-2.101498000	-1.206257000	5	4.746986338	-2.076564414	-1.195024471
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1	-5.891001000	-2.275794000	1.311085000	1	5.893087552	0.047075361	-2.533128940
1	-5.891036000	-2.275885000	-1.310740000	1	5.928034470	-2.212808659	-1.286899093
1	-5.918912000	-0.050032000	-2.596506000	1	5.928021929	-2.211754993	1.288975611
1	-5.958692000	2.199515000	-1.294858000	1	5.893077074	0.049470058	2.533093480
1	-5.958652000	2.199590000	1.294823000	1	5.862269433	2.299282921	1.293422996
1	5.660037000	1.078081000	2.133824000	1	-5.491740158	2.710718374	-0.001184324
1	5.552205000	-1.289070000	2.138544000	1	-5.536325088	1.251548893	-1.987006446
1	5.555116000	-2.467176000	0.000014000	1	-5.582474424	-1.235962406	-2.001532573
1	5.552142000	-1.289228000	-2.138606000	1	-5.565321408	-2.541060545	0.001089729
1	5.659981000	1.077918000	-2.134038000	1	-5.582513477	-1.233892318	2.002410933
1	5.746663000	2.249202000	-0.000147000	1	-5.536275822	1.253666402	1.986095785
5	-2.617975000	2.433416000	-0.000082000	5	2.533189308	1.194593081	2.034941792
5	0.344046000	2.921093000	-0.000140000	7	-1.782635388	2.752010335	-0.001249736
N₂@B_{As} (Schrock)				N₂@B_{As} (Enzymatic)			

7	-3.248887529	-2.329383258	-3.931489868	7	-2.455434000	-2.361339000	-1.245489000
5	-4.691168529	-2.240607258	-3.878675868	5	-3.897687000	-2.271236000	-1.192629000
7	-1.104915529	-1.361070258	-4.786042868	7	-0.312270000	-1.385507000	-2.090640000
5	-2.542673529	-1.314034258	-4.695248868	5	-1.750037000	-1.337709000	-1.998311000
7	-3.253577529	-0.104678258	-5.071526868	7	-2.459201000	-0.124495000	-2.363114000
5	-4.703842529	-0.150163258	-5.037168868	5	-3.910615000	-0.175093000	-2.342100000
7	-1.103483529	1.138967742	-4.686353868	7	-0.310595000	1.111130000	-1.939798000
5	-2.569147529	1.108625742	-4.638790868	5	-1.781827000	1.089914000	-1.920453000
7	-3.366458529	2.095881742	-3.922769868	7	-2.590391000	2.085699000	-1.234732000
5	-4.802728529	1.916645742	-3.877830868	5	-4.024668000	1.896787000	-1.191080000
5	-2.725391529	2.528890742	-2.685591868	5	-1.952224000	2.539319000	0.000175000
7	-3.366426529	2.095810742	-1.448424868	7	-2.590337000	2.085315000	1.234969000
5	-4.802698529	1.916581742	-1.493333868	5	-4.024624000	1.896491000	1.191356000
7	-1.103429529	1.138883742	-0.684921868	7	-0.310528000	1.110772000	1.940110000
5	-2.569095529	1.108535742	-0.732454868	5	-1.781757000	1.089521000	1.920656000
7	-3.253513529	-0.104785258	-0.299747868	7	-2.459146000	-0.124940000	2.363178000
5	-4.703778529	-0.150274258	-0.334071868	5	-3.910556000	-0.175536000	2.342146000
7	-1.104856529	-1.361161258	-0.585347868	7	-0.312219000	-1.385897000	2.090461000
5	-2.542617529	-1.314125258	-0.676097868	5	-1.749988000	-1.338092000	1.998172000
7	-3.248851529	-2.329442258	-1.439880868	7	-2.455401000	-2.361597000	1.245183000
5	-4.691134529	-2.240665258	-1.492647868	5	-3.897655000	-2.271478000	1.192370000
7	-1.103370529	-2.706189258	-2.685724868	7	-0.310495000	-2.745271000	-0.000217000
5	-2.541125529	-2.576249258	-2.685700868	5	-1.748335000	-2.611770000	-0.000186000
7	1.041462471	-2.330734258	-3.932999868	7	1.833653000	-2.362699000	-1.247156000
5	-0.396570529	-2.237556258	-3.868529868	5	0.395721000	-2.270714000	-1.181065000
7	3.194718471	-1.409301258	-4.826960868	7	3.985357000	-1.439276000	-2.140768000
5	1.750528471	-1.339156258	-4.724528868	5	2.541785000	-1.366317000	-2.033420000
7	1.043809471	-0.125753258	-5.109390868	7	1.835911000	-0.148088000	-2.405585000
5	-0.396164529	-0.107328258	-4.962929868	5	0.396141000	-0.130347000	-2.246448000
7	3.241343471	1.067413742	-4.824313868	7	4.041328000	1.037873000	-2.139961000
5	1.794703471	1.052417742	-4.720433868	5	2.595110000	1.028671000	-2.029762000
7	1.114963471	2.076339742	-3.950222868	7	1.926238000	2.056785000	-1.255346000
5	-0.334814529	2.108321742	-3.930011868	5	0.482162000	2.061054000	-1.188199000
7	3.270755471	2.318664742	-2.685664868	7	4.090984000	2.286494000	0.000274000
7	1.115001471	2.076290742	-1.421053868	7	1.926318000	2.056625000	1.255985000
5	-0.334777529	2.108286742	-1.441218868	5	0.482256000	2.060922000	1.188766000
7	3.241403471	1.067321742	-0.547069868	7	4.041411000	1.037447000	2.140269000
5	1.794760471	1.052330742	-0.650911868	5	2.595187000	1.028293000	2.030120000
7	1.043875471	-0.125860258	-0.261997868	7	1.835976000	-0.148554000	2.405640000
5	-0.396101529	-0.107426258	-0.408426868	5	0.396197000	-0.130762000	2.246515000
7	3.194778471	-1.409392258	-0.544551868	7	3.985411000	-1.439702000	2.140497000
5	1.750584471	-1.339243258	-0.646937868	5	2.541835000	-1.366705000	2.033197000
7	1.041497471	-2.330787258	-1.438491868	7	1.833683000	-2.362923000	1.246742000
5	-0.396537529	-2.237607258	-1.502918868	5	0.395749000	-2.270929000	1.180705000
7	3.196591471	-2.662670258	-2.685782868	7	3.988929000	-2.693951000	-0.000260000
5	1.753300471	-2.560053258	-2.685760868	5	2.545733000	-2.593098000	-0.000235000
7	-5.356624529	-1.437876258	-4.886652868	7	-4.560101000	-1.465893000	-2.200120000
7	-5.433996529	1.091333742	-4.886134868	7	-4.648572000	1.061363000	-2.195637000
7	-5.503585529	2.362051742	-2.685561868	7	-4.729202000	2.340790000	0.000205000
7	-5.433940529	1.091224742	-0.485053868	7	-4.648517000	1.060931000	2.195799000
7	-5.356561529	-1.437985258	-0.484610868	7	-4.560046000	-1.466323000	2.200026000
7	-5.369394529	-2.713734258	-2.685663868	7	-4.576490000	-2.745307000	-0.000170000
5	3.927364471	-0.182979258	-5.082336868	5	4.721091000	-0.216047000	-2.400385000
5	3.971525471	1.900987742	-3.887891868	5	4.783321000	1.864018000	-1.205509000
5	3.971559471	1.900939742	-1.483473868	5	4.783368000	1.863779000	1.205951000

5	3.927431471	-0.183084258	-0.289131868	5	4.721168000	-0.216542000	2.400373000
5	3.903165471	-2.264461258	-1.481283868	5	4.694511000	-2.295977000	1.204989000
5	3.903131471	-2.264410258	-3.890285868	5	4.694485000	-2.295732000	-1.205444000
1	5.106116471	-0.205444258	-5.276387868	1	5.898642000	-0.242930000	-2.600204000
1	5.080549471	-2.438493258	-3.994672868	1	5.871682000	-2.470043000	-1.311250000
1	5.080586471	-2.438546258	-1.376936868	1	5.871710000	-2.470310000	1.310732000
1	5.106187471	-0.205560258	-0.095112868	1	5.898725000	-0.243489000	2.600147000
1	5.153561471	2.044262742	-1.383042868	1	5.966066000	1.996481000	1.310285000
1	5.153526471	2.044311742	-3.988347868	1	5.966014000	1.996740000	-1.309865000
1	-6.437400529	0.988604742	-4.796472868	1	-5.651548000	0.952461000	-2.108682000
1	-6.365135529	-1.392810258	-4.806733868	1	-5.569115000	-1.423119000	-2.125455000
1	-6.374145529	-2.586830258	-2.685645868	1	-5.581064000	-2.616883000	-0.000143000
1	-6.365074529	-1.392915258	-0.564503868	1	-5.569061000	-1.423527000	2.125371000
1	-6.437346529	0.988498742	-0.574691868	1	-5.651498000	0.952057000	2.108871000
1	-6.502474529	2.195666742	-2.685552868	1	-5.727072000	2.168136000	0.000206000
5	1.822665471	2.276354742	-2.685643868	5	2.646078000	2.251621000	0.000312000
5	-1.109138529	2.991813742	-2.685578868	5	-0.342234000	2.978390000	0.000447000
7	-0.781226529	4.404159742	-2.685576868	7	0.201302000	4.519244000	0.575303000
7	-0.528658549	5.494406862	-2.686040948	7	0.202166000	4.518571000	-0.576381000
N₂H@B_{AS}				N₂H₂@B_{AS}			
7	-2.430587000	-2.406480000	-1.245769000	7	-2.418365000	-2.435618000	-1.245391000
5	-3.873312000	-2.325663000	-1.192843000	5	-3.860674000	-2.359543000	-1.191703000
7	-0.292639000	-1.422712000	-2.097757000	7	-0.285689000	-1.433909000	-2.087068000
5	-1.730637000	-1.384860000	-2.007217000	5	-1.722842000	-1.401782000	-1.995082000
7	-2.448684000	-0.179471000	-2.381700000	7	-2.444803000	-0.195283000	-2.357284000
5	-3.898619000	-0.234044000	-2.349917000	5	-3.894197000	-0.260688000	-2.335426000
7	-0.307480000	1.076684000	-1.984715000	7	-0.309717000	1.062879000	-1.924433000
5	-1.772736000	1.038041000	-1.945754000	5	-1.777126000	1.025740000	-1.911888000
7	-2.578656000	2.022670000	-1.237736000	7	-2.596773000	2.016252000	-1.232192000
5	-4.013575000	1.834036000	-1.192983000	5	-4.027078000	1.813845000	-1.187254000
5	-1.945667000	2.460242000	0.000104000	5	-1.960134000	2.493661000	0.000055000
7	-2.578633000	2.022612000	1.237931000	7	-2.596731000	2.016211000	1.232309000
5	-4.013552000	1.833977000	1.193196000	5	-4.027038000	1.813814000	1.187415000
7	-0.307435000	1.076595000	1.984803000	7	-0.309658000	1.062829000	1.924499000
5	-1.772692000	1.037949000	1.945879000	5	-1.777067000	1.025690000	1.911974000
7	-2.448629000	-0.179585000	2.381781000	7	-2.444734000	-0.195340000	2.357366000
5	-3.898565000	-0.234159000	2.350029000	5	-3.894129000	-0.260743000	2.335544000
7	-0.292591000	-1.422807000	2.097724000	7	-0.285627000	-1.433962000	2.087067000
5	-1.730590000	-1.384955000	2.007222000	5	-1.722783000	-1.401832000	1.995121000
7	-2.430557000	-2.406538000	1.245741000	7	-2.418329000	-2.435650000	1.245424000
5	-3.873284000	-2.325722000	1.192854000	5	-3.860639000	-2.359572000	1.191779000
7	-0.282698000	-2.771804000	-0.000047000	7	-0.269735000	-2.799351000	-0.000019000
5	-1.721370000	-2.649669000	-0.000028000	5	-1.708266000	-2.679498000	0.000004000
7	1.859833000	-2.380870000	-1.247237000	7	1.870203000	-2.392903000	-1.247196000
5	0.421029000	-2.296791000	-1.182332000	5	0.431584000	-2.314345000	-1.180395000
7	4.007080000	-1.442785000	-2.138841000	7	4.012596000	-1.441338000	-2.135550000
5	2.562170000	-1.381946000	-2.035776000	5	2.567587000	-1.384356000	-2.029023000
7	1.847880000	-0.172445000	-2.416929000	7	1.849159000	-0.174399000	-2.398156000
5	0.407789000	-0.163119000	-2.267828000	5	0.410041000	-0.168808000	-2.236158000
7	4.038689000	1.034458000	-2.133385000	7	4.041967000	1.036768000	-2.126136000
5	2.591195000	1.010883000	-2.028800000	5	2.593647000	1.011401000	-2.016115000
7	1.907645000	2.032338000	-1.261996000	7	1.915910000	2.031838000	-1.251408000
5	0.457851000	2.049148000	-1.227340000	5	0.472624000	2.023756000	-1.164992000
7	4.062909000	2.297140000	0.000023000	7	4.077847000	2.315819000	-0.000026000
7	1.907673000	2.032279000	1.262077000	7	1.915948000	2.031807000	1.251425000

5	0.457873000	2.049105000	1.227461000	5	0.472657000	2.023726000	1.165056000
7	4.038737000	1.034363000	2.133375000	7	4.042034000	1.036715000	2.126056000
5	2.591240000	1.010792000	2.028820000	5	2.593710000	1.011352000	2.016087000
7	1.847935000	-0.172556000	2.416911000	7	1.849234000	-0.174458000	2.398122000
5	0.407841000	-0.163221000	2.267840000	5	0.410108000	-0.168864000	2.236173000
7	4.007130000	-1.442881000	2.138707000	7	4.012663000	-1.441390000	2.135414000
5	2.562216000	-1.382037000	2.035681000	5	2.567650000	-1.384405000	2.028935000
7	1.859862000	-2.380925000	1.247111000	7	1.870241000	-2.392933000	1.247104000
5	0.421056000	-2.296844000	1.182242000	5	0.431620000	-2.314374000	1.180350000
7	4.016973000	-2.700098000	-0.000095000	7	4.028284000	-2.704661000	-0.000083000
5	2.572885000	-2.606212000	-0.000076000	5	2.584040000	-2.616554000	-0.000059000
7	-4.543326000	-1.526310000	-2.200453000	7	-4.532179000	-1.557979000	-2.196660000
7	-4.637899000	1.002191000	-2.200774000	7	-4.646000000	0.967901000	-2.186179000
7	-4.717798000	2.271812000	0.000125000	7	-4.737468000	2.265579000	0.000097000
7	-4.637852000	1.002081000	2.200960000	7	-4.645933000	0.967850000	2.186340000
7	-4.543274000	-1.526419000	2.200520000	7	-4.532116000	-1.558031000	2.196772000
7	-4.548962000	-2.803304000	0.000002000	7	-4.535294000	-2.842555000	0.000041000
5	4.732059000	-0.211540000	-2.391766000	5	4.735352000	-0.207808000	-2.386263000
5	4.764515000	1.875314000	-1.200519000	5	4.772773000	1.882625000	-1.200238000
5	4.764542000	1.875262000	1.200533000	5	4.772811000	1.882592000	1.200153000
5	4.732114000	-0.211648000	2.391678000	5	4.735427000	-0.207866000	2.386135000
5	4.720745000	-2.295506000	1.203884000	5	4.729470000	-2.294375000	1.203712000
5	4.720717000	-2.295453000	-1.204072000	5	4.729433000	-2.294345000	-1.203889000
1	5.911157000	-0.226552000	-2.585413000	1	5.914211000	-0.222186000	-2.582498000
1	5.899162000	-2.462804000	-1.309276000	1	5.908413000	-2.458016000	-1.310509000
1	5.899193000	-2.462858000	1.309052000	1	5.908454000	-2.458047000	1.310291000
1	5.911216000	-0.226670000	2.585300000	1	5.914292000	-0.222250000	2.582333000
1	5.946170000	2.023248000	1.302291000	1	5.955105000	2.023612000	1.306744000
1	5.946141000	2.023301000	-1.302297000	1	5.955063000	2.023646000	-1.306863000
1	-5.640491000	0.891757000	-2.110983000	1	-5.647241000	0.847337000	-2.094719000
1	-5.552084000	-1.487218000	-2.120486000	1	-5.541323000	-1.524180000	-2.119096000
1	-5.554274000	-2.680877000	0.000017000	1	-5.540779000	-2.721366000	0.000058000
1	-5.552034000	-1.487323000	2.120578000	1	-5.541262000	-1.524228000	2.119235000
1	-5.640446000	0.891648000	2.111186000	1	-5.647178000	0.847291000	2.094908000
1	-5.715243000	2.097174000	0.000130000	1	-5.732866000	2.078412000	0.000112000
5	2.614344000	2.243513000	0.000041000	5	2.630989000	2.264202000	0.000001000
5	-0.327013000	2.958995000	0.000092000	5	-0.360031000	2.996681000	0.000058000
7	0.040519000	4.335714000	-0.000083000	7	0.269721000	4.276593000	-0.000058000
7	-0.278184000	5.496420000	-0.000453000	7	-0.425905000	5.347735000	-0.000177000
1	0.529835000	6.142263000	-0.000374000	1	0.048426000	6.242024000	-0.000169000
				1	-1.446166000	5.332215000	-0.000302000
N₂H₃@B_{AS}				NHNH₃@B_{AS}			
7	-2.380664000	-1.829642000	-1.905665000	7	-2.576277000	-2.071953000	-1.518156000
5	-3.822070000	-1.800645000	-1.828582000	5	-4.011852000	-1.934218000	-1.470498000
7	-0.263341000	-0.561316000	-2.321552000	7	-0.381541000	-1.066689000	-2.156927000
5	-1.696911000	-0.594685000	-2.241734000	5	-1.813427000	-0.980908000	-2.100330000
7	-2.432521000	0.654848000	-2.182553000	7	-2.463160000	0.297515000	-2.321132000
5	-3.879755000	0.576794000	-2.187768000	5	-3.914469000	0.297123000	-2.338012000
7	-0.304647000	1.813669000	-1.472563000	7	-0.254816000	1.440806000	-1.879547000
5	-1.759074000	1.673215000	-1.389880000	5	-1.732177000	1.431607000	-1.755537000
7	-2.594201000	2.356552000	-0.374134000	7	-2.550297000	2.303359000	-0.883081000
5	-4.030400000	2.102334000	-0.409821000	5	-3.994470000	2.144776000	-0.904720000
5	-1.971481000	2.245367000	0.992080000	5	-2.004622000	2.550497000	0.453855000
7	-2.614718000	1.322853000	1.901956000	7	-2.655402000	1.943422000	1.590087000
5	-4.036667000	1.158678000	1.792158000	5	-4.084229000	1.778218000	1.479847000

7	-0.304597000	0.296414000	2.301956000	7	-0.360640000	0.839140000	2.086313000
5	-1.760307000	0.202304000	2.260127000	5	-1.834020000	0.845530000	2.101936000
7	-2.419526000	-1.108518000	2.264674000	7	-2.555530000	-0.399919000	2.362178000
5	-3.865294000	-1.180196000	2.192238000	5	-4.009636000	-0.417321000	2.337574000
7	-0.241136000	-2.099363000	1.552281000	7	-0.448164000	-1.667769000	1.910177000
5	-1.677029000	-2.080887000	1.485478000	5	-1.879708000	-1.572029000	1.831080000
7	-2.362740000	-2.776647000	0.401108000	7	-2.614920000	-2.459779000	0.942162000
5	-3.804775000	-2.710817000	0.381344000	5	-4.048977000	-2.309434000	0.892848000
7	-0.223814000	-2.604062000	-0.891267000	7	-0.478701000	-2.759508000	-0.330788000
5	-1.659910000	-2.516329000	-0.842641000	5	-1.902134000	-2.551513000	-0.321365000
7	1.898967000	-1.758927000	-1.916209000	7	1.691574000	-2.310840000	-1.496233000
5	0.465527000	-1.709925000	-1.806944000	5	0.267272000	-2.133281000	-1.412284000
7	4.031551000	-0.570591000	-2.457061000	7	3.898249000	-1.397674000	-2.237658000
5	2.586452000	-0.545206000	-2.319540000	5	2.460897000	-1.248686000	-2.120803000
7	1.866135000	0.720942000	-2.257809000	7	1.829567000	0.047003000	-2.318372000
5	0.425562000	0.694444000	-2.090102000	5	0.392229000	0.157389000	-2.197741000
7	4.075753000	1.727409000	-1.551871000	7	4.100678000	1.038447000	-1.863099000
5	2.627270000	1.673467000	-1.465054000	5	2.652736000	1.120507000	-1.788641000
7	1.954435000	2.379432000	-0.415297000	7	2.041173000	2.181806000	-1.055724000
5	0.514690000	2.595232000	-0.508358000	5	0.650972000	2.430253000	-1.267881000
7	4.082907000	2.182896000	0.881922000	7	4.181371000	2.209035000	0.334768000
7	1.900911000	1.478096000	1.927147000	7	1.910707000	1.797654000	1.463608000
5	0.438118000	1.530712000	1.917250000	5	0.483083000	1.885062000	1.472420000
7	4.045348000	0.268962000	2.447712000	7	3.981495000	0.578070000	2.208498000
5	2.595748000	0.272017000	2.312164000	5	2.538045000	0.646976000	2.054357000
7	1.874562000	-0.987660000	2.272390000	7	1.739009000	-0.541047000	2.310920000
5	0.432902000	-0.943887000	2.137941000	5	0.303156000	-0.456494000	2.199693000
7	4.051290000	-2.050125000	1.574924000	7	3.835402000	-1.886610000	1.955465000
5	2.604967000	-1.976963000	1.500571000	5	2.398755000	-1.747032000	1.843999000
7	1.916883000	-2.655676000	0.411962000	7	1.658932000	-2.648526000	0.973715000
5	0.479201000	-2.575898000	0.386488000	5	0.232088000	-2.473517000	0.908963000
7	4.066059000	-2.480728000	-0.870485000	7	3.808186000	-2.936162000	-0.292496000
5	2.622675000	-2.408970000	-0.833283000	5	2.374099000	-2.755488000	-0.289277000
7	-4.510147000	-0.695369000	-2.472229000	7	-4.620530000	-0.969962000	-2.366642000
7	-4.634264000	1.702430000	-1.664799000	7	-4.611956000	1.537914000	-2.063758000
7	-4.743335000	2.024014000	0.850618000	7	-4.731857000	2.383792000	0.326650000
7	-4.650914000	0.016903000	2.426988000	7	-4.738456000	0.836617000	2.357574000
7	-4.481865000	-2.365588000	1.616323000	7	-4.691722000	-1.659865000	2.019259000
7	-4.483376000	-2.702069000	-0.905425000	7	-4.730257000	-2.546918000	-0.368050000
5	4.763669000	0.666098000	-2.250331000	5	4.712136000	-0.195788000	-2.289297000
5	4.795109000	2.190932000	-0.378791000	5	4.862603000	1.745128000	-0.849008000
5	4.774558000	1.383413000	1.873259000	5	4.791768000	1.500075000	1.431070000
5	4.754334000	-0.977868000	2.257980000	5	4.607547000	-0.718092000	2.342070000
5	4.771564000	-2.502915000	0.399958000	5	4.517586000	-2.680777000	0.950668000
5	4.754043000	-1.686997000	-1.871850000	5	4.545026000	-2.417649000	-1.432929000
1	5.940536000	0.723900000	-2.451816000	1	5.890538000	-0.268703000	-2.478306000
1	5.931682000	-1.805253000	-2.039063000	1	5.710449000	-2.648409000	-1.563392000
1	5.955149000	-2.667305000	0.435104000	1	5.686778000	-2.910774000	1.045517000
1	5.932060000	-1.051265000	2.450773000	1	5.779281000	-0.815609000	2.559521000
1	5.953344000	1.496949000	2.040340000	1	5.981814000	1.495037000	1.569586000
1	5.979403000	2.353985000	-0.417818000	1	6.059552000	1.740392000	-0.905150000
1	-5.633942000	1.542961000	-1.619784000	1	-5.620227000	1.452678000	-2.018541000
1	-5.519343000	-0.701901000	-2.391651000	1	-5.628202000	-0.892708000	-2.304725000
1	-5.490366000	-2.606741000	-0.857051000	1	-5.728855000	-2.379381000	-0.356730000
1	-5.491438000	-2.317292000	1.549847000	1	-5.698669000	-1.575573000	1.951161000
1	-5.649305000	-0.085948000	2.295487000	1	-5.740006000	0.745971000	2.239337000

1	-5.735706000	1.838571000	0.767783000	1	-5.731283000	2.234508000	0.261711000
5	2.627494000	2.125654000	0.847293000	5	2.690415000	2.490234000	0.310410000
5	-0.448469000	2.781531000	1.248237000	5	-0.411004000	2.991227000	0.504370000
7	0.079692000	3.798543000	0.259630000	7	0.059753000	3.666996000	-0.679489000
7	-0.990150000	4.590715000	-0.322254000	1	-0.729949000	4.007134000	-1.224405000
1	-0.648088000	5.069884000	-1.157539000	7	2.588037530	4.899466460	0.589741780
1	-1.830957000	3.998399000	-0.546888000	1	3.032735240	5.653483610	0.069265620
1	-1.261486000	5.292255000	0.369896000	1	2.441489170	5.209580750	1.548712880
				1	1.683134750	4.668115020	0.150310020
NH@B_{As}				NH₂@B_{As}			
7	-2.401194000	-1.859255000	-1.779816000	7	-2.445089000	-2.322986000	-1.244559000
5	-3.843514000	-1.796759000	-1.730280000	5	-3.887538000	-2.233954000	-1.190172000
7	-0.253810000	-0.682910000	-2.284552000	7	-0.304473000	-1.336849000	-2.083876000
5	-1.691075000	-0.669496000	-2.218278000	5	-1.742609000	-1.292350000	-1.991044000
7	-2.401000000	0.593806000	-2.270625000	7	-2.453958000	-0.079480000	-2.349777000
5	-3.850507000	0.529211000	-2.292083000	5	-3.904632000	-0.131079000	-2.329122000
7	-0.249767000	1.761767000	-1.682506000	7	-0.310562000	1.157066000	-1.908301000
5	-1.724230000	1.671266000	-1.550321000	5	-1.780161000	1.136501000	-1.902795000
7	-2.569606000	2.376346000	-0.563014000	7	-2.583794000	2.138780000	-1.230952000
5	-4.008059000	2.170564000	-0.620574000	5	-4.016312000	1.951486000	-1.186154000
5	-2.049918000	2.514934000	0.806757000	5	-1.939540000	2.620451000	-0.000898000
7	-2.681066000	1.721797000	1.840753000	7	-2.583522000	2.138885000	1.229427000
5	-4.100888000	1.512055000	1.691751000	5	-4.016099000	1.951793000	1.184993000
7	-0.352005000	0.656608000	2.213597000	7	-0.310310000	1.157723000	1.907951000
5	-1.828319000	0.599767000	2.211975000	5	-1.779893000	1.137151000	1.902126000
7	-2.488668000	-0.700665000	2.300728000	7	-2.453740000	-0.078546000	2.349881000
5	-3.940865000	-0.776876000	2.248958000	5	-3.904393000	-0.130125000	2.329231000
7	-0.320525000	-1.803241000	1.718814000	7	-0.304275000	-1.336086000	2.084412000
5	-1.755964000	-1.758380000	1.626433000	5	-1.742421000	-1.291590000	1.991648000
7	-2.437410000	-2.547854000	0.613704000	7	-2.444981000	-2.322507000	1.245619000
5	-3.878480000	-2.465081000	0.565697000	5	-3.887439000	-2.233488000	1.191305000
7	-0.276447000	-2.566639000	-0.653746000	7	-0.297971000	-2.705141000	0.000521000
5	-1.711706000	-2.441442000	-0.640489000	5	-1.736910000	-2.573319000	0.000551000
7	1.878934000	-1.870814000	-1.724864000	7	1.845695000	-2.309010000	-1.246339000
5	0.443998000	-1.786110000	-1.647155000	5	0.406523000	-2.223588000	-1.179002000
7	4.043775000	-0.783404000	-2.345193000	7	3.993273000	-1.369727000	-2.135955000
5	2.597970000	-0.718301000	-2.238648000	5	2.549094000	-1.304400000	-2.026759000
7	1.902111000	0.560314000	-2.319816000	7	1.838295000	-0.087923000	-2.391699000
5	0.456667000	0.573682000	-2.176030000	5	0.399153000	-0.077391000	-2.226743000
7	4.120213000	1.599982000	-1.704331000	7	4.038047000	1.108770000	-2.135033000
5	2.671855000	1.588925000	-1.646302000	5	2.590843000	1.094005000	-2.021643000
7	1.996667000	2.452845000	-0.708945000	7	1.919288000	2.123293000	-1.251554000
5	0.582622000	2.691211000	-0.908062000	5	0.474077000	2.119379000	-1.165397000
7	4.079050000	2.322075000	0.660929000	7	4.086675000	2.367966000	-0.000568000
7	1.874612000	1.740767000	1.719230000	7	1.919493000	2.123786000	1.250818000
5	0.429011000	1.789122000	1.710877000	5	0.474268000	2.119758000	1.164542000
7	3.992991000	0.572404000	2.411980000	7	4.038321000	1.109534000	2.134392000
5	2.551882000	0.575420000	2.254937000	5	2.591108000	1.094747000	2.021169000
7	1.804632000	-0.662368000	2.349782000	7	1.838572000	-0.087076000	2.391649000
5	0.367711000	-0.617133000	2.193958000	5	0.399395000	-0.076586000	2.226832000
7	3.972280000	-1.830092000	1.808342000	7	3.993514000	-1.368978000	2.136082000
5	2.529889000	-1.746815000	1.701946000	5	2.549309000	-1.303674000	2.027046000
7	1.843270000	-2.521770000	0.682622000	7	1.845821000	-2.308554000	1.247048000
5	0.407838000	-2.418188000	0.621779000	5	0.406637000	-2.223156000	1.179810000
7	4.015311000	-2.523263000	-0.574906000	7	4.002977000	-2.630811000	0.000295000

5	2.573626000	-2.420965000	-0.571113000	5	2.558774000	-2.536684000	0.000361000
7	-4.495199000	-0.754032000	-2.498425000	7	-4.552612000	-1.423724000	-2.191969000
7	-4.598462000	1.687433000	-1.849766000	7	-4.642813000	1.104387000	-2.180904000
7	-4.763893000	2.237266000	0.620538000	7	-4.723079000	2.410304000	-0.000573000
7	-4.720849000	0.431521000	2.423368000	7	-4.642541000	1.105273000	2.180265000
7	-4.560325000	-1.994460000	1.755591000	7	-4.552431000	-1.422836000	2.192822000
7	-4.536369000	-2.579824000	-0.723440000	7	-4.565149000	-2.714695000	0.000689000
5	4.799477000	0.452675000	-2.263403000	5	4.722642000	-0.142790000	-2.394387000
5	4.822093000	2.189087000	-0.579987000	5	4.778617000	1.940564000	-1.205234000
5	4.743631000	1.616534000	1.739934000	5	4.778765000	1.940984000	1.204161000
5	4.685795000	-0.699722000	2.375349000	5	4.722934000	-0.141969000	2.393985000
5	4.702048000	-2.422905000	0.700767000	5	4.706601000	-2.225738000	1.204245000
5	4.734923000	-1.850258000	-1.642185000	5	4.706478000	-2.226110000	-1.203857000
1	5.980917000	0.463648000	-2.441115000	1	5.900600000	-0.164208000	-2.593633000
1	5.911136000	-2.008890000	-1.779485000	1	5.884422000	-2.395475000	-1.310930000
1	5.880883000	-2.603265000	0.775736000	1	5.884561000	-2.395035000	1.311235000
1	5.859357000	-0.765317000	2.589851000	1	5.900924000	-0.163337000	2.593065000
1	5.920326000	1.731710000	1.913576000	1	5.961125000	2.077217000	1.310732000
1	6.007461000	2.337199000	-0.607439000	1	5.960960000	2.076778000	-1.312016000
1	-5.602994000	1.561065000	-1.824931000	1	-5.645495000	0.995792000	-2.090649000
1	-5.505585000	-0.733628000	-2.435473000	1	-5.561461000	-1.382126000	-2.114371000
1	-5.542453000	-2.466412000	-0.705161000	1	-5.569648000	-2.585261000	0.000704000
1	-5.569780000	-1.950835000	1.686693000	1	-5.561279000	-1.381212000	2.115193000
1	-5.716972000	0.318482000	2.281084000	1	-5.645235000	0.996661000	2.090150000
1	-5.757227000	2.065082000	0.526285000	1	-5.720555000	2.235036000	-0.000461000
5	2.628659000	2.297937000	0.593127000	5	2.641058000	2.322323000	-0.000458000
5	-0.469130000	3.014129000	0.905536000	5	-0.354234000	3.162262000	-0.000234000
7	-0.045900000	3.804760000	-0.207999000	7	0.081760000	4.546324000	0.001265000
1	-0.849735000	4.187045000	-0.700202000	1	1.052222000	4.828545000	0.003318000
				1	-0.554650000	5.329429000	-0.000419000
NH₃@B_{As}				NHNH@B_{As}			
7	-2.444773000	-2.327840000	-1.245468000	7	-2.412488000	-2.433403000	-1.245671000
5	-3.886512000	-2.242098000	-1.191275000	5	-3.855845000	-2.360446000	-1.192752000
7	-0.304035000	-1.347873000	-2.095083000	7	-0.281054000	-1.431690000	-2.091526000
5	-1.741747000	-1.303393000	-2.002989000	5	-1.720021000	-1.401549000	-2.000653000
7	-2.456071000	-0.095628000	-2.373207000	7	-2.443450000	-0.199763000	-2.370467000
5	-3.904551000	-0.146441000	-2.340029000	5	-3.893547000	-0.266147000	-2.344689000
7	-0.307445000	1.152299000	-1.987356000	7	-0.309059000	1.066162000	-1.955209000
5	-1.772638000	1.123293000	-1.938506000	5	-1.780054000	1.024617000	-1.925943000
7	-2.575987000	2.111956000	-1.233765000	7	-2.596856000	2.004571000	-1.233475000
5	-4.006821000	1.926060000	-1.187269000	5	-4.027257000	1.802397000	-1.190544000
5	-1.917613000	2.577675000	-0.000561000	5	-1.957552000	2.476429000	0.000055000
7	-2.576041000	2.113331000	1.233090000	7	-2.596825000	2.004524000	1.233586000
5	-4.006857000	1.927260000	1.186710000	5	-4.027227000	1.802355000	1.190685000
7	-0.307486000	1.153716000	1.986739000	7	-0.309012000	1.066102000	1.955265000
5	-1.772641000	1.124776000	1.938047000	5	-1.780006000	1.024556000	1.926017000
7	-2.456142000	-0.093983000	2.373168000	7	-2.443395000	-0.199836000	2.370520000
5	-3.904638000	-0.144593000	2.340034000	5	-3.893492000	-0.266219000	2.344772000
7	-0.304168000	-1.346390000	2.095589000	7	-0.281006000	-1.431755000	2.091494000
5	-1.741899000	-1.301927000	2.003469000	5	-1.719975000	-1.401611000	2.000655000
7	-2.444886000	-2.326794000	1.246515000	7	-2.412459000	-2.433443000	1.245658000
5	-3.886615000	-2.241046000	1.192062000	5	-3.855817000	-2.360483000	1.192773000
7	-0.298406000	-2.700617000	0.000751000	7	-0.263036000	-2.789894000	-0.000037000
5	-1.736548000	-2.572753000	0.000651000	5	-1.702977000	-2.673598000	-0.000018000
7	1.844883000	-2.313750000	-1.246498000	7	1.876460000	-2.381418000	-1.246914000

5	0.405680000	-2.224201000	-1.181020000	5	0.436507000	-2.305985000	-1.180767000
7	3.994989000	-1.386476000	-2.141015000	7	4.016980000	-1.434477000	-2.142460000
5	2.549394000	-1.316433000	-2.035200000	5	2.571657000	-1.377815000	-2.034470000
7	1.841309000	-0.104968000	-2.416793000	7	1.851937000	-0.169420000	-2.409692000
5	0.399286000	-0.087516000	-2.264142000	5	0.410488000	-0.166640000	-2.251256000
7	4.038769000	1.090494000	-2.143083000	7	4.041796000	1.042717000	-2.143984000
5	2.588655000	1.077134000	-2.032519000	5	2.593996000	1.015974000	-2.032134000
7	1.912004000	2.104067000	-1.268335000	7	1.911571000	2.037109000	-1.259661000
5	0.444574000	2.146906000	-1.228146000	5	0.455888000	2.041693000	-1.200917000
7	4.069066000	2.334422000	-0.000751000	7	4.072281000	2.283866000	0.000000000
7	1.912030000	2.104938000	1.267129000	7	1.911604000	2.037081000	1.259713000
5	0.444700000	2.147682000	1.226777000	5	0.455918000	2.041671000	1.200997000
7	4.038766000	1.091617000	2.142192000	7	4.041848000	1.042650000	2.143946000
5	2.588638000	1.078312000	2.031827000	5	2.594045000	1.015914000	2.032129000
7	1.841224000	-0.103464000	2.416847000	7	1.851993000	-0.169495000	2.409656000
5	0.399193000	-0.086011000	2.264115000	5	0.410540000	-0.166708000	2.251252000
7	3.994831000	-1.385351000	2.142210000	7	4.017030000	-1.434544000	2.142330000
5	2.549267000	-1.315239000	2.036118000	5	2.571704000	-1.377877000	2.034375000
7	1.844781000	-2.312962000	1.247926000	7	1.876489000	-2.381454000	1.246803000
5	0.405590000	-2.223399000	1.182254000	5	0.436535000	-2.306020000	1.180691000
7	4.000956000	-2.639086000	0.000917000	7	4.035827000	-2.685746000	-0.000085000
5	2.556346000	-2.539770000	0.000818000	5	2.590632000	-2.602079000	-0.000067000
7	-4.555083000	-1.437700000	-2.195768000	7	-4.528756000	-1.565087000	-2.200777000
7	-4.641299000	1.090769000	-2.188259000	7	-4.644697000	0.961589000	-2.197553000
7	-4.714242000	2.383675000	-0.000515000	7	-4.739415000	2.235159000	0.000087000
7	-4.641286000	1.092752000	2.188456000	7	-4.644646000	0.961521000	2.197685000
7	-4.555291000	-1.435723000	2.195678000	7	-4.528705000	-1.565155000	2.200838000
7	-4.563964000	-2.721692000	0.000571000	7	-4.528772000	-2.842899000	0.000011000
5	4.724610000	-0.159675000	-2.398941000	5	4.736876000	-0.203228000	-2.403963000
5	4.769107000	1.916870000	-1.202673000	5	4.771810000	1.872014000	-1.205594000
5	4.769123000	1.917426000	1.201345000	5	4.771839000	1.871977000	1.205566000
5	4.724529000	-0.158374000	2.399134000	5	4.736933000	-0.203306000	2.403862000
5	4.705145000	-2.237672000	1.205351000	5	4.736212000	-2.280497000	1.205314000
5	4.705256000	-2.238224000	-1.203628000	5	4.736184000	-2.280460000	-1.205487000
1	5.903647000	-0.181373000	-2.595659000	1	5.914854000	-0.214719000	-2.604546000
1	5.883643000	-2.409305000	-1.308295000	1	5.915590000	-2.441163000	-1.311275000
1	5.883497000	-2.408829000	1.310263000	1	5.915620000	-2.441203000	1.311069000
1	5.903546000	-0.179963000	2.595977000	1	5.914916000	-0.214806000	2.604419000
1	5.951973000	2.062469000	1.301637000	1	5.953084000	2.022278000	1.307891000
1	5.951917000	2.062092000	-1.303147000	1	5.953052000	2.022318000	-1.307943000
1	-5.643236000	0.981291000	-2.090222000	1	-5.646044000	0.841089000	-2.106757000
1	-5.563264000	-1.393077000	-2.111208000	1	-5.537809000	-1.531769000	-2.121539000
1	-5.568416000	-2.591960000	0.000469000	1	-5.534524000	-2.723942000	0.000025000
1	-5.563465000	-1.391147000	2.111096000	1	-5.537760000	-1.531834000	2.121622000
1	-5.643214000	0.983169000	2.090344000	1	-5.645995000	0.841025000	2.106910000
1	-5.710645000	2.201898000	-0.000452000	1	-5.734632000	2.048394000	0.000096000
5	2.615497000	2.283951000	-0.000729000	5	2.624793000	2.223008000	0.000019000
5	-0.308315000	3.047578000	-0.000984000	5	-0.363371000	2.960931000	0.000070000
7	0.084043000	4.618150000	-0.001414000	7	0.073353000	4.370198000	0.000019000
1	1.095822000	4.753563000	-0.001505000	7	-0.657051000	5.394950000	-0.000076000
1	-0.282609000	5.098352000	-0.822387000	1	-0.057958000	6.229425000	-0.000099000
1	-0.282523000	5.098829000	0.819318000	1	1.091126000	4.519534000	0.000069000
NH₂NH@B_{As}				NH₂NH₂@B_{As}			
7	-2.386046000	-2.473023000	-1.245821000	7	-2.410151000	-2.319688000	-1.461458000
5	-3.829123000	-2.411422000	-1.191554000	5	-3.852773000	-2.254351000	-1.396120000

7	-0.262338000	-1.455695000	-2.093402000	7	-0.281499000	-1.234292000	-2.206054000
5	-1.700407000	-1.436254000	-2.001761000	5	-1.719644000	-1.214437000	-2.107293000
7	-2.434502000	-0.239534000	-2.370378000	7	-2.446790000	0.018051000	-2.348085000
5	-3.882200000	-0.314738000	-2.337534000	5	-3.895192000	-0.049365000	-2.322776000
7	-0.308747000	1.042882000	-1.969217000	7	-0.310906000	1.240477000	-1.839790000
5	-1.773059000	0.989257000	-1.932755000	5	-1.776876000	1.192510000	-1.791355000
7	-2.592332000	1.965191000	-1.231634000	7	-2.588171000	2.099377000	-0.991543000
5	-4.020503000	1.758273000	-1.185458000	5	-4.017907000	1.890904000	-0.965052000
5	-1.944893000	2.440831000	0.000070000	5	-1.936956000	2.431129000	0.289207000
7	-2.592301000	1.965132000	1.231765000	7	-2.585937000	1.827354000	1.462359000
5	-4.020473000	1.758224000	1.185619000	5	-4.015031000	1.631918000	1.398446000
7	-0.308699000	1.042809000	1.969277000	7	-0.302473000	0.825038000	2.109230000
5	-1.773012000	0.989180000	1.932841000	5	-1.768662000	0.782974000	2.060594000
7	-2.434446000	-0.239625000	2.370438000	7	-2.435962000	-0.482154000	2.368714000
5	-3.882144000	-0.314828000	2.337623000	5	-3.884332000	-0.546209000	2.333449000
7	-0.262287000	-1.455773000	2.093363000	7	-0.270992000	-1.672912000	1.957838000
5	-1.700359000	-1.436331000	2.001758000	5	-1.709546000	-1.636667000	1.874361000
7	-2.386016000	-2.473072000	1.245796000	7	-2.402783000	-2.585464000	1.015950000
5	-3.829094000	-2.411469000	1.191566000	5	-3.845786000	-2.509524000	0.973754000
7	-0.233474000	-2.811624000	-0.000045000	7	-0.255852000	-2.802379000	-0.266349000
5	-1.673604000	-2.707513000	-0.000026000	5	-1.695664000	-2.690103000	-0.250209000
7	1.902901000	-2.386750000	-1.247190000	7	1.880060000	-2.260761000	-1.468202000
5	0.462641000	-2.322397000	-1.181404000	5	0.440063000	-2.195109000	-1.391455000
7	4.036451000	-1.420384000	-2.140452000	7	4.017691000	-1.221350000	-2.264558000
5	2.590327000	-1.376120000	-2.034207000	5	2.571905000	-1.179087000	-2.148970000
7	1.860943000	-0.175933000	-2.412297000	7	1.849659000	0.058390000	-2.399568000
5	0.420042000	-0.183895000	-2.256481000	5	0.408055000	0.043021000	-2.244580000
7	4.037963000	1.057302000	-2.139742000	7	4.034651000	1.242738000	-2.007635000
5	2.589099000	1.018257000	-2.029089000	5	2.585786000	1.201584000	-1.896299000
7	1.896197000	2.031943000	-1.261692000	7	1.900050000	2.136660000	-1.027309000
5	0.436679000	2.039732000	-1.212836000	5	0.433907000	2.153654000	-0.981394000
7	4.052098000	2.306767000	0.000006000	7	4.058025000	2.252812000	0.254738000
7	1.896229000	2.031905000	1.261750000	7	1.906509000	1.869785000	1.494113000
5	0.436708000	2.039697000	1.212926000	5	0.439748000	1.901579000	1.462015000
7	4.038015000	1.057223000	2.139706000	7	4.045400000	0.793659000	2.256857000
5	2.589148000	1.018185000	2.029087000	5	2.595553000	0.775746000	2.146793000
7	1.861001000	-0.176023000	2.412258000	7	1.860811000	-0.447031000	2.405049000
5	0.420096000	-0.183979000	2.256475000	5	0.418395000	-0.429283000	2.255807000
7	4.036503000	-1.420464000	2.140312000	7	4.027586000	-1.669814000	1.997232000
5	2.590375000	-1.376195000	2.034104000	5	2.581260000	-1.605027000	1.900087000
7	1.902931000	-2.386794000	1.247064000	7	1.886241000	-2.522525000	1.012235000
5	0.462670000	-2.322440000	1.181315000	5	0.445873000	-2.442765000	0.957709000
7	4.064349000	-2.675094000	-0.000094000	7	4.043080000	-2.689741000	-0.264733000
5	2.618496000	-2.601411000	-0.000075000	5	2.597409000	-2.608868000	-0.252568000
7	-4.510712000	-1.616707000	-2.195033000	7	-4.531857000	-1.355043000	-2.308892000
7	-4.640072000	0.909499000	-2.182950000	7	-4.642573000	1.160494000	-2.051827000
7	-4.733518000	2.212086000	0.000098000	7	-4.728845000	2.199141000	0.265412000
7	-4.640020000	0.909414000	2.183094000	7	-4.636160000	0.690607000	2.309707000
7	-4.510660000	-1.616792000	2.195091000	7	-4.519610000	-1.824179000	2.059578000
7	-4.498315000	-2.902833000	0.000004000	7	-4.521816000	-2.865533000	-0.261518000
5	4.744947000	-0.180880000	-2.397482000	5	4.733083000	0.033516000	-2.395637000
5	4.756787000	1.897953000	-1.202437000	5	4.759238000	1.971338000	-0.985433000
5	4.756816000	1.897910000	1.202417000	5	4.765371000	1.719607000	1.406119000
5	4.745004000	-0.180970000	2.397378000	5	4.744752000	-0.469295000	2.382529000
5	4.761618000	-2.261628000	1.204456000	5	4.745366000	-2.410302000	0.974877000
5	4.761589000	-2.261585000	-1.204645000	5	4.740114000	-2.157570000	-1.421537000

1	5.923925000	-0.181906000	-2.594657000	1	5.911215000	0.046756000	-2.597657000
1	5.942384000	-2.413691000	-1.310247000	1	5.919985000	-2.303830000	-1.544880000
1	5.942415000	-2.413738000	1.310023000	1	5.925787000	-2.577829000	1.059706000
1	5.923987000	-0.182005000	2.594527000	1	5.923798000	-0.499093000	2.577368000
1	5.937103000	2.059414000	1.304517000	1	5.946960000	1.865065000	1.518403000
1	5.937071000	2.059460000	-1.304560000	1	5.940493000	2.136303000	-1.071147000
1	-5.640291000	0.784138000	-2.086937000	1	-5.643446000	1.031900000	-1.966202000
1	-5.519604000	-1.589685000	-2.111581000	1	-5.540383000	-1.330631000	-2.220616000
1	-5.504862000	-2.790660000	0.000019000	1	-5.527588000	-2.747616000	-0.245669000
1	-5.519553000	-1.589767000	2.111662000	1	-5.528486000	-1.782619000	1.981812000
1	-5.640241000	0.784058000	2.087102000	1	-5.637277000	0.580316000	2.204709000
1	-5.727780000	2.018725000	0.000107000	1	-5.723337000	2.008810000	0.245942000
5	2.602008000	2.232212000	0.000023000	5	2.605666000	2.188784000	0.252220000
5	-0.353469000	2.972633000	0.000075000	5	-0.332988000	2.911031000	0.335633000
7	0.037194000	4.413784000	0.000071000	7	0.024902000	4.461149000	0.466793000
7	-0.826574000	5.447315000	-0.000072000	7	-0.623386000	5.278163000	-0.532170000
1	-0.494334000	6.395097000	-0.000257000	1	0.033927000	5.979179000	-0.864592000
1	1.000576000	4.725546000	0.000162000	1	1.041392000	4.566793000	0.435071000
1	-1.806363000	5.223650000	-0.000336000	1	-0.833374000	4.643546000	-1.299133000
				1	-0.282943000	4.819081000	1.369483000
NH₃NH₂@B_{As}				N₂H@B_{As}_TS (-235.3 cm⁻¹)			
7	-2.197355000	-2.531905000	-1.382521000	7	-2.459079000	-2.365858000	-1.248909000
5	-3.640833000	-2.554490000	-1.313184000	5	-3.903000000	-2.279245000	-1.195898000
7	-0.143206000	-1.335318000	-2.160429000	7	-0.313145000	-1.393683000	-2.104768000
5	-1.578840000	-1.402072000	-2.056244000	5	-1.753160000	-1.345049000	-2.012376000
7	-2.380661000	-0.220589000	-2.321210000	7	-2.466760000	-0.131829000	-2.384134000
5	-3.822632000	-0.378909000	-2.291262000	5	-3.919818000	-0.186248000	-2.355884000
7	-0.323845000	1.134778000	-1.813133000	7	-0.308806000	1.113863000	-2.019269000
5	-1.786857000	1.008295000	-1.800699000	5	-1.783828000	1.089575000	-1.957086000
7	-2.655379000	1.908777000	-1.063797000	7	-2.600227000	2.076262000	-1.243877000
5	-4.067579000	1.618550000	-1.016032000	5	-4.036476000	1.878938000	-1.198150000
5	-2.021477000	2.329297000	0.200364000	5	-1.970209000	2.516831000	0.000166000
7	-2.624974000	1.714215000	1.390642000	7	-2.600161000	2.076008000	1.244179000
5	-4.039348000	1.445791000	1.340497000	5	-4.036409000	1.878730000	1.198492000
7	-0.281042000	0.862318000	2.007203000	7	-0.308729000	1.113561000	2.019661000
5	-1.743784000	0.733873000	1.995658000	5	-1.783744000	1.089236000	1.957269000
7	-2.331002000	-0.555287000	2.356599000	7	-2.466691000	-0.132242000	2.384102000
5	-3.773312000	-0.708548000	2.329437000	5	-3.919744000	-0.186644000	2.355869000
7	-0.098356000	-1.631879000	1.995902000	7	-0.313074000	-1.394016000	2.104504000
5	-1.536286000	-1.686405000	1.914281000	5	-1.753099000	-1.345400000	2.012190000
7	-2.170187000	-2.712533000	1.100913000	7	-2.459035000	-2.366100000	1.248580000
5	-3.615093000	-2.725697000	1.058876000	5	-3.902965000	-2.279503000	1.195638000
7	-0.015141000	-2.846787000	-0.180597000	7	-0.312256000	-2.743230000	-0.000240000
5	-1.458692000	-2.820774000	-0.162751000	5	-1.751482000	-2.613860000	-0.000201000
7	2.079978000	-2.207810000	-1.407207000	7	1.834474000	-2.370049000	-1.250648000
5	0.639807000	-2.231165000	-1.325975000	5	0.394849000	-2.274378000	-1.186288000
7	4.145870000	-1.057604000	-2.240426000	7	3.992959000	-1.458691000	-2.148652000
5	2.701895000	-1.102677000	-2.118306000	5	2.546664000	-1.380221000	-2.047123000
7	1.902619000	0.082395000	-2.391060000	7	1.842783000	-0.161436000	-2.435870000
5	0.468195000	-0.021077000	-2.218538000	5	0.398140000	-0.139163000	-2.290241000
7	4.014722000	1.411032000	-2.057810000	7	4.053777000	1.020023000	-2.148999000
5	2.573484000	1.285119000	-1.936244000	5	2.604887000	1.015764000	-2.047823000
7	1.839951000	2.202864000	-1.088456000	7	1.931053000	2.046065000	-1.275618000
5	0.399106000	2.093158000	-0.998450000	5	0.479345000	2.085481000	-1.270812000
7	3.998277000	2.512703000	0.163650000	7	4.084377000	2.265251000	0.000348000

7	1.869974000	2.030539000	1.411881000	7	1.931210000	2.046176000	1.276606000
5	0.424526000	1.941523000	1.336264000	5	0.479527000	2.085530000	1.271685000
7	4.063378000	1.105518000	2.204047000	7	4.053903000	1.019651000	2.149472000
5	2.618697000	0.997862000	2.098101000	5	2.605006000	1.015494000	2.048378000
7	1.954705000	-0.259141000	2.384716000	7	1.842868000	-0.161853000	2.435904000
5	0.516101000	-0.337195000	2.227472000	5	0.398208000	-0.139532000	2.290279000
7	4.192181000	-1.363272000	2.024646000	7	3.993031000	-1.459062000	2.148264000
5	2.745554000	-1.391450000	1.928295000	5	2.546735000	-1.380533000	2.046794000
7	2.107043000	-2.385438000	1.080129000	7	1.834517000	-2.370160000	1.250106000
5	0.665116000	-2.398816000	1.027104000	5	0.394886000	-2.274538000	1.185847000
7	4.267534000	-2.461507000	-0.198663000	7	3.990032000	-2.710830000	-0.000311000
5	2.820718000	-2.471459000	-0.183608000	5	2.545931000	-2.602585000	-0.000288000
7	-4.375741000	-1.720355000	-2.245126000	7	-4.567963000	-1.478386000	-2.207782000
7	-4.649463000	0.785341000	-2.046091000	7	-4.660637000	1.050959000	-2.210419000
7	-4.787759000	1.977969000	0.202444000	7	-4.740381000	2.310336000	0.000223000
7	-4.602912000	0.476314000	2.254220000	7	-4.660545000	1.050607000	2.210663000
7	-4.329326000	-2.033046000	2.113792000	7	-4.567908000	-1.478756000	2.207616000
7	-4.268296000	-3.173047000	-0.159129000	7	-4.581000000	-2.751141000	-0.000170000
5	4.783193000	0.234407000	-2.412904000	5	4.734243000	-0.235582000	-2.406111000
5	4.704915000	2.221678000	-1.071755000	5	4.786422000	1.844274000	-1.202982000
5	4.732755000	2.049183000	1.328815000	5	4.786503000	1.844083000	1.203567000
5	4.836454000	-0.109429000	2.368135000	5	4.734351000	-0.236061000	2.406118000
5	4.953377000	-2.096449000	1.028375000	5	4.698643000	-2.315212000	1.206845000
5	4.927520000	-1.923650000	-1.374809000	5	4.698607000	-2.315021000	-1.207426000
1	5.957254000	0.313174000	-2.621344000	1	5.909185000	-0.264699000	-2.598689000
1	6.113330000	-2.002282000	-1.499894000	1	5.872933000	-2.487290000	-1.305990000
1	6.141338000	-2.191550000	1.116159000	1	5.872978000	-2.487476000	1.305330000
1	6.015015000	-0.061561000	2.560079000	1	5.909309000	-0.265274000	2.598584000
1	5.905334000	2.254818000	1.434145000	1	5.967545000	1.969977000	1.292600000
1	5.875197000	2.441628000	-1.173676000	1	5.967454000	1.970217000	-1.292087000
1	-5.639418000	0.595320000	-1.950227000	1	-5.665019000	0.938517000	-2.122509000
1	-5.383843000	-1.758892000	-2.157413000	1	-5.578659000	-1.435612000	-2.131799000
1	-5.279466000	-3.117597000	-0.143910000	1	-5.587919000	-2.628392000	-0.000141000
1	-5.338975000	-2.058602000	2.039734000	1	-5.578603000	-1.435957000	2.131642000
1	-5.596029000	0.303713000	2.159741000	1	-5.664939000	0.938222000	2.122806000
1	-5.772282000	1.738450000	0.197530000	1	-5.739152000	2.132909000	0.000241000
5	2.557747000	2.368370000	0.171782000	5	2.632394000	2.237127000	0.000429000
5	-0.485009000	2.970728000	0.251784000	5	-0.334184000	2.823134000	0.000602000
7	-0.256200000	4.398740000	0.299893000	7	0.227659000	4.846698000	0.554688000
7	-3.172244000	5.029928000	-0.323787000	7	0.235008000	4.845827000	-0.556304000
1	-3.876331000	4.437521000	0.114041000				
1	0.648533000	4.843893000	0.365380000				
1	-3.592963000	5.947429000	-0.444774000				
1	-1.061052000	5.021318000	0.254826000				
1	-3.024745000	4.639973000	-1.251423000				
N₂H@B_{As}_TS (-1291.7 cm⁻¹)				N₂H₂@B_{As}_TS (-1028.2 cm⁻¹)			
7	2.450247000	-2.399700000	1.248715000	7	2.396749000	-2.456327000	1.248635000
5	3.894708000	-2.312526000	1.194592000	5	3.841880000	-2.390315000	1.193536000
7	0.305064000	-1.424332000	2.105951000	7	0.267826000	-1.439340000	2.096444000
5	1.745482000	-1.380221000	2.014592000	5	1.708520000	-1.417338000	2.004525000
7	2.460259000	-0.168757000	2.389108000	7	2.441107000	-0.214569000	2.369394000
5	3.912336000	-0.216990000	2.351541000	5	3.891812000	-0.288610000	2.337662000
7	0.309209000	1.081524000	2.005171000	7	0.309667000	1.065418000	1.963533000
5	1.777084000	1.048579000	1.956409000	5	1.779071000	1.014836000	1.929027000
7	2.574655000	2.038695000	1.239464000	7	2.597478000	1.997983000	1.233518000

5	4.013148000	1.856242000	1.193165000	5	4.029569000	1.790646000	1.187209000
5	1.934381000	2.475931000	-0.000008000	5	1.973186000	2.498654000	-0.000037000
7	2.574628000	2.038705000	-1.239499000	7	2.597434000	1.997940000	-1.233595000
5	4.013122000	1.856249000	-1.193232000	5	4.029530000	1.790617000	-1.187334000
7	0.309165000	1.081530000	-2.005158000	7	0.309604000	1.065388000	-1.963553000
5	1.777041000	1.048588000	-1.956428000	5	1.779009000	1.014802000	-1.929087000
7	2.460208000	-0.168746000	-2.389146000	7	2.441031000	-0.214604000	-2.369476000
5	3.912286000	-0.216978000	-2.351612000	5	3.891736000	-0.288646000	-2.337778000
7	0.305019000	-1.424326000	-2.105956000	7	0.267758000	-1.439371000	-2.096442000
5	1.745439000	-1.380213000	-2.014624000	5	1.708456000	-1.417368000	-2.004570000
7	2.450221000	-2.399696000	-1.248768000	7	2.396707000	-2.456350000	-1.248690000
5	3.894683000	-2.312521000	-1.194674000	5	3.841841000	-2.390340000	-1.193640000
7	0.300639000	-2.771450000	-0.000004000	7	0.242142000	-2.800501000	0.000012000
5	1.741169000	-2.645945000	-0.000019000	5	1.684267000	-2.694127000	-0.000013000
7	-1.846977000	-2.391028000	1.250228000	7	-1.898645000	-2.381347000	1.250191000
5	-0.406238000	-2.301647000	1.186291000	5	-0.456673000	-2.313234000	1.184465000
7	-4.001662000	-1.461565000	2.144030000	7	-4.038057000	-1.414690000	2.140853000
5	-2.555127000	-1.395401000	2.043752000	5	-2.590341000	-1.368748000	2.037311000
7	-1.844706000	-0.180619000	2.430212000	7	-1.862323000	-0.162373000	2.413569000
5	-0.402224000	-0.166123000	2.283394000	5	-0.419597000	-0.167793000	2.257802000
7	-4.042824000	1.019241000	2.141093000	7	-4.047369000	1.066990000	2.134518000
5	-2.593780000	1.002437000	2.039012000	5	-2.597240000	1.031630000	2.027898000
7	-1.910876000	2.027164000	1.266605000	7	-1.906677000	2.050154000	1.260672000
5	-0.458693000	2.052708000	1.245481000	5	-0.455797000	2.043492000	1.206473000
7	-4.069393000	2.277112000	0.000057000	7	-4.065513000	2.339340000	0.000055000
7	-1.910905000	2.027163000	-1.266538000	7	-1.906716000	2.050134000	-1.260628000
5	-0.458722000	2.052710000	-1.245446000	5	-0.455833000	2.043472000	-1.206480000
7	-4.042872000	1.019245000	-2.140982000	7	-4.047438000	1.066955000	-2.134386000
5	-2.593826000	1.002441000	-2.038935000	5	-2.597304000	1.031600000	-2.027818000
7	-1.844759000	-0.180611000	-2.430162000	7	-1.862401000	-0.162405000	-2.413506000
5	-0.402273000	-0.166115000	-2.283374000	5	-0.419670000	-0.167826000	-2.257786000
7	-4.001707000	-1.461561000	-2.143946000	7	-4.038125000	-1.414726000	-2.140716000
5	-2.555171000	-1.395397000	-2.043696000	5	-2.590406000	-1.368779000	-2.037217000
7	-1.847004000	-2.391027000	-1.250192000	7	-1.898685000	-2.381369000	-1.250107000
5	-0.406264000	-2.301645000	-1.186284000	5	-0.456711000	-2.313253000	-1.184426000
7	-4.005051000	-2.720015000	0.000041000	7	-4.061341000	-2.678652000	0.000079000
5	-2.559954000	-2.620239000	0.000026000	5	-2.614680000	-2.600721000	0.000055000
7	4.562816000	-1.507371000	2.201414000	7	4.521629000	-1.591293000	2.197304000
7	4.643966000	1.025029000	2.199076000	7	4.647837000	0.937892000	2.183063000
7	4.714429000	2.304490000	-0.000040000	7	4.740397000	2.247625000	-0.000081000
7	4.643918000	1.025041000	-2.199160000	7	4.647768000	0.937855000	-2.183199000
7	4.562769000	-1.507358000	-2.201505000	7	4.521558000	-1.591330000	-2.197438000
7	4.571704000	-2.788456000	-0.000049000	7	4.511971000	-2.879851000	-0.000058000
5	-4.732836000	-0.231477000	2.398213000	5	-4.752419000	-0.174315000	2.392685000
5	-4.772274000	1.855039000	1.202659000	5	-4.769255000	1.915245000	1.201340000
5	-4.772301000	1.855038000	-1.202527000	5	-4.769295000	1.915221000	-1.201196000
5	-4.732888000	-0.231472000	-2.398100000	5	-4.752495000	-0.174351000	-2.392526000
5	-4.712365000	-2.316553000	-1.205400000	5	-4.761505000	-2.261527000	-1.204902000
5	-4.712339000	-2.316554000	1.205497000	5	-4.761469000	-2.261500000	1.205070000
1	-5.908317000	-0.250950000	2.588609000	1	-5.928055000	-0.178934000	2.584664000
1	-5.887754000	-2.480924000	1.303747000	1	-5.939300000	-2.408118000	1.304414000
1	-5.887781000	-2.480928000	-1.303628000	1	-5.939339000	-2.408149000	-1.304207000
1	-5.908374000	-0.250944000	-2.588470000	1	-5.928138000	-0.178971000	-2.584468000
1	-5.951982000	1.989380000	-1.295553000	1	-5.947944000	2.059723000	-1.297587000
1	-5.951952000	1.989387000	1.295714000	1	-5.947900000	2.059759000	1.297771000
1	5.649195000	0.921658000	2.110080000	1	5.650718000	0.815877000	2.092228000

1	5.573130000	-1.463848000	2.120862000	1	5.532439000	-1.563079000	2.116280000
1	5.578619000	-2.665366000	-0.000059000	1	5.520214000	-2.767759000	-0.000076000
1	5.573085000	-1.463835000	-2.120973000	1	5.532370000	-1.563112000	-2.116438000
1	5.649149000	0.921669000	-2.110183000	1	5.650651000	0.815842000	-2.092396000
1	5.714778000	2.136369000	-0.000051000	1	5.737394000	2.059501000	-0.000096000
5	-2.619757000	2.232618000	0.000042000	5	-2.616109000	2.276622000	0.000032000
5	0.313929000	2.941333000	0.000006000	5	0.341865000	2.974082000	-0.000017000
7	-0.042069000	4.341787000	-0.000040000	7	-0.103524000	4.339673000	-0.000053000
7	-0.271611000	5.446927000	-0.000115000	7	0.610918000	5.314276000	-0.000083000
1	1.003823000	6.389617000	-0.001002000	1	0.280269000	6.279906000	-0.000133000
				1	2.277552000	4.977201000	-0.000099000
NHNH@B_{As}_TS (-896.6 cm⁻¹)				NH₂NH@B_{As}_TS (-501.7 cm⁻¹)			
7	2.428312000	-2.429316000	1.248780000	7	2.408640000	-2.419792000	1.316362000
5	3.873181000	-2.349825000	1.194320000	5	3.853938000	-2.352528000	1.258057000
7	0.288914000	-1.439836000	2.104196000	7	0.278092000	-1.384708000	2.136813000
5	1.729655000	-1.403632000	2.012386000	5	1.718948000	-1.361326000	2.041905000
7	2.451685000	-0.195941000	2.384568000	7	2.448678000	-0.146131000	2.369501000
5	3.903379000	-0.252645000	2.348808000	5	3.900296000	-0.217896000	2.339920000
7	0.309148000	1.065439000	1.995088000	7	0.313828000	1.113825000	1.922283000
5	1.776608000	1.026025000	1.950525000	5	1.784860000	1.067032000	1.892156000
7	2.580681000	2.014124000	1.239674000	7	2.601124000	2.028918000	1.162869000
5	4.017592000	1.822298000	1.193070000	5	4.034125000	1.820228000	1.121026000
5	1.945524000	2.460479000	-0.000127000	5	1.957610000	2.456292000	-0.087047000
7	2.580704000	2.014329000	-1.240011000	7	2.597138000	1.945638000	-1.307427000
5	4.017597000	1.822385000	-1.193354000	5	4.030382000	1.741821000	-1.257180000
7	0.309153000	1.065378000	-1.995082000	7	0.308196000	0.989353000	-2.009974000
5	1.776624000	1.026042000	-1.950635000	5	1.778825000	0.942337000	-1.975805000
7	2.451687000	-0.195968000	-2.384541000	7	2.442374000	-0.299057000	-2.376715000
5	3.903386000	-0.252665000	-2.348834000	5	3.893889000	-0.368702000	-2.344920000
7	0.288920000	-1.439891000	-2.104145000	7	0.272474000	-1.517984000	-2.057298000
5	1.729661000	-1.403653000	-2.012310000	5	1.713562000	-1.490353000	-1.969132000
7	2.428323000	-2.429288000	-1.248661000	7	2.404917000	-2.500875000	-1.179074000
5	3.873194000	-2.349811000	-1.194199000	5	3.850355000	-2.430028000	-1.128999000
7	0.276303000	-2.789690000	0.000045000	7	0.252732000	-2.809329000	0.083181000
5	1.717709000	-2.671850000	0.000054000	5	1.695047000	-2.699520000	0.077337000
7	-1.869252000	-2.395158000	1.250300000	7	-1.887356000	-2.354872000	1.322729000
5	-0.427715000	-2.314210000	1.186058000	5	-0.445327000	-2.287181000	1.252549000
7	-4.018917000	-1.447232000	2.138394000	7	-4.026545000	-1.369473000	2.191805000
5	-2.571375000	-1.391543000	2.039607000	5	-2.579682000	-1.322333000	2.081877000
7	-1.853438000	-0.181201000	2.423458000	7	-1.854011000	-0.101621000	2.417635000
5	-0.410447000	-0.176274000	2.276452000	5	-0.411337000	-0.110601000	2.258829000
7	-4.043896000	1.034236000	2.127970000	7	-4.042678000	1.110422000	2.108834000
5	-2.593838000	1.007014000	2.029758000	5	-2.593634000	1.075978000	1.997447000
7	-1.904158000	2.027192000	1.263783000	7	-1.906410000	2.068009000	1.185298000
5	-0.456731000	2.039333000	1.236141000	5	-0.450063000	2.064865000	1.131589000
7	-4.061786000	2.320282000	0.000040000	7	-4.071810000	2.280776000	-0.080342000
7	-1.904105000	2.027084000	-1.263596000	7	-1.910614000	1.990347000	-1.337448000
5	-0.456694000	2.039191000	-1.236049000	5	-0.453381000	1.994754000	-1.283711000
7	-4.043862000	1.034235000	-2.127893000	7	-4.048559000	0.972382000	-2.189641000
5	-2.593813000	1.006983000	-2.029657000	5	-2.598993000	0.945702000	-2.079704000
7	-1.853432000	-0.181233000	-2.423412000	7	-1.860293000	-0.257953000	-2.419250000
5	-0.410444000	-0.176340000	-2.276421000	5	-0.417092000	-0.254618000	-2.262645000
7	-4.018920000	-1.447230000	-2.138295000	7	-4.032268000	-1.507319000	-2.101852000
5	-2.571378000	-1.391565000	-2.039527000	5	-2.585005000	-1.453051000	-1.999371000
7	-1.869252000	-2.395172000	-1.250216000	7	-1.890730000	-2.433404000	-1.175908000

5	-0.427712000	-2.314236000	-1.185976000	5	-0.448488000	-2.362104000	-1.115201000
7	-4.028861000	-2.714463000	0.000049000	7	-4.052030000	-2.689579000	0.085371000
5	-2.583129000	-2.621325000	0.000045000	5	-2.605236000	-2.612726000	0.081036000
7	4.546179000	-1.547426000	2.200026000	7	4.531944000	-1.522931000	2.237552000
7	4.642884000	0.984603000	2.198055000	7	4.653345000	1.004911000	2.147459000
7	4.722687000	2.264228000	-0.000122000	7	4.742614000	2.228296000	-0.083833000
7	4.642881000	0.984617000	-2.198297000	7	4.647053000	0.864057000	-2.232027000
7	4.546193000	-1.547419000	-2.199908000	7	4.526229000	-1.664620000	-2.161176000
7	4.547568000	-2.830863000	0.000058000	7	4.523406000	-2.876644000	0.079372000
5	-4.742795000	-0.211204000	2.383946000	5	-4.742684000	-0.125092000	2.413823000
5	-4.765985000	1.885860000	1.198107000	5	-4.772788000	1.908872000	1.140055000
5	-4.765964000	1.885849000	-1.198029000	5	-4.776081000	1.832389000	-1.273244000
5	-4.742774000	-0.211197000	-2.383893000	5	-4.749209000	-0.281036000	-2.406754000
5	-4.733923000	-2.302917000	-1.203903000	5	-4.754279000	-2.317865000	-1.132918000
5	-4.733912000	-2.302951000	1.204024000	5	-4.751125000	-2.241084000	1.279447000
1	-5.919442000	-0.222559000	2.568833000	1	-5.916186000	-0.125870000	2.616615000
1	-5.910109000	-2.461440000	1.303369000	1	-5.928677000	-2.385144000	1.384066000
1	-5.910128000	-2.461371000	-1.303228000	1	-5.932338000	-2.466680000	-1.224474000
1	-5.919415000	-0.222537000	-2.568811000	1	-5.923365000	-0.295535000	-2.605388000
1	-5.945366000	2.024326000	-1.292204000	1	-5.954741000	1.972671000	-1.370664000
1	-5.945388000	2.024336000	1.292265000	1	-5.951530000	2.052901000	1.230811000
1	5.647336000	0.874515000	2.108221000	1	5.656253000	0.880726000	2.059488000
1	5.556650000	-1.509510000	2.118676000	1	5.542887000	-1.496466000	2.157760000
1	5.554958000	-2.711555000	0.000065000	1	5.531571000	-2.764183000	0.074108000
1	5.556665000	-1.509504000	-2.118579000	1	5.537105000	-1.631396000	-2.082722000
1	5.647330000	0.874522000	-2.108428000	1	5.650739000	0.747659000	-2.142346000
1	5.721478000	2.087220000	-0.000120000	1	5.739758000	2.041532000	-0.079351000
5	-2.611252000	2.267735000	0.000076000	5	-2.623482000	2.220265000	-0.081224000
5	0.328863000	2.939363000	0.000049000	5	0.359495000	2.951028000	-0.107730000
7	-0.006354000	4.340700000	-0.000272000	7	-0.094147000	4.363865000	-0.112779000
7	0.562435000	5.407854000	-0.000207000	7	0.532127000	5.454329000	-0.086160000
1	-0.068119000	6.214556000	-0.000831000	1	0.801851000	6.143641000	1.883686000
1	-1.930875000	4.506607000	-0.000558000	1	-1.106646000	4.532821000	-0.124941000
				1	1.533877000	5.213877000	-0.077109000