

Supporting Information

Exploration of iron borides as electrochemical catalysts for nitrogen reduction reaction

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Section 1. Computational tests

Before running the calculations, cutoff energy and k-points have been tested, using FeB and FeB-N₂ as an example. The tested results are shown below:

	Cutoff energy test with K=1×1×1			K-point test with Cutoff energy=380 eV		
	380 eV	420 eV	450 eV	1×1×1	3×3×1	5×5×1
E(FeB) (eV)	-227.486	-227.464	-227.461	-227.486	-229.753	-229.696
E(FeB-N ₂) (eV)	-248.744	-248.746	-248.747	-248.744	-250.946	-250.892

Based on the tests, cutoff energy of 380 eV and k-space has been sampled with 3×3×1 as higher setting can only improve the reaction energy slightly (<0.06 eV).

Section 2. Space groups and lattice parameters for four Fe-B compounds

	Space Group	Lattice parameters	
FeB	Pnma	a= 4.00 Å b=5.41 Å; c= 2.95 Å(this work) $\alpha = \beta = \gamma = 90^\circ$ a=4.05 Å; b= 5.49 Å; c= 2.95 Å [1,2]	Note
FeB2	P6/mmm	a= b= 3.01 Å (this work) $\alpha = \beta = 90^\circ; \gamma = 120^\circ$ a=b=3.05 Å [2] a= b = 3.18 [3] a= b = 3.02 [4]	FeB+FeB2 mixed; AlB2-type
FeB6(α)	P6/mmm	a= b = 4.46 Å $\alpha = \beta = 90^\circ; \gamma = 88.05^\circ$ (this work) a= b = 4.45 Å [5] $\alpha = \beta = 90^\circ; \gamma = 88.05^\circ$	Jahn–Teller effect
FeB6(β)	P6/mmm	a=b=4.80 (this work) $\alpha = \beta = 90^\circ; \gamma = 120^\circ$ a=b=4.75 [6] $\alpha = \beta = 90^\circ; \gamma = 120^\circ$	

References:

- [1] Z. Kristallogr. 2006, 221, 477–481 (Experiments)
- [2] *Metal Science and Heat Treatment*. 2013, 55, 68–72. (Experiments)
- [3] Nano Lett. 2016, 16, 6124-6129 (Computational work)
- [4] Materials Project. (No. mp-569376) <https://materialsproject.org/materials/mp-569376/>
- [5] J. Am. Chem. Soc. 2016, 138, 5644–5651.
- [6] J. Mater. Chem. C, 2016, 4, 9613—9621.

Section 3. Tests for N₂ adsorption on four compounds. Calculated total energies are listed in unit of eV. The bold numbers are the total energies for most stable configurations.

Tested N₂ adsorption

	Fe-site	Fe-B sites	Fe-Fe sites	Enzymatic	Dissociative	B-Site
FeB-N ₂	-250.892	-248.611	-248.865	-248.074	-247.751	-249.241
FeB ₂ -N ₂	-202.791	-202.790*	-202.764	-201.796	-203.472	-200.332
FeB ₆ (α)-N ₂	-111.527	-111.408	Fe-Fe is too far	-110.833	-108.384	-109.484
FeB ₆ (β)-N ₂	-111.464	-111.241	Fe-Fe is too far	-111.194	-105.886	-110.546

* It changes to sole Fe-site adsorption.

Calculated N₂H dissociation on four compounds.

Catalysts	N ₂ H*	N*+NH*	deltaE(N ₂ H*→N*+NH*)
FeB	-253.486	-251.961	1.525
FeB ₂	-204.812	-207.208	-2.396
FeB ₆ (α)	-204.328	-202.481	1.847
FeB ₆ (β)	-111.655	-110.003	1.652

Section 4. Optimized geometries of intermediate states for NRR over FeB and FeB₂

FeB-N₂

FeB

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N
16	16	2

Direct

0.099082001	0.123988003	0.216748998
0.156790003	0.375999987	0.321002990
0.399646997	0.375845999	0.359100014
0.334643006	0.127841994	0.253030986
0.595624983	0.128560007	0.216481999
0.659142017	0.375465989	0.320706993
0.896109998	0.375903010	0.353872001
0.833307981	0.127298996	0.250367999
0.099118002	0.627067983	0.216768995
0.159118995	0.876092970	0.321204990
0.398624003	0.875706971	0.356276989
0.334652990	0.623579979	0.253060013
0.595618010	0.622617006	0.216484994
0.658738017	0.875446022	0.319867998
0.896992028	0.875715017	0.353850007
0.833329976	0.623947024	0.250366986
0.008607000	0.125642002	0.309311986
0.222923994	0.375642985	0.218208000
0.482634008	0.375613987	0.262683004
0.273443997	0.128610998	0.352901012
0.509130001	0.125404999	0.310169995
0.720992029	0.375562996	0.214589000
0.985091984	0.375690997	0.260650992
0.772283018	0.124618001	0.354211986
0.008645000	0.625760972	0.309271008
0.224805996	0.875606000	0.216774002
0.483206987	0.875575006	0.261413008
0.273335993	0.623404980	0.352990001
0.509214997	0.625868022	0.310209990
0.718932986	0.875588000	0.218308002
0.984547973	0.875651002	0.260843992
0.772217989	0.626761019	0.354313999
0.437159985	0.375670999	0.448709011
0.460045010	0.376168013	0.504028976

FeB-N2H

FeB

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	2	1

Direct

0.098531000	0.125376999	0.216820002
0.155615002	0.376457006	0.320672989
0.396097004	0.376026005	0.366349012
0.333303988	0.130244002	0.254940003
0.591969013	0.120411001	0.219667003
0.658770025	0.376217008	0.322663993
0.896687984	0.376107007	0.354274005
0.830669999	0.125637993	0.251284987
0.098569997	0.627089977	0.216822997
0.157122999	0.876049995	0.321289003
0.396176010	0.872823000	0.358644009
0.333241999	0.622227013	0.254947007
0.591938019	0.631994009	0.219670996
0.656138003	0.876146019	0.322632015
0.895784974	0.876376987	0.354043990
0.830649972	0.626818001	0.251282007
0.006913000	0.125729993	0.308943987
0.222848997	0.376347989	0.218596995
0.482829988	0.376246005	0.265437990
0.269872010	0.126748994	0.353000998
0.506729007	0.127197996	0.312655002
0.712929010	0.376239985	0.221773997
0.983088017	0.376367986	0.260224015
0.771723986	0.126001000	0.355984986
0.006816000	0.626721978	0.308932006
0.224286005	0.876227021	0.218484998
0.478073001	0.876276016	0.264120996
0.269908994	0.625588000	0.353222013
0.506677985	0.625051022	0.312698007
0.718915999	0.876242995	0.216216996
0.983319998	0.876209021	0.260740995
0.771827996	0.626416028	0.355883986
0.421858013	0.374837995	0.449014008
0.427311003	0.372693002	0.509396970
0.515053988	0.377732009	0.529217005

FeB-NHNH

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	2	2

Direct

0.095663004	0.154369995	0.222624004
0.157414004	0.410899013	0.326384008
0.401596993	0.391216010	0.362962991
0.330996990	0.154159993	0.255661994
0.593113005	0.154306993	0.218158007
0.654193997	0.407808989	0.322474003
0.890419006	0.402220011	0.358440012
0.830864012	0.154384002	0.254673004
0.094844997	0.654004991	0.222027004
0.157386005	0.897499025	0.326391011
0.401472986	0.917021990	0.362978011
0.329901010	0.654034972	0.257784009
0.592576027	0.654223025	0.218560994
0.654182017	0.900843024	0.322461993
0.890453994	0.906522989	0.358464986
0.831351995	0.654340982	0.254442990
0.006692000	0.154277995	0.315095007
0.220328003	0.404626995	0.221367002
0.478715003	0.407151014	0.264665991
0.270857990	0.154149994	0.353549987
0.507344007	0.154257998	0.309289992
0.717473984	0.403580010	0.220605999
0.982553005	0.404038996	0.266728014
0.764545023	0.154385999	0.357849985
0.004822000	0.654309988	0.315494001
0.220111996	0.903654993	0.221579000
0.478675991	0.901126027	0.264687985
0.282687008	0.654102027	0.358202010
0.499879003	0.654202998	0.315281004
0.717424989	0.905035019	0.220615000
0.982635021	0.904509008	0.266705006
0.767104983	0.654327989	0.358067989
0.451747000	0.265498012	0.445964009
0.451400995	0.042390000	0.446056992
0.495299011	0.969371021	0.486230999
0.496812999	0.338378996	0.485864997

FeB-NNH2

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	2	2

Direct

0.107326001	0.125227004	0.218647003
0.165530995	0.374862999	0.322007000
0.407649010	0.374902993	0.368598014
0.341751993	0.128191993	0.256381005
0.600585997	0.118308000	0.219301000
0.668896019	0.374565989	0.321794003
0.905430973	0.374392003	0.354911000
0.840213001	0.123595998	0.251450002
0.107395001	0.624471009	0.218563005
0.166906998	0.874577999	0.323372006
0.406544000	0.874844015	0.359943986
0.341937989	0.621538997	0.256375998
0.600580990	0.631527007	0.219313994
0.665130973	0.875473022	0.322982997
0.903630018	0.875479996	0.354799002
0.840022981	0.626219988	0.251563996
0.016403001	0.124369003	0.310618997
0.232274994	0.374890000	0.219634995
0.492231011	0.374972999	0.265747011
0.280423999	0.126580000	0.354797989
0.516270995	0.126212001	0.312669992
0.722276986	0.374980003	0.221992999
0.991841972	0.375003010	0.261638999
0.779760003	0.125516996	0.356693000
0.016155001	0.625310004	0.310665011
0.232302994	0.874835014	0.220135003
0.486797005	0.874715984	0.264697999
0.280712008	0.622587979	0.354939997
0.516364992	0.623728991	0.312844992
0.728079975	0.874804974	0.216372997
0.993203998	0.874776006	0.262293994
0.780156016	0.624489009	0.355924010
0.426613986	0.372860014	0.454694003
0.359604001	0.389721006	0.507317007
0.265617013	0.412501991	0.504734993
0.400316000	0.380194992	0.553363979

FeB-NHNH2

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	2	3

Direct

0.101081997	0.120151997	0.221663997
0.162028998	0.371753007	0.324800014
0.407413006	0.374673009	0.362437993
0.336867005	0.122706003	0.255584002
0.597676992	0.127753004	0.217584997
0.661596000	0.373163998	0.321806997
0.896826029	0.373546004	0.357468992
0.837181985	0.126376003	0.252995014
0.100869000	0.627771020	0.221454993
0.162266999	0.876350999	0.325946003
0.403672993	0.873803020	0.359272987
0.337336987	0.624355972	0.254920006
0.599237025	0.620480001	0.217810005
0.661217988	0.875096023	0.321709007
0.897579014	0.874687016	0.357405007
0.836952984	0.622380972	0.253565997
0.010958000	0.124352999	0.314043999
0.224102005	0.373768985	0.223300993
0.484553993	0.373712003	0.263401985
0.279680014	0.128479004	0.357066005
0.511982977	0.125360996	0.311010003
0.725302994	0.374559999	0.217225999
0.988615990	0.374251992	0.265280008
0.772130013	0.123498999	0.357937992
0.011199000	0.623717010	0.314141005
0.227472007	0.873861015	0.218419001
0.487733990	0.873947024	0.263334006
0.278488994	0.620540023	0.353349000
0.512802005	0.623944998	0.310838997
0.722571015	0.873812020	0.221015006
0.986748993	0.873854995	0.265505999
0.772682011	0.625024021	0.356837988
0.454656005	0.406994998	0.449274004
0.394419014	0.335420996	0.506130993
0.305620015	0.292373002	0.494531006
0.398528993	0.448136985	0.545002997
0.536529005	0.483527005	0.460815996

FeB-NH2NH2

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	2	4

Direct

0.085437000	0.140604004	0.224924996
0.147648007	0.393332988	0.328298986
0.391158015	0.394333988	0.361826003
0.321884990	0.145636007	0.257382989
0.584456980	0.145744994	0.219727993
0.647189975	0.392910004	0.323226988
0.880917013	0.394163013	0.360592008
0.822251976	0.144554004	0.256238014
0.085616998	0.646443009	0.224972993
0.148425996	0.893383026	0.328981996
0.388359994	0.892723024	0.359064013
0.322223008	0.641059995	0.257346004
0.584612012	0.640893996	0.219859004
0.645891011	0.893360019	0.324678004
0.881280005	0.892603993	0.360446006
0.822251022	0.641930997	0.256265998
0.995884001	0.143640995	0.317539990
0.208414003	0.393381000	0.224409997
0.470894009	0.393359005	0.265747011
0.265105993	0.146705002	0.359495014
0.497905999	0.143546999	0.313407004
0.710328996	0.393150002	0.220586002
0.973178029	0.393355012	0.268611997
0.756877005	0.143095002	0.359856009
0.996268988	0.643157005	0.317440987
0.211652994	0.893423021	0.222532004
0.472541004	0.893230975	0.265091002
0.264746010	0.640376985	0.360002011
0.498365015	0.643396020	0.313717991
0.708050013	0.893441021	0.223844007
0.971853018	0.893441021	0.268902987
0.755891025	0.643483996	0.360642999
0.459475011	0.396723002	0.457138985
0.496463001	0.180666000	0.488555998
0.418280989	0.081811003	0.484508008
0.556595981	0.110459000	0.454133004
0.537693977	0.495460004	0.456966996
0.399610996	0.472171992	0.489989996

FeB-N

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N
16	16	1

Direct

0.100511000	0.122534998	0.216279998
0.163140997	0.375546008	0.319561005
0.406037003	0.375389010	0.366584986
0.335364997	0.122813001	0.251354009
0.595521986	0.119066998	0.217603996
0.660800993	0.375512004	0.321397990
0.898998022	0.375663012	0.352654994
0.834231973	0.123741999	0.249309003
0.100458004	0.628247023	0.216236994
0.162106007	0.875231028	0.320089012
0.402267009	0.875572979	0.357769012
0.335303009	0.627848029	0.251408011
0.595596015	0.631950974	0.217620999
0.658451021	0.875626028	0.320648998
0.897904992	0.875458002	0.351929009
0.834218979	0.627400994	0.249289006
0.010844000	0.125485003	0.307940006
0.225091994	0.375369012	0.218710005
0.483971000	0.378845990	0.260704011
0.277561009	0.126389995	0.350423008
0.506974995	0.128040001	0.309150994
0.716723979	0.375582993	0.221397996
0.986923993	0.375443012	0.259335011
0.773549974	0.125345007	0.353617996
0.010800000	0.625411987	0.307895988
0.227421999	0.875322998	0.213189006
0.481604010	0.875643015	0.261996001
0.277610987	0.624260008	0.350609004
0.506963015	0.622664988	0.309210002
0.723267972	0.875581980	0.213108003
0.986048996	0.875523984	0.259656012
0.773441017	0.625774980	0.353615999
0.449178010	0.375452995	0.440135986

FeB-NH

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	1	1

Direct

0.101538002	0.124429002	0.215307996
0.161440000	0.374725014	0.318545997
0.399836987	0.376672000	0.367350996
0.336971998	0.126369998	0.251976997
0.596184015	0.119012997	0.216938004
0.662567973	0.375034004	0.319788992
0.900484025	0.375384986	0.351985991
0.835393012	0.122639000	0.248576999
0.101632997	0.625977993	0.215381995
0.162202001	0.875808001	0.319175005
0.401611000	0.874414980	0.357387990
0.336970001	0.624239028	0.251922011
0.596313000	0.631280005	0.216940001
0.659377992	0.875274003	0.320719987
0.899480999	0.874942005	0.351841003
0.835471988	0.627649009	0.248541996
0.011332000	0.124955997	0.307503998
0.226523995	0.371834010	0.216739997
0.486474007	0.375144988	0.261736989
0.276403010	0.125916004	0.350207001
0.509482026	0.128984004	0.309785008
0.717772007	0.375102997	0.219812006
0.986752987	0.375178993	0.258534014
0.775250971	0.125117004	0.352851987
0.011575000	0.625416994	0.307487994
0.227603003	0.875280976	0.214873999
0.483303994	0.875274003	0.262681007
0.275485009	0.624718010	0.350071013
0.509769976	0.621357977	0.309637010
0.723084986	0.875196993	0.213042006
0.987425983	0.875160992	0.258971006
0.775038004	0.625172019	0.353040993
0.404193997	0.381054997	0.450533003
0.343692005	0.389201999	0.489239991

FeB-NH2

1.0

10.8163995743	0.0000000000	0.0000000000
0.0000000000	5.8972001076	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
16	16	1	2

Direct

0.099152997	0.120787002	0.215849996
0.157795995	0.374060988	0.319359988
0.401872009	0.375961006	0.364602000
0.332814008	0.125195995	0.253724009
0.590267003	0.127412006	0.216718003
0.657480001	0.375519007	0.319846004
0.894169986	0.376552999	0.351727009
0.830488026	0.127324998	0.248377994
0.099110998	0.629369020	0.215939000
0.157868996	0.876160979	0.320867002
0.397592008	0.874414027	0.359847009
0.332709998	0.624916971	0.253681004
0.590521991	0.622729003	0.216665998
0.657012999	0.874732971	0.319382012
0.894303977	0.873579979	0.351696014
0.830578029	0.622705996	0.248346999
0.006721000	0.125434995	0.307460010
0.222128004	0.375090986	0.218282998
0.479012012	0.375027001	0.263301015
0.273514003	0.128603995	0.352232993
0.506792009	0.126877993	0.311199009
0.715699971	0.374823004	0.214532003
0.984768987	0.374927014	0.258612007
0.770501018	0.124949001	0.352854013
0.007570000	0.624719977	0.307240993
0.226554006	0.875083029	0.214636996
0.480504990	0.875102997	0.263913006
0.272756010	0.621502995	0.351612002
0.506877005	0.623355985	0.310923994
0.713882029	0.875379026	0.218134999
0.983199000	0.875281990	0.259283990
0.769200981	0.625522017	0.354645997
0.440627009	0.382243991	0.454268992
0.375743985	0.384308010	0.491167992
0.527848005	0.394612014	0.471067995

FeB2-N2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N
9	18	2

Direct

0.000567000	0.000842000	0.404238999
0.365200013	0.031567000	0.431297988
0.666601002	0.031909999	0.431230009
0.968870997	0.333003014	0.432101995
0.363918006	0.332938999	0.432289004
0.666752994	0.333896011	0.421348989
0.969112992	0.635182023	0.431484997
0.332643986	0.665466011	0.404688001
0.666384995	0.635312021	0.431281000
0.113342002	0.226763994	0.442133993
0.210921004	0.104891002	0.454216003
0.451234996	0.223174006	0.494603008
0.559252024	0.118357003	0.494985998
0.773423016	0.225875005	0.494874001
0.894092977	0.104969002	0.454061002
0.122385003	0.561092973	0.454602003
0.219609007	0.439256012	0.442191005
0.438854992	0.561249971	0.454468995
0.559683025	0.440546006	0.494080991
0.774071991	0.548097014	0.493842989
0.880895972	0.440326989	0.494369000
0.113756999	0.886318982	0.440486997
0.220042005	0.780288994	0.441078007
0.438919991	0.877604008	0.453642011
0.560500979	0.780497015	0.440815002
0.772799015	0.886533022	0.440358996
0.894712985	0.789309025	0.453267008
0.666393995	0.331968993	0.328357995
0.666592002	0.332663000	0.271643996

FeB2-N2H

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	2	1

Direct

0.998694003	0.000655000	0.406803012
0.364093006	0.030673999	0.431697994
0.666651011	0.029468000	0.433256000
0.969152987	0.332040995	0.433174014
0.362740010	0.333297998	0.433932006
0.667505980	0.333608001	0.397964001
0.968235016	0.634806991	0.431448996
0.333898991	0.665493011	0.406998992
0.665392995	0.636196017	0.432958007
0.112999000	0.226278007	0.443497986
0.211133003	0.104790002	0.455572009
0.451025993	0.225070000	0.494132996
0.558317006	0.118065000	0.494222999
0.773054004	0.225966007	0.494361997
0.893679976	0.105063997	0.457352996
0.121168002	0.560769022	0.455552012
0.219170004	0.439357013	0.443179995
0.438481003	0.560267985	0.457253993
0.559072018	0.439857990	0.494004995
0.773950994	0.547828019	0.493912995
0.881395996	0.440968007	0.494244993
0.112942003	0.885958016	0.440521002
0.219275996	0.779645979	0.440789014
0.438152999	0.877830029	0.455839008
0.559578001	0.779758990	0.443664998
0.772719026	0.885948002	0.443192989
0.894110024	0.787833989	0.455199003
0.682458997	0.345322013	0.314336002
0.712100983	0.369053990	0.254981011
0.615670979	0.289669991	0.222714007

FeB2-NHNH

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	2	2

Direct

0.960491002	0.981303990	0.418583006
0.370086014	0.027136000	0.418978989
0.671384990	0.009029000	0.460224986
0.961376011	0.323302001	0.408574998
0.376300991	0.347184002	0.409404010
0.668829978	0.334307998	0.427349001
0.970308006	0.646945000	0.418258995
0.380488008	0.693584979	0.415176988
0.667069972	0.664736986	0.457846999
0.116714001	0.229877993	0.417320013
0.210523993	0.108268000	0.421730012
0.437794000	0.223463997	0.478228003
0.550140977	0.120755002	0.485799015
0.799390018	0.243480995	0.486925989
0.913228989	0.131644994	0.467730999
0.129537001	0.565476000	0.415600002
0.222736001	0.444117993	0.411738008
0.425399989	0.542733014	0.464394003
0.540661991	0.430792987	0.485466987
0.786366999	0.550806999	0.482798010
0.901610017	0.449755996	0.476615012
0.117040999	0.892408013	0.428153008
0.222287998	0.780062973	0.427239001
0.430056006	0.885685980	0.470743001
0.545678020	0.774846017	0.487237990
0.791311979	0.896987021	0.488514006
0.907863975	0.784790993	0.471266001
0.666359007	0.353814006	0.333431989
0.636964977	0.245006993	0.286565006
0.653214991	0.304484010	0.240517005
0.702183008	0.477396995	0.318747997

FeB2-NNH2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	2	2

Direct

0.998999000	0.998064995	0.406181991
0.363404006	0.030439001	0.429280996
0.667101026	0.030406000	0.429280013
0.968909025	0.333303005	0.428961992
0.364452004	0.333332002	0.428905010
0.666575015	0.333092004	0.408457011
0.970003009	0.636125982	0.429199010
0.334452003	0.668775022	0.406397015
0.666161001	0.636155009	0.429277003
0.113785997	0.227509007	0.439312994
0.212469995	0.106868997	0.453657001
0.454712003	0.227519006	0.492101014
0.560585022	0.121136002	0.492255002
0.772840023	0.227521002	0.492114991
0.894442976	0.106882997	0.453729987
0.120862998	0.559741974	0.453777999
0.219624996	0.439199001	0.439348012
0.438908011	0.559688985	0.453824013
0.560486019	0.439166993	0.492101014
0.772780001	0.545485020	0.492150009
0.878717005	0.439186990	0.492096990
0.113485999	0.886139989	0.441132009
0.219825000	0.780498981	0.441361994
0.440429002	0.880809009	0.455058008
0.560727000	0.780512989	0.441435009
0.772718012	0.886152983	0.441233993
0.893009007	0.785889030	0.454728991
0.666310012	0.332046002	0.325466007
0.665865004	0.330487013	0.260919005
0.610216022	0.217665002	0.235550001
0.721606016	0.442270994	0.233855993

FeB2-NHNH2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	2	3

Direct

0.990544975	0.981257975	0.406798005
0.357836008	0.024072999	0.432197988
0.661073983	0.025345000	0.429998994
0.966454983	0.341937989	0.410356998
0.371050000	0.340288013	0.411962003
0.670418978	0.345364004	0.419586986
0.972033024	0.655689001	0.440847993
0.339428991	0.689357996	0.405943006
0.679538012	0.654142022	0.437799007
0.113578998	0.230848998	0.414559990
0.214995995	0.119052999	0.441846997
0.445131004	0.233014002	0.483601987
0.563403010	0.129372999	0.485139012
0.784488022	0.232493997	0.482858002
0.899380028	0.118574001	0.438937992
0.117209002	0.559504986	0.446330011
0.220669001	0.445165008	0.418655008
0.438686013	0.561639011	0.443114012
0.546312988	0.441035986	0.486736000
0.765293002	0.536327004	0.492922008
0.890761971	0.439244986	0.486761004
0.117505997	0.898813009	0.455565989
0.218484998	0.782209992	0.451745987
0.440935999	0.884398997	0.463117987
0.559435010	0.781801999	0.447234005
0.775933981	0.898104012	0.451710999
0.897623003	0.802320004	0.472764999
0.698252976	0.384122998	0.328761011
0.631699979	0.278889000	0.274794996
0.585354984	0.154756993	0.288246989
0.704984009	0.316062003	0.232563004
0.762320995	0.509061992	0.313109010

FeB2-NH2NH2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	2	4

Direct

0.956216991	0.971175015	0.400225013
0.359676987	0.039027002	0.433108002
0.650403023	0.003288000	0.429726005
0.939480007	0.327176005	0.397588015
0.354626000	0.346967012	0.414730996
0.637324989	0.347658992	0.492572010
0.963348985	0.655638993	0.417290986
0.352153003	0.682927012	0.401582003
0.646565020	0.628633976	0.470115006
0.095559999	0.223578006	0.404938996
0.194034994	0.111929998	0.429538012
0.377891988	0.212543994	0.493921995
0.553506970	0.104652002	0.489450008
0.766470015	0.229893997	0.470218986
0.886565983	0.116756000	0.440499008
0.108329996	0.560500026	0.419829994
0.200086996	0.438098013	0.406370997
0.400967002	0.548575997	0.463813007
0.454430997	0.416406989	0.508876026
0.828217030	0.586843014	0.498867005
0.883849978	0.445726007	0.469280005
0.111239001	0.896884978	0.429646999
0.214774996	0.784074008	0.425787002
0.421757996	0.878051996	0.460857987
0.541788995	0.770223975	0.462904990
0.763347030	0.882604003	0.460373998
0.891795993	0.791383982	0.468149006
0.747412980	0.329991013	0.329919994
0.739347994	0.333431989	0.256945997
0.742935002	0.228385001	0.239552006
0.851466000	0.434017003	0.240859002
0.730009973	0.428822011	0.346285999
0.631615996	0.228504002	0.345853001

FeB2-N

FeB2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N
9	18	1

Direct

0.983170986	0.966647983	0.427170992
0.374933988	0.024754999	0.438901007
0.649478018	0.024561999	0.439121991
0.964865983	0.323345006	0.435826004
0.358215988	0.322849005	0.435647994
0.669978976	0.339915991	0.418071002
0.949965000	0.630599976	0.419014990
0.312539011	0.624539971	0.382618010
0.681012988	0.630711973	0.419070989
0.104580000	0.209501997	0.451409012
0.211870000	0.093332000	0.465689987
0.451570988	0.229670003	0.498275012
0.567690015	0.135752007	0.502601027
0.778002977	0.229663998	0.498268992
0.881394029	0.093617000	0.465788990
0.116609998	0.557901978	0.439159989
0.213975996	0.427477002	0.442016006
0.441747993	0.557422996	0.439031005
0.570580006	0.447248995	0.492527008
0.784662008	0.569337010	0.511781991
0.876348019	0.447041988	0.492655009
0.123954996	0.872807026	0.453467011
0.217819005	0.770826995	0.418190002
0.431944013	0.863780975	0.398299009
0.552949011	0.770682991	0.418505013
0.748806000	0.872879028	0.453597009
0.883659005	0.766292989	0.484048992
0.764084995	0.528066993	0.363074988

FeB2-NH

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	1	1

Direct

0.028306000	0.056634001	0.387288004
0.383929014	0.044436999	0.412337989
0.660564005	0.044440001	0.412328005
0.979875982	0.341904998	0.443147004
0.362118989	0.341769993	0.443233997
0.659802020	0.319518000	0.437328994
0.963725984	0.644055009	0.426764995
0.343017012	0.685698986	0.425482005
0.680399001	0.644116998	0.426753998
0.117366999	0.234611005	0.453992009
0.218437001	0.105301999	0.444986999
0.441119999	0.207001999	0.493346006
0.550446987	0.100610003	0.507830024
0.766058981	0.206909001	0.493301004
0.887031019	0.105364002	0.444961995
0.119125001	0.577881992	0.467290014
0.228294000	0.456463009	0.461400986
0.458878011	0.577908993	0.467343986
0.564374030	0.452342987	0.493972003
0.773954988	0.547719002	0.493185997
0.887821019	0.452154011	0.493916005
0.120637998	0.900977015	0.410016000
0.215298995	0.797412992	0.441947013
0.452105999	0.904175997	0.472344011
0.582249999	0.797416985	0.441958994
0.780534029	0.901090980	0.409992993
0.907001019	0.813929021	0.394733995
0.585651994	0.171185002	0.362428993
0.604961991	0.209531993	0.313475013

FeB2-NH2

1.0

9.0576000214	0.0000000000	0.0000000000
-4.5288000107	7.8441117158	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Fe	B	N	H
9	18	1	2

Direct

0.016027000	0.980715990	0.409476012
0.373122007	0.016347000	0.446541011
0.668289006	0.020914000	0.434789985
0.979077995	0.336997986	0.416832000
0.389737993	0.329807997	0.408526003
0.672438979	0.330707997	0.410200000
0.993228972	0.653636992	0.440564007
0.352452993	0.691901028	0.409828991
0.693005025	0.647231996	0.435259014
0.129427999	0.228346005	0.417791009
0.234944001	0.119079001	0.450578004
0.461059004	0.233992994	0.490245014
0.584087014	0.131725997	0.494964987
0.798286021	0.228284001	0.487619996
0.910727978	0.110390998	0.438555986
0.133337006	0.553547978	0.450042993
0.236397997	0.442250997	0.416768014
0.453085989	0.556313992	0.435885996
0.567497015	0.439433008	0.486856997
0.785614014	0.541592002	0.491984010
0.900892019	0.438015997	0.488005996
0.131155998	0.893836975	0.463331997
0.233031005	0.774177015	0.464356989
0.455801994	0.872770011	0.474693000
0.573988974	0.775141001	0.449716985
0.790161014	0.893061996	0.446765006
0.908443987	0.793936014	0.471280992
0.526975989	0.319032997	0.333620995
0.472155005	0.205179006	0.309163004
0.565312028	0.415780991	0.299744993