

SUPPORTING INFORMATION

Density Functional Theory Study of Single Metal Atoms Embedded into MBenes for Electrocatalytic Conversion of N₂ to NH₃

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Supplementary Materials

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ADDITIONAL COMPUTATIONAL DETAILS

Settings PBE/DFT-D₃ optimisation

```

SYSTEM = MBene
ISTATRT = 0
ICHARG = 2
ENCUT = 450
ISMEAR = 0
SIGMA = 0.05
EDIFFG = -5E-02
ISIF = 2
LREAL = Auto
GGA = PBE
PREC = M
ALGO = Fast

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NSW = 200
IBRION = 2
POTIM = 0.02
EDIFF = 1E-05

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ISPIN = 2
IVDW=11

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LVDW = 11, zero damping DFT-D3 method of Grimme.

Pseudo-potentials applied:

Nitrogen: PAW_PBE N 08Apr2002

Technetium: PAW_PBE Tc_pv 04Feb2005

Hydrogen: PAW_PBE H 15Jun2001

Ruthenium: PAW_PBE Ru_pv 28Jan2005

Oxygen: PAW_PBE O 08Apr2002

Rhodium: PAW_PBE Rh_pv 25Jan2005

Titanium: PAW_PBE Ti_pv 07Sep2000

Palladium: PAW_PBE Pd_pv 28Jan2005

Vanadium: PAW_PBE V_pv 07Sep2000

Silver: PAW_PBE Ag_pv 09Dec2005

Chromium: PAW_PBE Cr_pv02Aug2007

Hafnium: PAW_PBE Hf_pv 06Sep2000

Manganese: PAW_PBE Mn_pv 02Aug2007

Tantalum: PAW_PBE Ta_pv 07Sep2000

Iron: PAW_PBE Fe_pv 02Aug2007

Tungsten: PAW_PBE W_sv 04Sep2015

Cobalt: PAW_PBE Co_pv 23Apr2009

Rhenium: PAW_PBE Re_pv 06Sep2000

Nickel: PAW_PBE Ni_pv 06Sep2000

Copper: PAW_PBE Cu_pv 06Sep2000

Zirconium: PAW_Zr_sv_GW 07Apr2010

Niobium: PAW_PBE Nb_pv 08Apr2002

Molybdenum: PAW_PBE Mo_pv 04Feb2005

Osmium: PAW_PBE Os_pv 20Jan2003

Iridium: PAW_PBE Ir 06Sep2000

Platinum: PAW_PBE Pt_pv 12Dec2005

Gold: PAW_PBE Au 04Oct2007

Table S1. The calculated E_{ZPE} and $-TS$ of the different adsorption species on $\text{Mo}_2\text{B}_2\text{O}_2$ - Re_{SA} and $-\text{Os}_{\text{SA}}$ ($T=298.15 \text{ K}$), where the * denotes the adsorption site.

Adsorption Species	$\text{Mo}_2\text{B}_2\text{O}_2\text{-Re}_{\text{SA}}$		$\text{Mo}_2\text{B}_2\text{O}_2\text{-Os}_{\text{SA}}$	
	E_{ZPE} (eV)	$-TS$ (eV)	E_{ZPE} (eV)	$-TS$ (eV)
N_2	0.16	-0.57	0.16	-0.57
* N_2	0.21	-0.14	0.21	-0.15
* N-NH	0.52	-0.11	0.52	-0.11
* N-NH_2	0.86	-0.11	0.86	-0.11
* N-NH_3	1.19	-0.09	1.06	-0.09
* $\text{NH}\cdot\text{NH}_3$	1.45	-0.10	1.36	-0.15
* NH_2	0.74	-0.05	0.74	-0.05
* NH_3	1.05	-0.09	1.06	-0.09
* NH-NH	0.83	-0.13	0.83	-0.12
* NH-NH_2	1.15	-0.12	1.17	-0.12
* $\text{NH}_2\text{-NH}_2$	1.55	-0.10	1.55	-0.09
* $\text{NH}_2\cdot\text{NH}_3$	1.68	-0.19	1.67	-0.19
H_2	0.28	-0.39	0.28	-0.39
NH_3	0.93	-0.58	0.93	-0.58

Table S2. The calculated valence states (electrons) of SA and the adjacent Mo atom in $\text{Mo}_2\text{B}_2\text{O}_2$ -SA systems.

metal atom	SA site	Mo site
Ti	1.39	1.02
V	1.21	1.05
Cr	0.99	1.05
Mn	0.77	1.05
Fe	0.54	1.02
Zr	1.63	0.95
Nb	1.55	1.02
Mo	1.04	1.04
Tc	0.65	1.07
Ru	0.29	1.04
Rh	0.08	1.04
Hf	1.65	0.97
Ta	1.51	1.02
W	1.18	1.05
Re	0.73	1.08
Os	0.24	1.08
Ir	-0.02	1.06
Pt	-0.06	1.06

Table S3. The E_{form} s of dominant SAs embedded in $\text{Mo}_2\text{B}_2\text{O}_2$ in activity screening, where Mo system indicates the pristine $\text{Mo}_2\text{B}_2\text{O}_2$ with one oxygen vacancy.

metal atom	Mo	Tc	Ru	Hf	Ta
E_{form} (eV)	0	+0.81	+2.95	-1.69	-0.83
metal atom	W	Re	Os	Ir	
E_{form} (eV)	-0.03	+0.50	+1.29	+0.93	

ADSORPTION MODELS

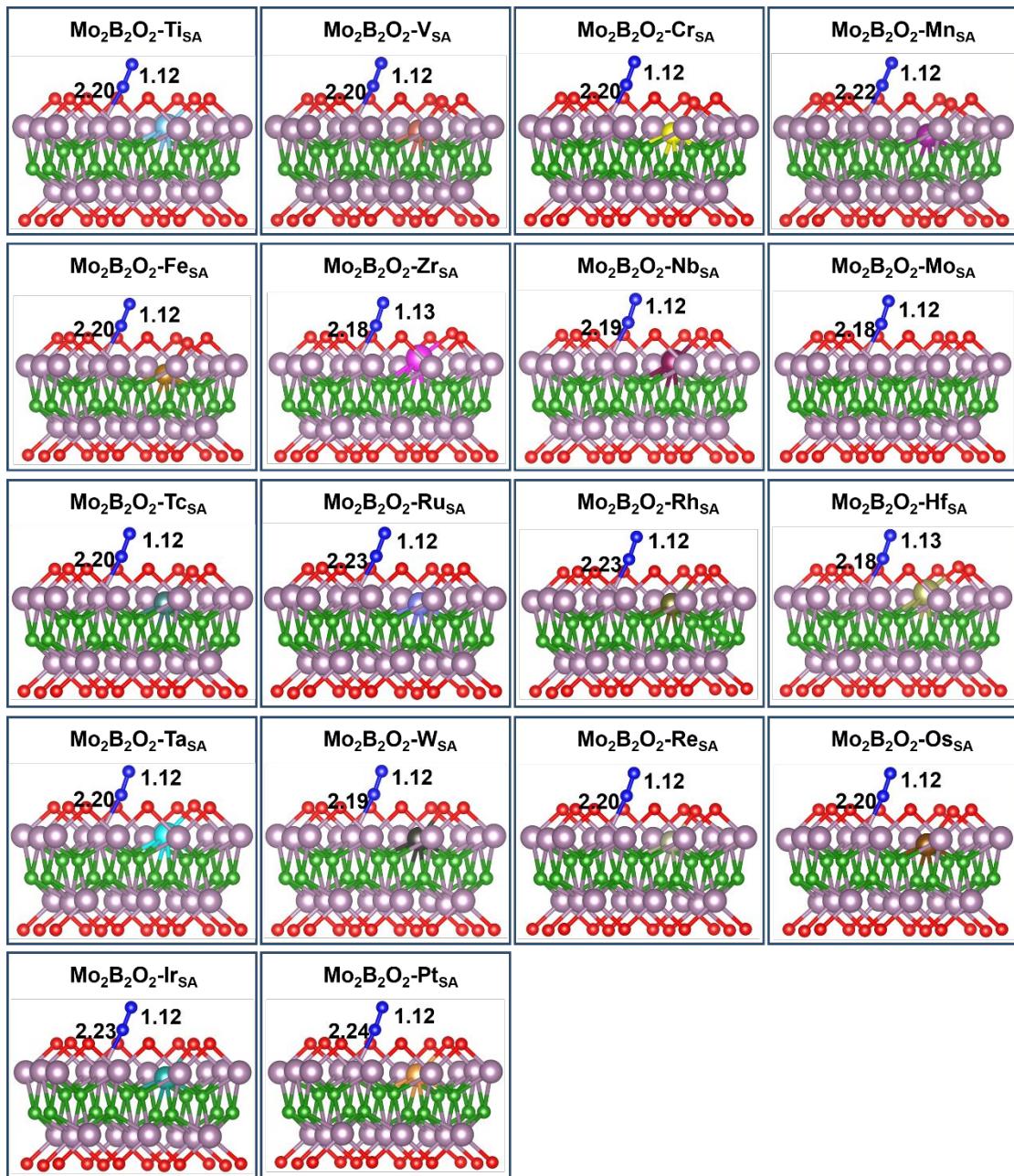


Figure S1. The N₂ adsorption models on Mo site of MBene embedded different SAs.

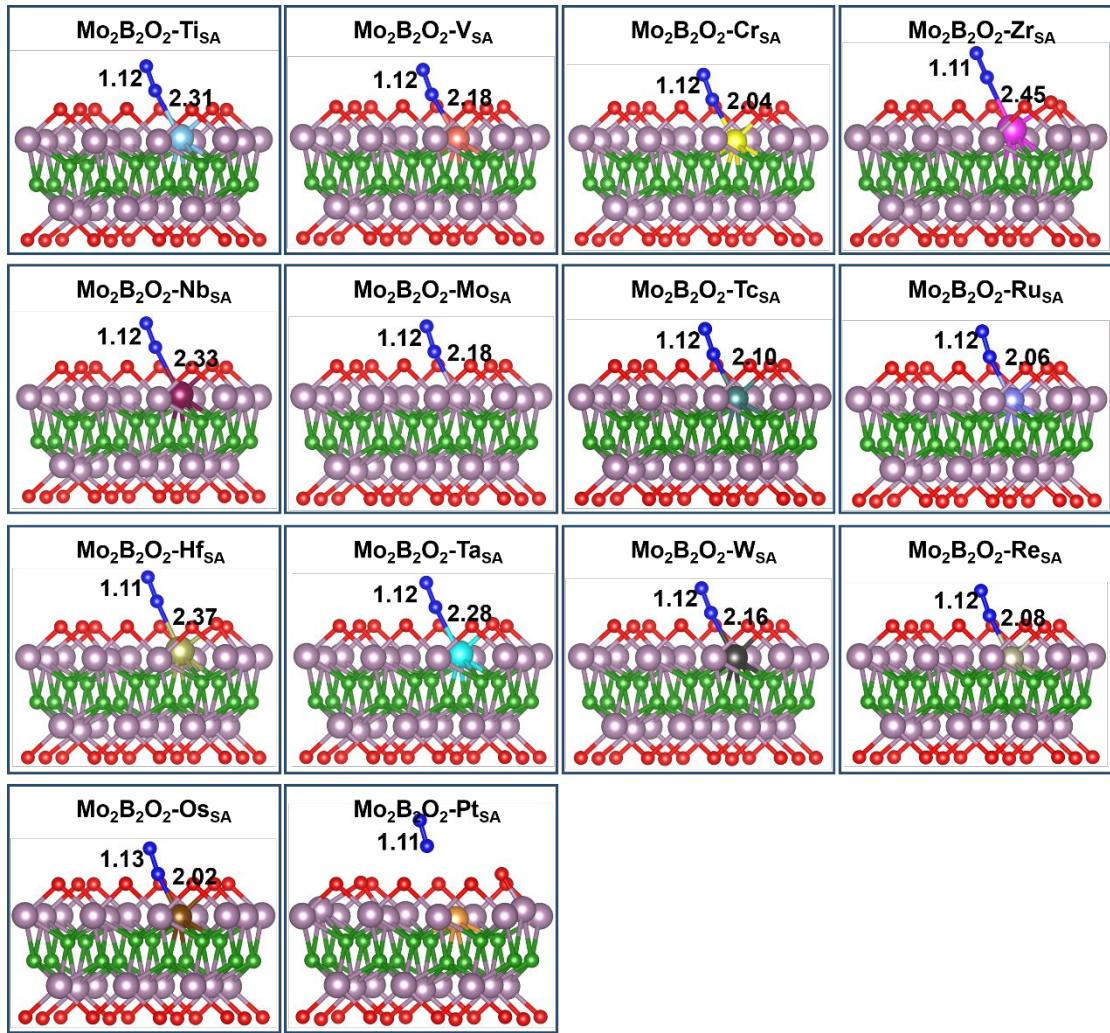


Figure S2. The N_2 adsorption models on SA site of MBene embedded different SAs.

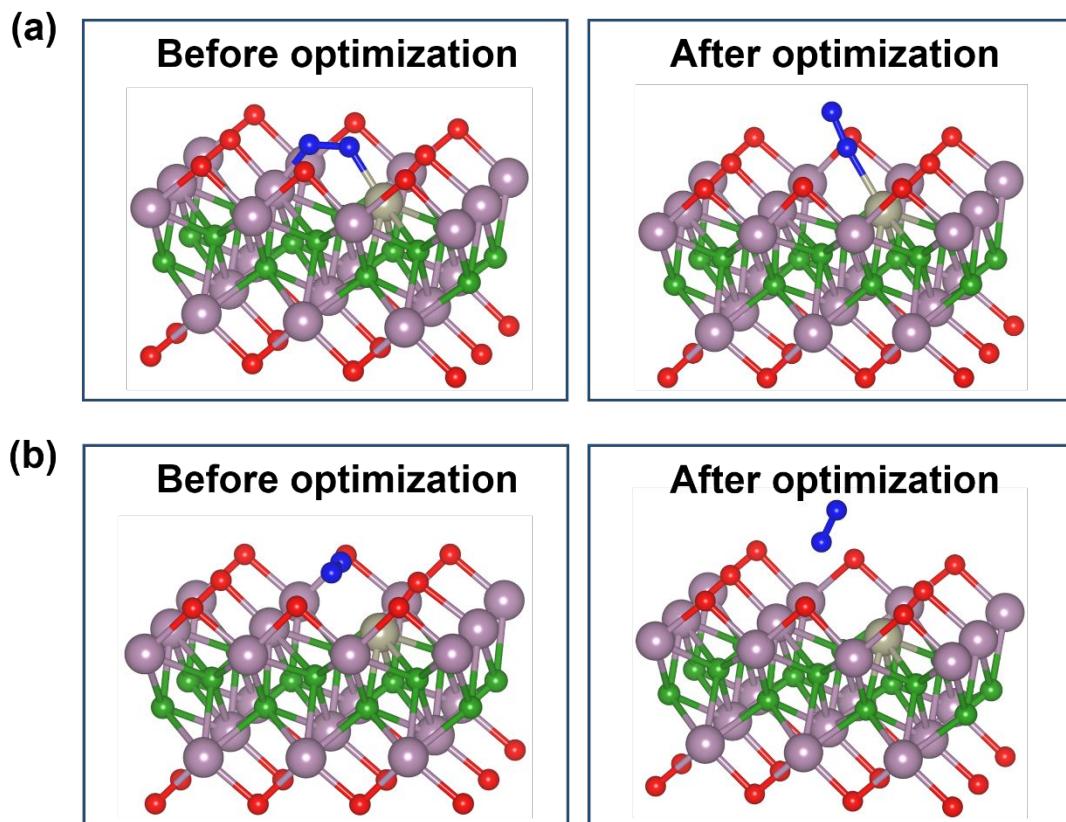


Figure S3. The initial tentative two side-on adsorption models, taking $\text{Mo}_2\text{B}_2\text{O}_2\text{-Re}_{\text{SA}}$ as an example. (a) and (b) correspond to the N_2 with horizontal and vertical direction, respectively.

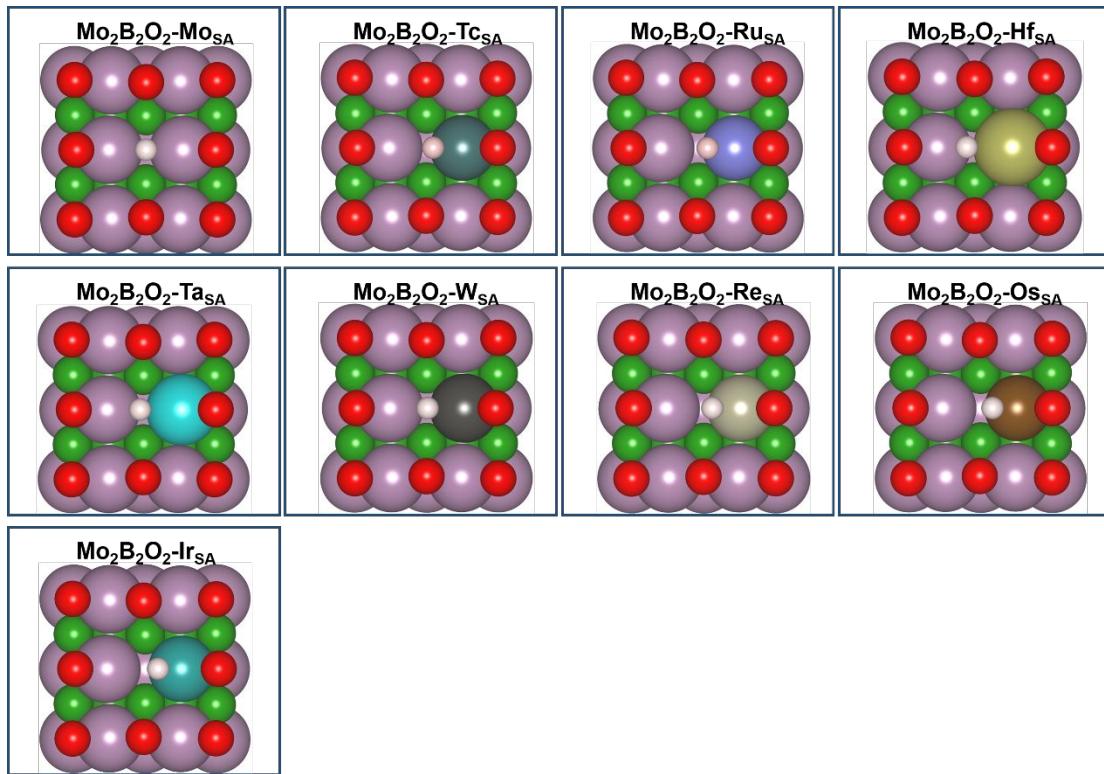


Figure S4. The H adsorption models on the bridge site of Mo-SA cluster embedded in MBene.

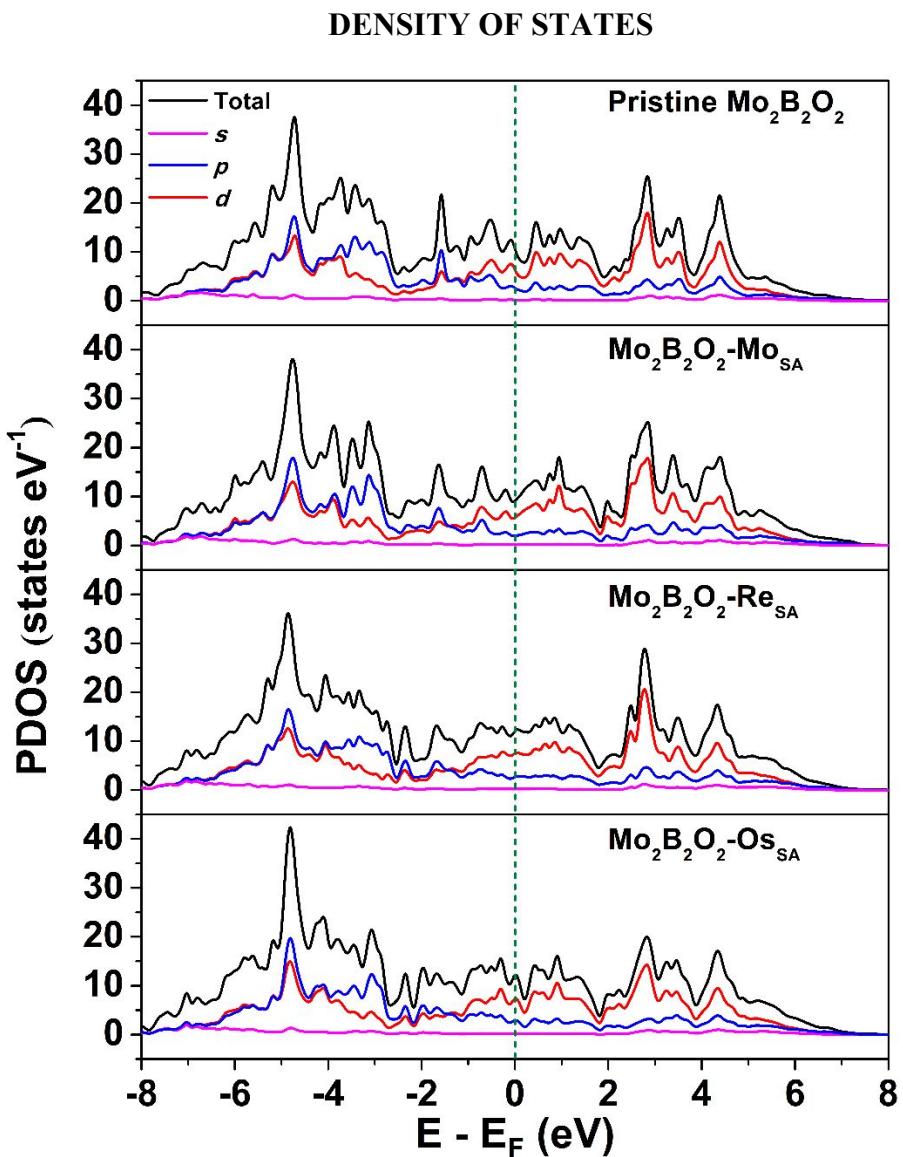


Figure S5. The projected DOSs of pristine $\text{Mo}_2\text{B}_2\text{O}_2$, $\text{Mo}_2\text{B}_2\text{O}_2\text{-Mo}_{\text{SA}}$, -Re_{SA} and -Os_{SA} .

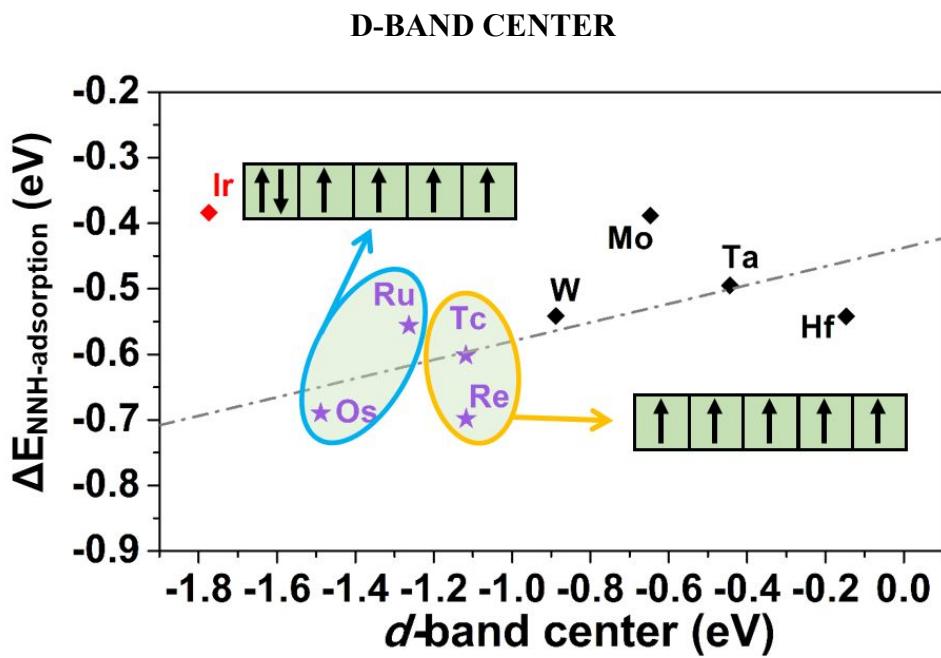


Figure S6. The relationship between NNH adsorption energies and *d*-band center of Mo-SA local cluster. SAs with four and five half occupied *d*-orbitals are in the blue and yellow circle, respectively.

CARTESIAN COORDINATES

The atomic coordinates of all the optimized NRR intermediates on the Mo₂B₂O₂-Re_{SA} (provided in the format of VASP input). The absolute energies are given in parenthesis.

1. Mo₂B₂O₂-Re_{SA} (-445.65592083 a.u.)

1.000000000000000

8.6025421979180567	-0.0001565003596935	0.0003384485662567
-0.0002068925001896	9.1281053549185120	-0.0093218991834330
0.0015614692367874	-0.0253378682072854	23.0531482380066315
Mo Re B O		
17 1 18 17		

Direct

0.2491667857284710	0.9974916097859137	0.5616117710628042
0.0832172469216042	0.0013253890814848	0.4392893802170280
0.5837173401024284	0.9972815974185976	0.5617024550282538
0.4159807988259732	0.0013757478033643	0.4392205567916925
0.9162169317113282	0.9980174404469109	0.5617340322954059
0.7492404816524678	0.0017743960819419	0.4392913735567058
0.2492756059751459	0.3356788967798103	0.5616306681648603
0.0831190905290329	0.3307779131590367	0.4393123614555128
0.5835731968388309	0.3357599360452528	0.5618242771207892
0.4160356190792509	0.3307012002511900	0.4392866887820872
0.9163379638417504	0.3351990004859073	0.5618335043704711
0.7490339486099178	0.3303527616117687	0.4393176362955183
0.2410217391324643	0.6667516645228210	0.5588981047678899
0.0833540424431184	0.6659895947143876	0.4380708723318000
0.4150195421874587	0.6658533138678830	0.4365436342783450
0.9151961696289861	0.6666688771117947	0.5603837983940718
0.7491985623005941	0.6659725340063761	0.4365589873532876
0.5906241731381150	0.6667462558886353	0.5539667292585106
0.0829584198251878	0.1657463703336398	0.5207592894194792
0.2493638088581513	0.1661720827130453	0.4824781088061916
0.4157394155422088	0.1663390963696036	0.5209749342770847
0.5828420196579799	0.1663081377658746	0.4827015006186386
0.7490836706677991	0.1664346643668707	0.5210408198256286
0.9161661014730349	0.1662035563797375	0.4827294774940235
0.0821890339542092	0.4995918561402726	0.5183556804461618
0.2509869117225855	0.5001030114146304	0.4808249898843697
0.4169925992365734	0.5042740586755793	0.5211071476273190
0.5810914884013567	0.4996795997542007	0.4793400182712415
0.7494216363513048	0.4981265129689827	0.5179964591221776
0.9159879144712161	0.5016122239232621	0.4801970715259323

0.0826309913877848	0.8331504254863558	0.5182470737023132
0.2513914529348792	0.8320181089384645	0.4805867367344315
0.4172226774983969	0.8281265603867892	0.5210000064813349
0.5813132476249548	0.8325826799024703	0.4792616065197093
0.7497429455872351	0.8348188909830166	0.5179118025750206
0.9164353845755056	0.8306011093464184	0.4801699459539157
0.0825848302574967	0.9954620817079135	0.6200965624358695
0.4155611171510342	0.9909739088017835	0.6202068767927049
0.7508087695566276	0.9951556605978819	0.6201839351430916
0.0823690195750798	0.3383007662800199	0.6201572733268131
0.4153979816247600	0.3424726561392893	0.6203240089544245
0.7508086153978381	0.3389933620346925	0.6202726841903252
0.0915419497249031	0.6671621157777583	0.6184864446865311
0.7314504042286233	0.6673339273084730	0.6166333250038553
0.2499059271539928	0.0025822173938373	0.3808175439458050
0.5819922776612094	0.0027942678897041	0.3807968846434076
0.9162033953297425	0.0047519222615663	0.3810831677949092
0.2498899281924393	0.3292090827806901	0.3808883315503341
0.5820244529987696	0.3288342878457854	0.3808176378803914
0.9162764514310370	0.3272253156744793	0.3810830622353853
0.2485732964499949	0.6658365444256472	0.3785460411187499
0.5828982626801429	0.6663860645147265	0.3781775968605959
0.9160541771689933	0.6664185456534821	0.3787489526268142

2.*N₂ (-462.88233805 a.u.)

1.000000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N
17	1	18	17	2

Direct

0.2563744716140841	0.9966318224361369	0.5597756840399394
0.0871830474682929	0.0004130405912415	0.4380082830173253
0.5861853335601219	0.9961199023777726	0.5589707686974295
0.4197452796061696	0.0006676489182177	0.4373519839720150
0.9201269598728681	0.9976199401943376	0.5617720212679436
0.7524338998126814	0.0004820604973684	0.4377480227840360
0.2556393831996622	0.3363933754411447	0.5601749953202666
0.0869820531967413	0.3320060752692885	0.4379646407819710
0.5862856635404918	0.3368145385744209	0.5598910887989431
0.4195156066449122	0.3319903360780890	0.4375234729590852
0.9203801174628518	0.3349155857552999	0.5618901485354371
0.7523569082931880	0.3319642134120262	0.4378285224885519

0.2407097321511263	0.6668599868031773	0.5608921466609385
0.0932650076057457	0.6657634334508499	0.4380193461135043
0.4145213228740331	0.6658586438445567	0.4374779601875099
0.9202640692936808	0.6665390901341505	0.5579241284886526
0.7540975290301341	0.6656297926311585	0.4307777640270805
0.6006198968680644	0.6664661173337320	0.5521933193090997
0.0873766181248721	0.1665805866257292	0.5169855740184147
0.2537135519280391	0.1664201559612772	0.4825953235558281
0.4205643002989024	0.1668446623440503	0.5170849616690407
0.5869830057883135	0.1667939103961251	0.4825131478183800
0.7535855817092838	0.1666898293435475	0.5173251406957549
0.9201296875361319	0.1662958767851543	0.4831045919921544
0.0866862132915908	0.4991523098715681	0.5163535231953105
0.2549619450197249	0.5013275264375622	0.4825338559004657
0.4214349888843680	0.5060217623402293	0.5181946003949317
0.5847799019203163	0.4975274973718731	0.4797067481903991
0.7537610447603544	0.4978187586842021	0.5138832264537206
0.9212260205384432	0.5006295993165935	0.4810192791804112
0.0866946063294871	0.8335213137405700	0.5160856246548670
0.2550848452241039	0.8313306393320842	0.4821568919728061
0.4216151919165735	0.8269310102820788	0.5178666232227311
0.5849410142144180	0.8347808342475810	0.4792375775792836
0.7536619416498567	0.8343778440292644	0.5136053566007031
0.9212916175420580	0.8316233648073005	0.4808412047054406
0.0877346513116039	0.9987314638848993	0.6160931854473815
0.4224712808855067	0.9911783145619536	0.6166916467510232
0.7557040653397782	0.9961054527293561	0.6159562515511633
0.0884537615245498	0.3342698374164099	0.6166169087706040
0.4234052216243681	0.3437923173671535	0.6171555222174615
0.7563736660273334	0.3358689100949045	0.6164820544732499
0.0723106510375507	0.6675812831366883	0.6165038498563086
0.7329127170728839	0.6659649475343088	0.6133514230954227
0.2549893137049086	0.0008734557362505	0.3818807101717181
0.5864944117076120	0.0028476852553579	0.3814283798534351
0.9221146743242263	0.0003949840154530	0.3823038387976572
0.2537587265073621	0.3306329924569474	0.3819908989340038
0.5852353901706085	0.3289107279223715	0.3816106744450083
0.9212112540320465	0.3303625041509721	0.3823750128134273
0.2531353669556194	0.6642428894297260	0.3798470995342957
0.5871245961207336	0.6640766592253039	0.3796904757208499
0.9207700908359026	0.6635156801507522	0.3800545652304958
0.3951208124560962	0.6709060613347746	0.6872523083191558
0.3537408975896664	0.6689408449366661	0.6429478497669614

3. *NNH (-466.36334487 a.u.)

1.000000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	1

Direct

0.2544022555386725	0.9986450271369844	0.5603541463577939
0.0841363378719404	-0.0002379123419614	0.4389735092742042
0.5817131781249396	0.9964567677140883	0.5604531118651030
0.4182316985806910	-0.0001810416615852	0.4379255982761410
0.9178101218569922	0.9979230933704458	0.5628858045892274
0.7509297854695890	-0.0013315044326348	0.4394880778399338
0.2541350696337628	0.3349264258914119	0.5600662467034559
0.0836487766230815	0.3326711262785081	0.4386165641478323
0.5815364324154232	0.3369082483094068	0.5609565734538032
0.4183705932598337	0.3321025432296092	0.4380118950052516
0.9181762384752111	0.3356357720778557	0.5627808166176796
0.7501598381843056	0.3334899690304139	0.4397045808926674
0.2421589708828012	0.6668834151461802	0.5605907149551140
0.0913822343000306	0.6662666889719485	0.4383590631001907
0.4111544473853188	0.6656465660979307	0.4387547684691218
0.9165275047425704	0.6668734883045840	0.5603037507304333
0.7505565890578463	0.6658581698743693	0.4307545520262503
0.5901995706775309	0.6667292962889416	0.5561669644342891
0.0846043483919185	0.1668115084511933	0.5172026144204407
0.2510537605461435	0.1663267110051336	0.4825732638710907
0.4178548252522318	0.1666616647034524	0.5173248205095436
0.5846266767990999	0.1664674294264429	0.4831378012217498
0.7503446852065619	0.1665580407645064	0.5180352931289143
0.9168564434896582	0.1666741713043678	0.4839154325170563
0.0836434538493928	0.5006167750904222	0.5169514988610361
0.2515651652569948	0.5011213257655124	0.4828527174272367
0.4180609560257363	0.5033631198167879	0.5181111155642442
0.5826659692477212	0.5000431386591563	0.4814037083449653
0.7502255066372316	0.5011387414817775	0.5156719184837661
0.9176470598289429	0.5017453743351682	0.4826053463431256
0.0839186713501000	0.8328064873486088	0.5170107000786063
0.2517311343187037	0.8316972748932556	0.4827621960084102
0.4181537766089162	0.8297354156738458	0.5179549048238324
0.5827968322843785	0.8318842499481478	0.4811950187685700
0.7501928769689824	0.8321529442762803	0.5156639358167399

0.9177888677005980	0.8319969900538366	0.4827489533729559
0.0842414428876108	0.0004394414713142	0.6166132212869215
0.4178466801924102	0.9938316369768699	0.6177951154616212
0.7524785850547099	0.9987145147011103	0.6167409335020038
0.0843012515366265	0.3337403460455781	0.6165526300239142
0.4180140819661397	0.3404098575618333	0.6178917555230941
0.7527702404396920	0.3351154928582555	0.6168160547386130
0.0807564670422825	0.6677262705397867	0.6176981852503399
0.7410762886378836	0.6668775718165130	0.6164466408463224
0.2506405202353960	-0.0018942918786141	0.3828880593816906
0.5830540304585751	-0.0027914237589718	0.3826698699452310
0.9182195505344533	-0.0003743863364572	0.3834724638625061
0.2500213696682185	0.3308808800150904	0.3829750478901210
0.5827908899444706	0.3297211036876251	0.3826580033596533
0.9181299209630382	0.3329228821995844	0.3834651982782636
0.2505884646151854	0.6627585140250275	0.3803790415223008
0.5845730960881459	0.6622941738594812	0.3803219679538121
0.9205839238342860	0.6665467915392767	0.3810611048579969
0.4328130968829550	0.6701110473086368	0.6734403070625278
0.4226934448116949	0.6682352404195345	0.6227108293178774
0.5465858173623918	0.6708566806641463	0.6869955156344013

4. *NNH2(-471.00542209 a.u.)

1.000000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	2

Direct

0.2521159292770638	0.9961513943774289	0.5613142817490346
0.0838338404692636	-0.0001568499643446	0.4386650235779559
0.5841658902745702	0.9944944603198151	0.5611249110928159
0.4184428029997059	-0.0007861353214766	0.4382600326191476
0.9178744598593139	0.9970093386260054	0.5620081751958577
0.7503266370733759	-0.0001336894432604	0.4392030386822525
0.2499834135518205	0.3349588085857407	0.5614347319705352
0.0855276958553691	0.3301063646597031	0.4369801452212222
0.5852887302856395	0.3366425865793534	0.5618032225214852
0.4188939532964845	0.3302354424065449	0.4397223815730733
0.9180083269785896	0.3344996995405174	0.5606248736159729
0.7475222271817029	0.3296753696755038	0.4380869668922727
0.2474687785747310	0.6651278659130714	0.5583237806606808
0.0823915763913417	0.6646889282405488	0.4390079787404566

0.4149338917027854	0.6646142453079765	0.4348169606338065
0.9171714787809979	0.6653274372331850	0.5615769740357720
0.7543772405622674	0.6646995136469181	0.4364696608804695
0.5861194961374413	0.6649558549656513	0.5549865662951284
0.0846818295488794	0.1662542792748875	0.5177025593779603
0.2513522813880050	0.1657534213929028	0.4835705462292474
0.4177255869069135	0.1651034296415215	0.5183027105629523
0.5840413721892573	0.1657444545085836	0.4839945210875058
0.7504026379633328	0.1661363297828699	0.5185116325690112
0.9171298371842301	0.1652238478547498	0.4837366381978506
0.0839838386951465	0.4976490173196578	0.5163824576155708
0.2508372300757755	0.4988106691510384	0.4817774024195644
0.4176866216641898	0.5002121230473510	0.5162622003887729
0.5837859958505286	0.4966568476546714	0.4806478319387079
0.7502021484485492	0.4980218620563833	0.5158422111453833
0.9172990646729292	0.5008296701159345	0.4822250771761226
0.0842264846987384	0.8333501989238229	0.5167185031716245
0.2510958107166397	0.8314067993396516	0.4819159512024780
0.4180084803431712	0.8307601490270138	0.5163462602034498
0.5839801678288526	0.8327531498783882	0.4808173218979275
0.7504827949390486	0.8327274838298765	0.5161336126152272
0.9176700851752935	0.8302099542644110	0.4823540591974066
0.0841290972450058	-0.0054937699606973	0.6175394432367770
0.4178384546849424	0.9929365716597655	0.6180053143481795
0.7516476491747812	0.9930085469295964	0.6175983267663842
0.0840163535675003	0.3374666138807603	0.6178313729502193
0.4165871101028095	0.3399003974518250	0.6180342754136259
0.7495524944710042	0.3386884390958481	0.6178427749326334
0.0827048290823844	0.6666377194287604	0.6165837179230961
0.7463913293138903	0.6658936489634443	0.6157027019181145
0.2507712893260791	0.9982862809176554	0.3829365153335398
0.5850739743068621	0.9972637401172711	0.3825212362982636
0.9179843146774062	0.0002783946841602	0.3832349072232074
0.2492647646479479	0.3274395024287175	0.3824345015399626
0.5850618251024368	0.3266461983987009	0.3819408020191448
0.9177643874500017	0.3278503111858092	0.3828877781935089
0.2505969371389302	0.6623140566546121	0.3809095070318174
0.5833120829270734	0.6622364854357026	0.3809364044037613
0.9173807677666931	0.6613734047663743	0.3807021954216963
0.4489840101435583	0.6564054269103720	0.6703243242615832
0.4274682476708467	0.6634259032218176	0.6176332200866355
0.5590028706194087	0.6518540313505121	0.6849696658046590
0.3572083850384778	0.6495139160663954	0.6965695849384959

5. *NNH3(-474.76025207 a.u.)

1.000000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	3

Direct

0.2477537960585956	-0.0041864233086094	0.5625931169305008
0.0856493010432804	-0.0008547905660154	0.4377131597812565
0.5849091892594446	-0.0045228388823641	0.5626085376943344
0.4180361554894355	-0.0011681509770740	0.4420985724562508
0.9161192911804046	-0.0029508954160824	0.5604855233400452
0.7461425152124198	-0.0006023162563209	0.4388282123466488
0.2510433563250755	0.3349630486126758	0.5619374548267720
0.0817206987758894	0.3301037374261392	0.4398471944256088
0.5824845168814062	0.3358106826617500	0.5608445081055363
0.4157372195902936	0.3298884228224527	0.4380655106275151
0.9152016676359084	0.3334601297524992	0.5628479695833108
0.7504815368605277	0.3295421189350400	0.4390594487519806
0.2447758427358414	0.6646654218447686	0.5605186882214204
0.0810275676414187	0.6645436967689389	0.4394194102438397
0.4141870278089608	0.6649103175668917	0.4353322730637017
0.9157818097301261	0.6650230466550970	0.5623703702861327
0.7524155038647807	0.6645352812328507	0.4372933092309542
0.5848909799679012	0.6644734942543645	0.5555906541296185
0.0830292136988209	0.1644638620328585	0.5182050790637734
0.2501312782375992	0.1654622910502375	0.4845647794829932
0.4163689421359612	0.1663787730694347	0.5193903951772001
0.5825556913289310	0.1649877207829194	0.4846696987010130
0.7492352690307390	0.1649388630024604	0.5187026377797963
0.9160676039136993	0.1663091253213862	0.4841908031696199
0.0822135010589113	0.4986436365897452	0.5175611750365720
0.2488919784638917	0.4996070797762582	0.4827388014439525
0.4165659475124756	0.4996700551578845	0.5161262183508699
0.5826595256887999	0.4968142540392683	0.4808984638623836
0.7488321858146335	0.4983565576394334	0.5165708634764011
0.9160720992663827	0.4997755063206943	0.4831849349880735
0.0822476915390578	0.8323719162170139	0.5172362560611909
0.2493207013139447	0.8303896308449297	0.4830368092759708
0.4164057423570284	0.8295528950041855	0.5172783390393718
0.5828993652234349	0.8325066498709661	0.4818899848859695
0.7493140643804068	0.8325610988104690	0.5168357096181482

0.9160808799738412	0.8291691015953453	0.4828993888828620
0.0834118282418869	-0.0049266927733339	0.6184015262291787
0.4151546326584072	-0.0075599668896371	0.6189644649189199
0.7480164459927487	-0.0055599065911722	0.6185414823011690
0.0828045597444812	0.3370766826891443	0.6180448098664947
0.4156444721858003	0.3393686992363067	0.6190885063999263
0.7499375757129129	0.3380799859233913	0.6182881216736787
0.0797724776164748	0.6625917148698722	0.6184629841322018
0.7393320402442851	0.6632272219404584	0.6174539079966594
0.2493772248365043	-0.0008573744403736	0.3839979307253164
0.5839349396477506	0.0000890155399680	0.3835032743276887
0.9169993051493689	-0.0014888784748728	0.3841318098315362
0.2496997051691199	0.3280921706359497	0.3832459308483439
0.5827073548443100	0.3269300922749053	0.3829187411188723
0.9165740523613384	0.3271611988893787	0.3831190664393091
0.2498302772417461	0.6614054397380345	0.3812781817155845
0.5823970585909966	0.6617542266891507	0.3811968680363154
0.9158715035768588	0.6623999659938846	0.3812962179717431
0.4672800960608994	0.6566102511062664	0.6729454795907923
0.4271540165680424	0.6639987680787965	0.6153900004620806
0.5876811117030341	0.6530959187860886	0.6742901568710128
0.4218746772594379	0.5557233582523955	0.6901476541860945
0.4276548615933309	0.7554454232729049	0.6932286720154728

6. *NH...NH₃ (-479.47262584 a.u.)

1.000000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	4

Direct

0.2504002038793738	0.0017167392571725	0.5615076807567984
0.0796306659070235	0.0025139195186616	0.4416100002128368
0.5797695319466688	0.9996491883704681	0.5606966270016378
0.4133519502875430	0.0032640521675958	0.4386748077096413
0.9138864328334357	0.0005506617887504	0.5646467127759965
0.7481105900166475	0.0027887158794604	0.4405372865153458
0.2476003447428199	0.3380593269318780	0.5612702788284210
0.0799213036354125	0.3353590282116062	0.4392897700505690
0.5819242458363806	0.3386813607680999	0.5612671441542648
0.4157187307822155	0.3352777485767461	0.4389798809836812
0.9149917174827706	0.3378218860256449	0.5639343415918535
0.7460273334450883	0.3352188254236870	0.4408731762207482

0.2387475683743774	0.6685879281017747	0.5623860727082869
0.0852317334219625	0.6688913146148815	0.4389309740154729
0.4096998746521596	0.6692506112639122	0.4399893617544714
0.9137094497022632	0.6688328501879711	0.5612406679004125
0.7451233120896990	0.6689801101286154	0.4348094258428324
0.5865495175450141	0.6698732851786092	0.5573100680686887
0.0813506128538781	0.1705461687436373	0.5189352567304831
0.2477702011846415	0.1690782040991678	0.4841963201847831
0.4144417641191435	0.1700419347401196	0.5189931613669908
0.5810620211247152	0.1695141068271973	0.4844634806795597
0.7473437981074463	0.1689227525391700	0.5195928184227910
0.9138326260890425	0.1693438099040643	0.4854260668667363
0.0807262443881949	0.5025853384483233	0.5180404373888676
0.2484205394770318	0.5039431932569278	0.4840287374157007
0.4149053730574378	0.5050612390971466	0.5195260909470237
0.5794763714133618	0.5027275861163076	0.4826926341466765
0.7468415296784180	0.5021054153299926	0.5173097587462774
0.9142283152086763	0.5021907539229062	0.4838355354839085
0.0808459020219615	0.8345456191966246	0.5186028846323202
0.2480836693743390	0.8335288997538354	0.4841373906184574
0.4144656322034351	0.8326663589958803	0.5193228696857973
0.5790933055057284	0.8349212749340874	0.4824525833498787
0.7465360942990167	0.8348297703818528	0.5172384438426136
0.9143167759975911	0.8340783500571194	0.4841608826333089
0.0803168432997654	0.0043050059487153	0.6185498277661803
0.4135798833989629	0.9954696970783619	0.6197385830186064
0.7477648776124618	0.9983931640611317	0.6185732607134170
0.0813737660262084	0.3388544201231730	0.6189861902060771
0.4147257835099344	0.3443612689712770	0.6208698579006157
0.7474805571435549	0.3391282903381461	0.6190573945256425
0.0802951846383925	0.6705739994072958	0.6193704782601150
0.7410682163785722	0.6669918658467300	0.6175703390090479
0.2471238995512625	0.0024570685504734	0.3844483705404615
0.5801383871662100	0.0039342586378330	0.3840565886116262
0.9143614683767440	0.0018783715813785	0.3848909076565046
0.2476892034516096	0.3352890249278858	0.3839094535995568
0.5797313995984725	0.3348967563939257	0.3833967174678430
0.9154111151668736	0.3340494041354941	0.3843425001247480
0.2454224116991224	0.6696889244634598	0.3818931178403976
0.5805047382780013	0.6713467504076235	0.3816983327985469
0.9130206651180193	0.6683938566375432	0.3827946423445627
0.4640879621375776	0.5902726924168045	0.6733256426883806
0.4277029571331823	0.6878878168948087	0.6258485141456033
0.5798882988855335	0.6022735329354494	0.6814007452224657

0.4391370931803533	0.4670608518121694	0.6580621210315430
0.3994285982524842	0.6212471481011679	0.7073954512593866
0.4273716893117958	0.8042177225892490	0.6389614350345286

7. *NH₂ (-463.58777185 a.u.)

1.00000000000000

8.7643003464000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5680999755999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	1	2

Direct

0.2565263532952173	0.0022024628445586	0.5602430725808215
0.0858147101400453	0.0039457252611979	0.4395012433747703
0.5843747906175849	-0.0004611688547306	0.5593800663669805
0.4179866002010252	0.0044669182075088	0.4377731094044337
0.9186971216806025	0.0011241228468377	0.5627186083800907
0.7532564574420056	0.0036841299908762	0.4387330622668446
0.2547028478183153	0.3376122619707019	0.5591751861930253
0.0845385503611516	0.3374205760268123	0.4378963332889148
0.5831241029187969	0.3387128382462822	0.5615348201960908
0.4204969630369906	0.3367411243359829	0.4377697878789331
0.9204500868756117	0.3386686132174224	0.5628572824366427
0.7522904616282264	0.3377384644580683	0.4401730951538713
0.2452345934830075	0.6697955329224385	0.5607246511668612
0.0923435299499391	0.6704225084652328	0.4382016046566305
0.4136729146994285	0.6701596277871156	0.4387898798141177
0.9183758822201554	0.6699492266902310	0.5590115422080408
0.7520667454614672	0.6702232400972271	0.4320467134929513
0.5914182190930755	0.6692649909877108	0.5566763454370611
0.0859359045255854	0.1708073205175222	0.5169497338104446
0.2526492623543451	0.1697573148631626	0.4824048097455533
0.4196219926338584	0.1697226081879489	0.5172892266775427
0.5864093290317484	0.1706228080323429	0.4830454996556759
0.7524623121582689	0.1692935511652827	0.5178954457773655
0.9186752957613519	0.1701380129759023	0.4836120752382647
0.0860218371538496	0.5033604885550162	0.5167433455600228
0.2535821363745687	0.5050730438095115	0.4825399684146823
0.4199067911869760	0.5053640572665392	0.5181566929596577
0.5846428418025960	0.5032713158138390	0.4818424759797095
0.7519816510330695	0.503435522975392	0.5159805850023342
0.9195785948289135	0.5039098968454476	0.4824299362928293
0.0860378079245828	0.8356468596099571	0.5168796409299666
0.2534705393144226	0.8351476106567725	0.4826529170323498

0.4200781708757199	0.8328366286743796	0.5178861519421285
0.5846400087432683	0.8352115521837169	0.4811932689382898
0.7516652683587520	0.8350860015642781	0.5155133803403982
0.9196355406171471	0.8362099840306322	0.4823797981667973
0.0866370566721144	0.0043308513816027	0.6162605685467583
0.4188262830858058	-0.0066364832686418	0.6174768800965581
0.7540486790403363	0.0014916094006451	0.6165634877922133
0.0853012636681228	0.3375752653524145	0.6168016621530674
0.4188950746517746	0.3413029998075291	0.6179922177844499
0.7535633744472091	0.3372107843740439	0.6169332645725489
0.0851871462887007	0.6718763607472091	0.6171209345215654
0.7485584212079884	0.6682475883825332	0.6153316118585919
0.2524675639345482	0.0062392551715336	0.3826108102895094
0.5846567505492366	0.0057810845630426	0.3827753898348900
0.9188592395977754	0.0063385337301087	0.3830847979989336
0.2526394892659022	0.3395237656938291	0.3826291094016388
0.5847122097246945	0.3389721571292869	0.3826370417137331
0.9203685798652238	0.3398460782744602	0.3828966989414401
0.2520601492954938	0.6721538567897885	0.3805003663101404
0.5861464850859234	0.6722277206453842	0.3807310120093556
0.9203997106507609	0.6730216224275187	0.3813324769095839
0.4269963390928797	0.6671705788615729	0.6232090415496824
0.4332985284874903	0.7641213490359356	0.6483371567234408
0.4317315677863430	0.5669992889489200	0.6467540132308162

8. *NH₃ (-467.24517125 a.u.)

1.00000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	1	3

Direct

0.2601176586835597	0.0006873006449140	0.5595682691130042
0.0906210926889712	0.0044299805118719	0.4383722777356786
0.5903682872615706	0.9996955327218054	0.5586477495969338
0.4226000335024395	0.0047594898310655	0.4366073031868138
0.9240522356206683	0.0015380068705262	0.5617403486160679
0.7572810267798229	0.0050778663808778	0.4371919220314676
0.2572677312643029	0.3390377737612287	0.5592897236889096
0.0904870569458133	0.3370889039559025	0.4365266865053937
0.5890917815305755	0.3393566659053637	0.5599338242449350
0.4247430036200147	0.3365883632866796	0.4375935736679573
0.9242190486774114	0.3384940645332300	0.5611739733002769

0.7544971339858616	0.3360049997524281	0.4380362859771982
0.2428806529398659	0.6697170924030809	0.5621250284872579
0.0955024686958190	0.6703495553071877	0.4377965714758835
0.4177458198005935	0.6703894072984914	0.4373406669548198
0.9225252062111016	0.6698136472830286	0.5579931211939752
0.7566534436984580	0.6705846261055285	0.4318063725152747
0.6026456866891162	0.6702063203866685	0.5518058317420356
0.0908896334721379	0.1705444610277631	0.5165987598765680
0.2571074031043107	0.1706498095814003	0.4820048607423277
0.4236775397442527	0.1699925487158811	0.5169966310717001
0.5902864207272825	0.1706530699943116	0.4822431758255468
0.7570927979959762	0.1697804470833905	0.5171359572884585
0.9236475505921105	0.1701571027734021	0.4827951109190650
0.0895003588185055	0.5034309625962071	0.5159268958479118
0.2580969772680107	0.5060337421760621	0.4824146192243017
0.4239932428880073	0.5102126195460097	0.5184400561285680
0.5875480939741465	0.5013329816934197	0.4797882165503548
0.7565179001180359	0.5010870760743189	0.5139063096965604
0.9237775611711067	0.5043927738847226	0.4807076976438659
0.0898834042831549	0.8361444905857488	0.5163338100582240
0.2579912690873719	0.8346331543244229	0.4824049095655872
0.4243112818647826	0.8297807460932757	0.5179692772203964
0.5878709031248416	0.8387017936480072	0.4792629571184047
0.7567630791422423	0.8391195875112830	0.5137106312044557
0.9243846706570030	0.8361565398560713	0.4809829159560704
0.0928522347993288	0.0018411339672237	0.6163346475165775
0.4272978777405521	0.9899414203451828	0.6172201975793294
0.7601768017392061	-0.0015610725823740	0.6162289562632371
0.0918125112848995	0.3377897244070154	0.6165579227957499
0.4266214966568753	0.3472058583792241	0.6174354998538277
0.7596758725751683	0.3393935472247984	0.6162909729914313
0.0741747646494426	0.6695401931129024	0.6170832297823549
0.7327705153707210	0.6684024401991137	0.6135275531989334
0.2571677330013131	0.0057348212386405	0.3815316837476203
0.5887340934010409	0.0065096013545376	0.3812261501574084
0.9246535483038940	0.0068772965737421	0.3819018169074921
0.2571155666962449	0.3381985817016433	0.3816015595204862
0.5890302290772924	0.3364011954958936	0.3810934167637466
0.9248929949151248	0.3365527572271374	0.3818569495677782
0.2561933331474729	0.6710157668427302	0.3798120015088097
0.5910522755905456	0.6708542350469510	0.3798190148967408
0.9228540728061198	0.6725928432902730	0.3802175760292241
0.3544122577892000	0.6683907263697252	0.6473060279534960
0.4185348075826190	0.7665764152977858	0.6553902548241504

0.4142822244875409	0.5671824938332828	0.6550642265879520
0.2614654027561351	0.6702364705689906	0.6735281405813979

9. *NHNH (-469.82021083 a.u.)

1.00000000000000

8.764300346400007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5680999755999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	2

Direct

0.2481336764357351	0.9953594135719115	0.5594549092416869
0.0803616823789355	0.9975345926639463	0.4381552649145632
0.5770597368399635	0.9949073831592870	0.5602623422581345
0.4143568928348031	0.9979927534174138	0.4378531584757042
0.9132578256622566	0.9965237700177312	0.5626242268755277
0.7460804584461158	0.9986376975903397	0.4387891413987788
0.2474802320805765	0.3338876231228198	0.5600840504052158
0.0797810903945830	0.3301886647803656	0.4390573436687433
0.5780470054272371	0.3342952160340005	0.5593890710639826
0.4132115498155358	0.3303769969915606	0.4375196426538182
0.9119409390446762	0.3332148435533497	0.5626548179503104
0.7472050410084847	0.3301866072864996	0.4384321894638603
0.2318131795187810	0.6657467672198933	0.5583451668929271
0.0815912466299054	0.6639245004437768	0.4344756770083222
0.4145515989639961	0.6639020485849088	0.4390202537441752
0.9129359526137719	0.6658838090026649	0.5579524613089930
0.7411848428876056	0.6638610133604459	0.4361635768568277
0.5881286869763329	0.6637603934337548	0.5591810448370538
0.0799716854668802	0.1647017061972491	0.5174338831348209
0.2465466968666092	0.1647197958170636	0.4826771093363433
0.4127995107580844	0.1647824341968942	0.5175794129021511
0.5796861335716699	0.1644491042770326	0.4829302216313991
0.7459266617898308	0.1646299289217410	0.5177423581116187
0.9130688555546485	0.1647143842056593	0.4836360040279786
0.0798656026386411	0.4980567881226676	0.5153364891932739
0.2483704920751109	0.4979038041867554	0.4818688832734992
0.4131920202996753	0.5033431268547019	0.5192211620005693
0.5782176500370682	0.5003080178808190	0.4821989261306854
0.7455972019592849	0.4975182300416350	0.5165565980719364
0.9123991918423826	0.4979690083778294	0.4820201377980169
0.0799442669248123	0.8326051143119173	0.5150566714456417
0.2488161618952276	0.8307978271638063	0.4816395675503315
0.4140114971702289	0.8252177909217764	0.5189621830292523

0.5786092154135147	0.8302972172044392	0.4818436453021917
0.7457756594735869	0.8315374135593103	0.5161163173082954
0.9124632507816273	0.8309065429296325	0.4816141700162078
0.0778693998619744	0.9982197478835459	0.6166109598724319
0.4130957822620687	0.9864641836822940	0.6176682325136298
0.7454022806533231	0.9943197839693028	0.6171680461013409
0.0774143491245525	0.3335423206134109	0.6167842317758385
0.4074257033364717	0.3421229051247110	0.6183904455133842
0.7455510223696038	0.3331325495756801	0.6169185716551269
0.0875149325950773	0.6672375463520837	0.6159828049494109
0.7556295142273584	0.6700166915285664	0.6154399989864814
0.2472927513020977	0.9959628413144301	0.3823118145827848
0.5784903349316508	0.9978040350728108	0.3822284460839569
0.9131305306175364	0.9970955670272588	0.3828530433555031
0.2478186800609450	0.3273964972084826	0.3824308967724264
0.5787797463015565	0.3292317489594865	0.3823934430908125
0.9119110644079953	0.3280347700592827	0.3827712307777205
0.2463893382370372	0.6620714592895212	0.3807901530058544
0.5809366996489018	0.6613250568640865	0.3802686526458672
0.9152114727389744	0.6613986394238651	0.3810385540747347
0.4987093466836683	0.7116217006124614	0.6828525472602820
0.4809900409491092	0.6358945579600572	0.6388387315181916
0.5646989989184732	0.8104931356091214	0.6754099102198765
0.4246344322934377	0.5276220664639482	0.6440130908842208

10. *NHNH₂ (-474.67630206 a.u.)

1.00000000000000

8.764300346400007	0.000000000000000	0.000000000000000
0.000000000000000	8.568099975599991	0.000000000000000
0.000000000000000	0.000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	3

Direct

0.2580601297852615	0.9996235422389542	0.5595304257137987
0.0875160376094217	-0.0007973967720199	0.4394468457052533
0.5867383376791984	0.9970807584403852	0.5575659480037514
0.4188161573277792	-0.0011656583028804	0.4366837229800523
0.9192404588066917	0.9986311232381705	0.5623541315675153
0.7557656851234340	-0.0018817572408618	0.4377268773566830
0.2542044001300713	0.3336761032972397	0.5573462923356007
0.0862349166509737	0.3327425463959277	0.4355559826323997
0.5850585008820689	0.3343236845803834	0.5606055461254004
0.4245042898619072	0.3327624975053473	0.4378165302293290
0.9220920954980344	0.3340178250440017	0.5618138677942490

0.7518323726646330	0.3328998097840408	0.4393903001165998
0.2468789040979148	0.6670497383595330	0.5609067896384793
0.0933349838517801	0.6658200047207162	0.4370982393412335
0.4154247974701284	0.6652350618843467	0.4382588903524749
0.9208299709860885	0.6661041179637935	0.5586249922017952
0.7535635515023023	0.6649331340126433	0.4313531845963242
0.5944290224938902	0.6687885265497497	0.5575742204041572
0.0874278760031627	0.1677768994091446	0.5158090704368521
0.2544330431719151	0.1659245757157007	0.4812035333108337
0.4210796432284491	0.1663394048158811	0.5162856136740102
0.5877223661141752	0.1666168093804203	0.4818112331208738
0.7533953613933737	0.1659221437488573	0.5167707676445467
0.9199778813586064	0.1664902159414191	0.4826241256123616
0.0871367092921784	0.5000322105889262	0.5155219759797467
0.2555302725266370	0.5025245080320702	0.4821762641513749
0.4216969859624133	0.5041096204629143	0.5183583142984547
0.5862619888079886	0.4997998064989851	0.4819334428767508
0.7537361065227458	0.5009299295305407	0.5155006852498740
0.9207212545165403	0.5004927491197484	0.4815219983886485
0.0882770948282490	0.8308498929406551	0.5164304524197414
0.2552193642653321	0.8304404195702904	0.4820193328001385
0.4219591309855354	0.8292506387473296	0.5175617073731398
0.5864571766272006	0.8290697888578346	0.4805669291386231
0.7534120863107966	0.8313576026850590	0.5151053143021214
0.9215736792294865	0.8315777439519869	0.4821141558652240
0.0874120389047484	0.0000328447262080	0.6155682583423727
0.4185307687365845	0.9959035680915109	0.6170648571025638
0.7551626433510870	0.9999863076910263	0.6158658134083445
0.0864607623860848	0.3328752654084355	0.6159057625870865
0.4205096189668519	0.3352538700658940	0.6168484937627339
0.7548710355672875	0.3315500998976876	0.6161718202251504
0.0898021073317515	0.6675636685224771	0.6172966880802042
0.7509278338711696	0.6665608739951187	0.6155401410567334
0.2551253405253643	0.9983443488134758	0.3818030913316831
0.5870041964004039	-0.0048836170465731	0.3821210635873578
0.9203660687042693	-0.0017167997892946	0.3824405565014684
0.2556102681420669	0.3339506394398978	0.3820855648522157
0.5865483336032656	0.3291993581388107	0.3815540643472855
0.9230713296157316	0.3331616431590765	0.3818792102176485
0.2545576905888804	0.6633002187250432	0.3797949567441700
0.5882875615366390	0.6625680059727443	0.3798636211989789
0.9221156011878833	0.6676910753738500	0.3802849790543841
0.4484026753767304	0.6024836921380330	0.6741063708711664
0.4331872849857861	0.6887079996909936	0.6265238900580760

0.4077936703691554	0.6545181340192807	0.7093788676035427
0.4296841795148256	0.4849211298453873	0.6685384777264554
0.4304362287670792	0.8069992814236822	0.6369757616019459

11. *NH₂NH₂ (-479.52145712 a.u.)

1.00000000000000

8.7643003464000007	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.5680999755999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	23.8917007446000014

Mo	Re	B	O	N	H
17	1	18	17	2	4

Direct

0.2602116561174208	0.9955094758060752	0.5610001711997521
0.0915442617436358	-0.0011600259890316	0.4396025937232332
0.5918992493444873	0.9951199317013105	0.5582926545031209
0.4210272406366783	-0.0019838585413051	0.4381155614133532
0.9224971541749127	0.9961286100964734	0.5620332278725997
0.7574042789748295	-0.0012933047610109	0.4369751551839635
0.2575598391533409	0.3329017375635557	0.5582444087608784
0.0904068658185920	0.3301890555012280	0.4359380142716550
0.5870608274885954	0.3344474072048022	0.5616539610164260
0.4271696744608905	0.3305875234303707	0.4382259006820149
0.9250033420041017	0.3328878634902290	0.5621652662465644
0.7551056909631044	0.3301717896303070	0.4395466147493394
0.2399154322052642	0.6622099677683063	0.5606538389393193
0.0973083232389065	0.6644316207661894	0.4366657478572113
0.4203085302808122	0.6640637572704066	0.4389919442188504
0.9237063001597607	0.6641720596758899	0.5565867211312403
0.7558323996852548	0.6642444503687416	0.4326934011836209
0.6019318987565406	0.6665334633419759	0.5571888381414233
0.0904629956207818	0.1652018222666694	0.5170415324109677
0.2575310280059620	0.1636549759958001	0.4826642046430202
0.4238643913725784	0.1647887998262488	0.5178947291866893
0.5900834305005920	0.1656745461137024	0.4830379011287764
0.7568060174449073	0.1644188297667109	0.5176895003142806
0.9232757666436046	0.1650145806678313	0.4832358517605754
0.0901350283865298	0.4958787967336564	0.5148418968105778
0.2596742119226543	0.4998899873129347	0.4819666631417400
0.4241969743940557	0.5041133585292972	0.5197629466748848
0.5882595620315015	0.4978000061574183	0.4821443152330080
0.7563914851801157	0.4966731912352003	0.5151531577929142
0.9234640752128265	0.4968774024913626	0.4807210425114581
0.0900277634351357	0.8321307893677882	0.5158740081160220
0.2587495004478090	0.8294358969936357	0.4829334754829441

0.4245475018052653	0.8249089836893713	0.5195308486110273
0.5882173602271193	0.8291521800543534	0.4811550440626829
0.7563431547240522	0.8331094917825425	0.5147000049544430
0.9240883863295362	0.8322964217996612	0.4810110101070889
0.0916759414698586	-0.0044484871701515	0.6168139613351906
0.4240276767518851	0.9869162485131037	0.6186649790999070
0.7592199240854958	0.9941287198579002	0.6170040990598037
0.0896067320548931	0.3325346290936376	0.6167901611516028
0.4251115634733437	0.3407966951174637	0.6191482910899454
0.7581399975631136	0.3343572515838810	0.6171280992450980
0.0763611633553134	0.6640538999677401	0.6164806025945094
0.7651100426139930	0.6621462847452649	0.6142809615411845
0.2578596703490498	-0.0013373933786597	0.3822581046375482
0.5887668819646921	-0.0035552301560000	0.3823286601100732
0.9235506870176955	-0.0002492199535561	0.3825520566495852
0.2585478654060463	0.3312945392333844	0.3820450800923834
0.5893498096824432	0.3288240872224808	0.3818596051805183
0.9260030801353445	0.3289669329044764	0.3820207896743411
0.2585375276172816	0.6639458783621278	0.3801605235056338
0.5922659636660242	0.6646739552094483	0.3803439412986895
0.9252012707835591	0.6660099717725341	0.3808604130496560
0.3477487599459528	0.6343876850709878	0.6435862807068625
0.5000092166431728	0.6932499718611987	0.6403704885035431
0.2838367158457179	0.6880455394216249	0.6741196636185159
0.3555793678709333	0.5135632797417462	0.6493701885567099
0.4917672719509004	0.8148001763861985	0.6460155470200527
0.5730412178611394	0.6423227164844512	0.6687953182409822