

Supplementary Information

Using $N\equiv N$ dipole as a theoretical indicator for estimating electrocatalytic performance of active sites in nitrogen reduction reaction: single transition metal atoms embedded in the two dimensional phthalocyanine

Fangfang Liu,^{‡a} Luying Song,^{‡a} Yunxia Liu,^a Fangfang Zheng,^a Lu Wang,^a Krisztián Palotás,^b
Haiping Lin,^{*a} Youyong Li^{*a}

^aInstitute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, 199 Ren'ai Road, Suzhou, 215123, Jiangsu, PR China.

^bWigner Research Center for Physics, Hungarian Academy of Sciences, 1525 Budapest, Hungary; MTA-SZTE Reaction Kinetics and Surface Chemistry Research Group, University of Szeged, 6720 Szeged, Hungary.

*Corresponding authors.

E-mail: hplin@suda.edu.cn and yyli@suda.edu.cn.

Table S1. The adsorption energies of N₂, N₂H and NH₂ on 2D Mo-Pc using different supercell.

Supercell	E _{ads} (N ₂)	E _{ads} (N ₂ H)	E _{ads} (NH ₂)
(2×2)	-0.94 eV	-1.05 eV	-2.25 eV
(3×3)	-0.94 eV	-1.07 eV	-2.30 eV
ΔE	0.00 eV	0.02 eV	0.05 eV

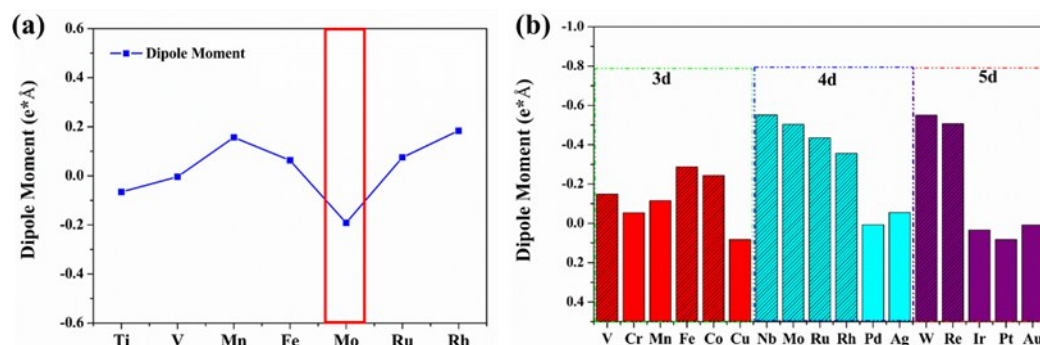


Fig. S1 (a) The dipole moments of a N₂ molecule adsorbing on 7 single transition metal atoms anchored on defective BN nanosheets. (b) The dipole moments of a N₂ molecule adsorbing on 17 transition metal atoms supported on g-C₃N₄. As can be seen, the Mo-BN has the best activity in (a), and the single Co, Fe, V, Ru, Rh, Mo, Nb, W and Re metal atoms on the g-C₃N₄ are the best catalysts in (b). These results are in consistent with Figure 1 in Chen et al's work¹ and Figure 2a in Qiao et al's work².

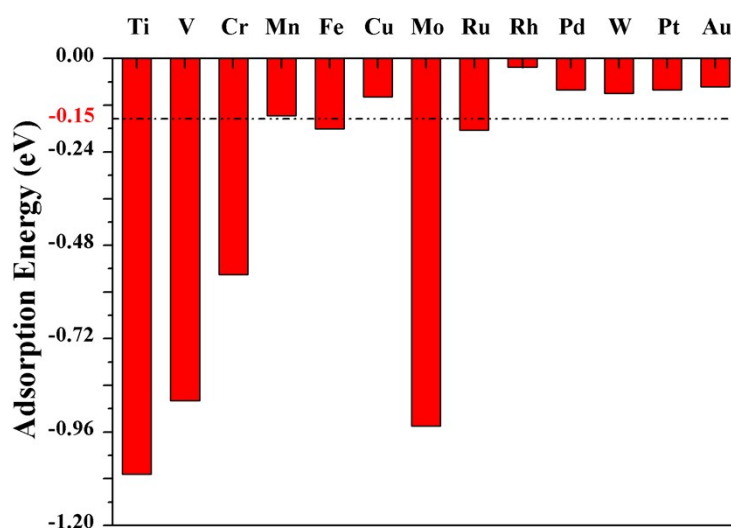


Fig. S2 Adsorption energies of the N₂ molecule on the 2D TM-Pc (TM = Ti, V, Cr, Fe, Mn, Cu, Mo, Ru, Rh, Pd, W, Pt, Au).

Table S2 The adsorption energies and Gibbs free energies for the N_2 molecule adsorbed on the 2D TM-Pc (TM = Ti, V, Cr, Fe, Mn, Cu, Mo, Ru, Rh, Pd, W, Pt, Au).

Catalysts	E_{ad} (eV)	ΔG (eV)	Catalyst	E_{ad} (eV)	ΔG (eV)
2D Ti-Pc	-1.07	-0.53	2D Ru-Pc	-0.18	0.34
2D V-Pc	-0.88	-0.34	2D Rh-Pc	-0.02	—
2D Cr-Pc	-0.56	-0.13	2D Pd-Pc	-0.08	—
2D Mn-Pc	-0.15	—	2D W-Pc	-0.09	—
2D Fe-Pc	-0.18	0.30	2D Pt-Pc	-0.08	—
2D Cu-Pc	-0.10	—	2D Au-Pc	-0.07	—
2D Mo-Pc	-0.94	-0.38			

E_{ad} and ΔG are the adsorption energies and Gibbs free energies of a N_2 molecule adsorbed on the 2D TM-Pc

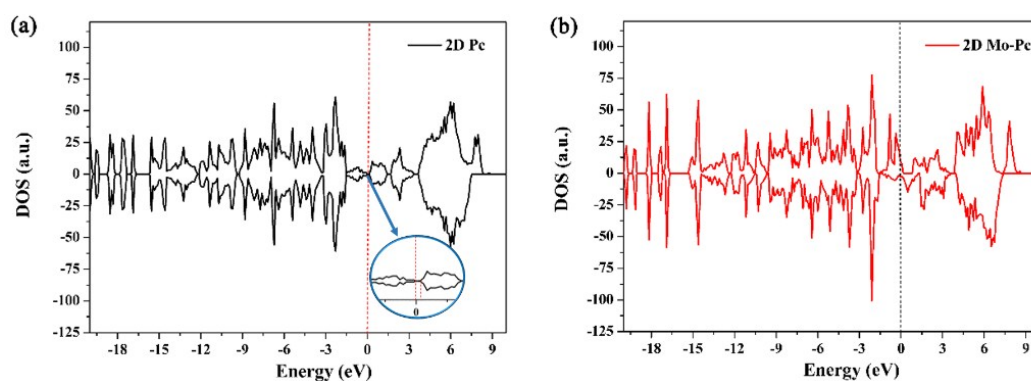


Fig. S3 The densities of states of (a) 2D Pc and (b) 2D Mo-Pc.

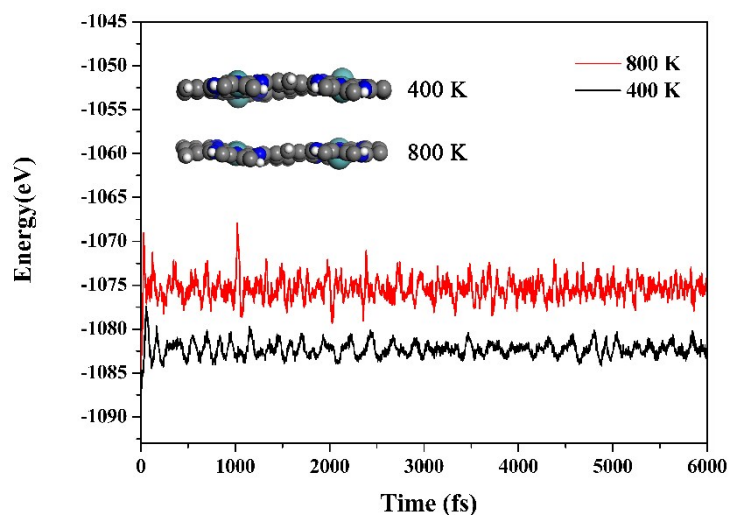


Fig. S4 AIMD simulations of 2D Mo-Pc at 400 and 800 K for 6000 fs. The inserted images are the side views of final 2D Mo-Pc structures at 400 and 800 K, respectively.

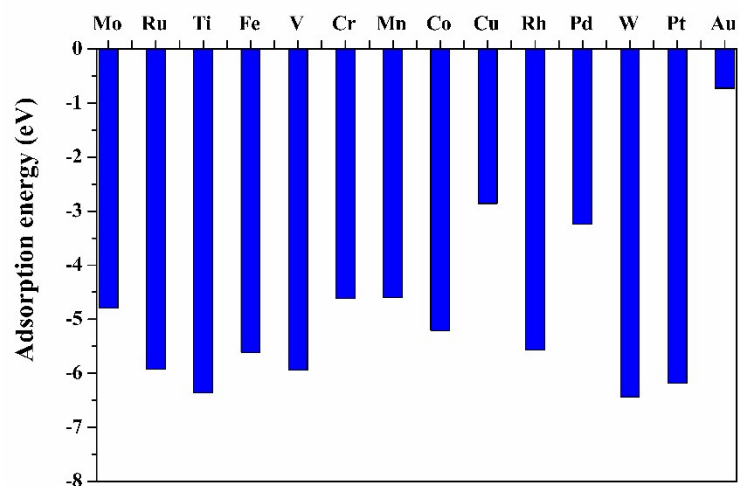


Fig. S5 Adsorption energies of single transition metal (TM) atom anchored on the 2D Pc (TM = Ti, V, Cr, Fe, Mn, Cu, Mo, Ru, Rh, Pd, W, Pt, Au).

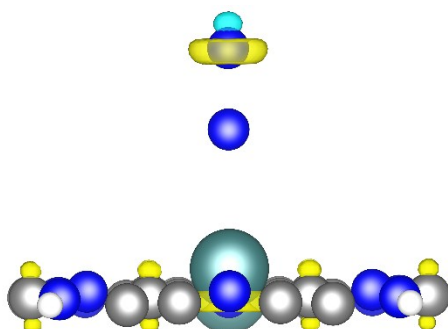


Fig. S6 The differential charge density between the negatively charged and neutral systems. The differential charge density is obtained by $\Delta\rho = \Delta\rho_{N_2^{ad} + e^-} - \Delta\rho_{N_2^{ad}}$, where $\Delta\rho_{N_2^{ad} + e^-}$ and $\Delta\rho_{N_2^{ad}}$ are the total charge densities of the negatively charged system and the neutral system. The yellow and blue contours represent electron accumulation and depletion, respectively.

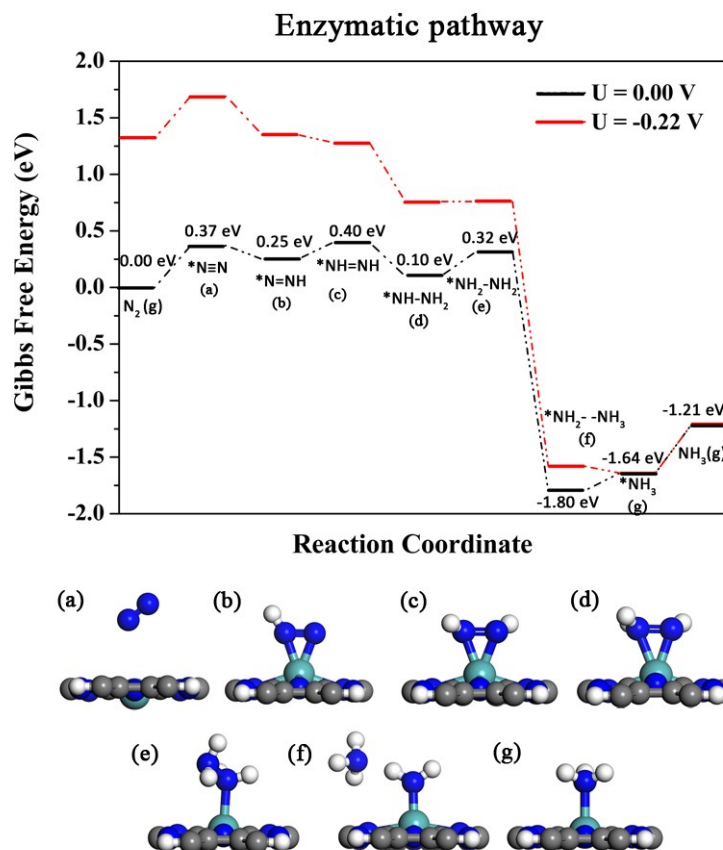


Fig. S7 The free energy profile along the enzymatic pathway of NRR on the 2D Mo-Pc at the zero (the black line) and limiting potential (the red line).

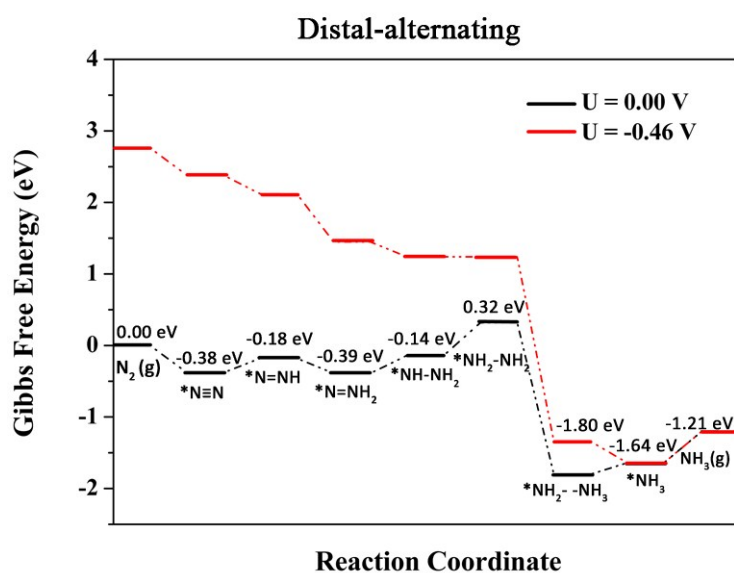


Fig. S8 The free energy profile along the distal-alternating hybrid pathway of NRR on the 2D Mo-Pc at the zero (the black line) and limiting potential (the red line).

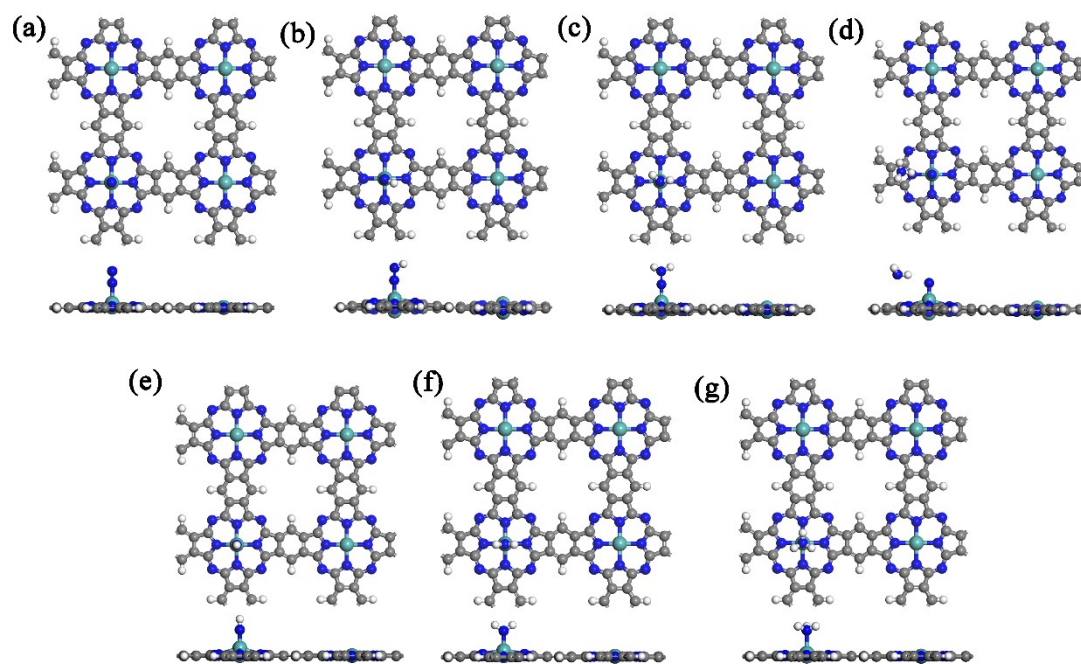


Fig. S9 The optimized structures of NRR intermediates along the distal pathway on 2D Mo-Pc.

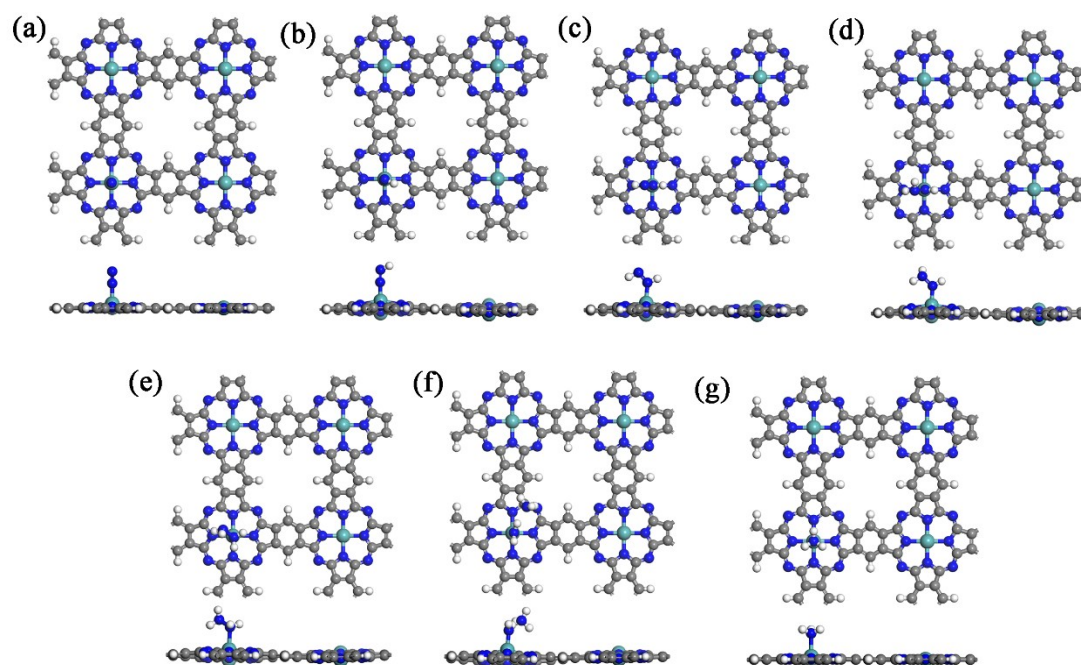


Fig. S10 The optimized structures of NRR intermediates along the alternating pathway on 2D Mo-Pc.

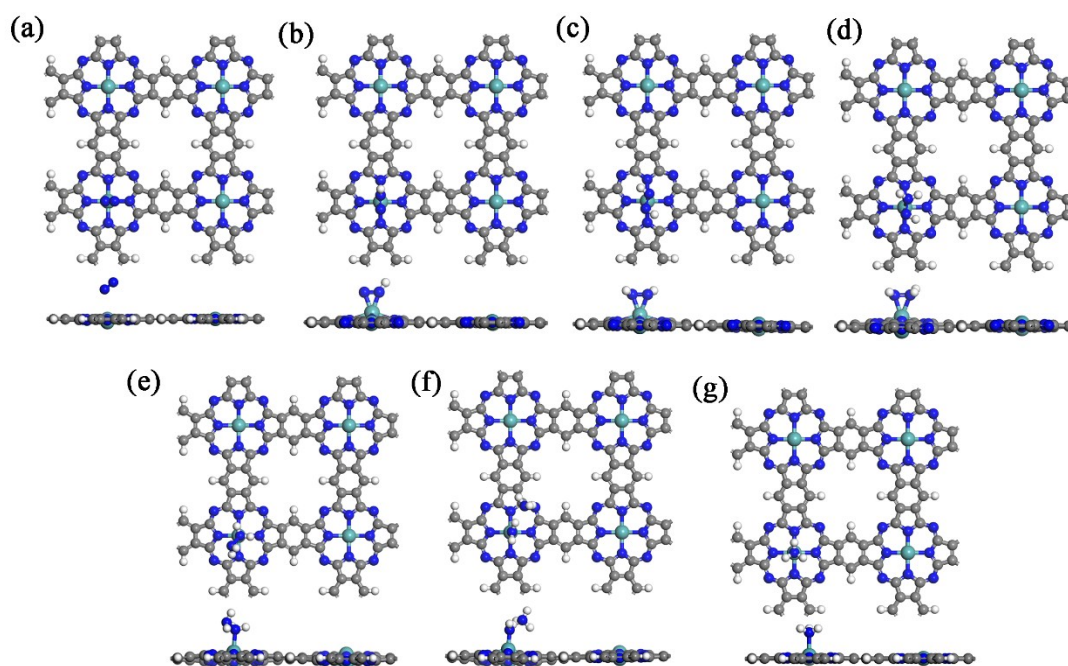


Fig. S11 The optimized structures of NRR intermediates along the enzymatic pathway on 2D Mo-Pc.

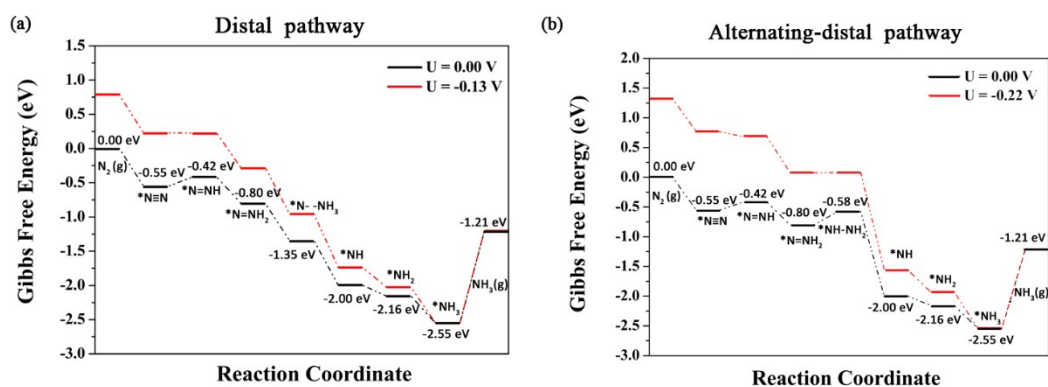


Fig. S12 The free energy profiles along (a) the distal and (b) alternating-distal pathway of NRR after considering the solvation effects on the 2D Mo-Pc.

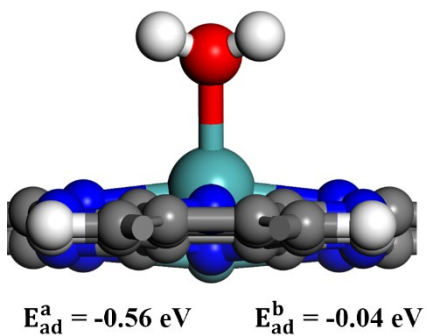


Fig. S13 The adsorption configurations for H₂O on 2D Mo-Pc. (E_{ad}^a is the adsorption energy without the effect of hydrogen bond, E_{ad}^b is the adsorption energy with the effect of hydrogen bond.)

Table S3 The calculated total energy of the coupled structure ($E_{H_2O-Mo-Pc}$), the clean surface (E_{Mo-Pc}), the H₂O molecule (E_{H_2O}) and the hydrogen bond (E_{H-bond}). E_{ad}^b is the adsorption energy of H₂O with the effect of hydrogen bond.

	$E_{H_2O-Mo-Pc}$	E_{Mo-Pc}	E_{H_2O}	E_{H-bond}	E_{ad}^b
H ₂ O	-1104.15 eV	-1089.37 eV	-14.22 eV	-0.26 eV	-0.04 eV

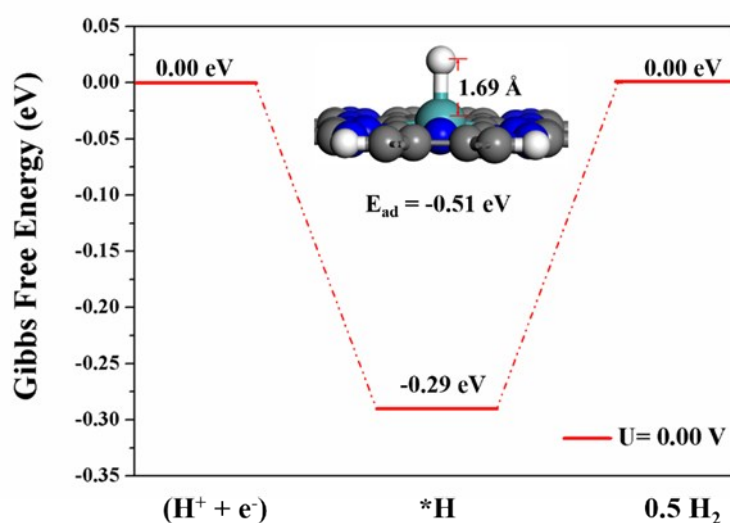


Fig. S14 The Gibbs free energy diagram for the HER on the 2D Mo-Pc at the zero potential.

Table S4 The calculated energy, the zero-point energy (ZPE), entropy, and free energy of intermediate states in NRR at 0.00 V.

Intermediate state	Energy (eV)	ZPE (eV)	Entropy (eV)	Free Energy (eV)	Relative Free Energy(eV)
N ₂	-16.61	0.15	0.67	-17.12	—
H ₂	-6.69	0.27	0.40	-6.83	—
NH ₃	-19.52	0.91	0.80	-19.41	-0.6

Mo-Pc	-1089.37	—	—	—	—
1-N ₂ -Mo (end)	-1106.92	0.21	0.16	-17.50	-0.38
1-N ₂ -Mo (side)	-1106.09	0.16	0.20	-16.75	0.37
2-N ₂ H-Mo (end)	-1110.38	0.45	0.17	-20.72	-0.18
2-N ₂ H-Mo (side)	-1110.00	0.46	0.12	-20.29	0.25
Alternating pathway					
3-NH-NH-Mo	-1113.46	0.82	0.14	-23.40	0.55
4-NH-NH ₂ -Mo	-1117.80	1.13	0.21	-27.50	-0.14
5-NH ₂ -NH ₂ -Mo	-1121.04	1.49	0.27	-30.45	0.32
6-NH ₂ -NH ₃ -Mo	-1126.66	1.65	0.36	-36.00	-1.80
Distal pathway					
3-NH ₂ -N-Mo	-1114.30	0.81	0.22	-24.34	-0.39
4-NH ₃ -N-Mo	-1118.61	1.03	0.27	-28.48	-1.11
5-NH ₃ (g) +NH-Mo	-1102.85	0.35	0.09	-32.63	-1.85
6-NH ₃ (g) + NH ₂ -Mo	-1106.62	0.68	0.11	-36.08	-1.89
Enzymatic pathway					
3-NH-NH-Mo	-1113.57	0.79	0.15	-23.55	0.40
4-NH-NH ₂ -Mo	-1117.63	1.16	0.16	-27.26	0.10
5-NH ₂ -NH ₂ -Mo	-1121.04	1.49	0.27	-30.45	0.32
6-NH ₃ -NH ₂ -Mo	-1126.66	1.65	0.36	-36.00	-1.80
7-NH ₃ (g) +NH ₃ -Mo	-1110.12	1.03	0.12	-39.25	-1.64

The atomic coordinates of all the optimized systems for the intermediate states.

(1) 2D Mo-Pc (POSACR)

C H Mo N

1.0000000000000000

21.5339999999999989 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.533999999999989 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.0000000000000000

80 16 4 32

Cartesian

4.5235413598656953	0.6097010852923684	6.9536556707098187
5.2620268832919610	10.1960679250272346	6.9494199933507854
7.1265849098808776	3.1692729461543485	6.9573036836542412
4.8365869620045512	3.1714531240781465	6.9573678596264203
3.1588503008905104	4.8491697082269178	6.9529056498845003
7.1225951881230358	8.8121837199423876	6.9453720246151018
8.7996045629091810	7.1351633566647186	6.9460527820053404
3.1566831092942467	7.1391492806522221	6.9458076518591954
6.6959310555715916	10.1946187665339814	6.9491907310013756
4.8329083559576445	8.8145317452117276	6.9455334917689822
7.4366781383381717	0.6069986376944241	6.9531031798863872
8.8019615695375215	4.8454942001587353	6.9532357654581940
1.7750032512426146	6.7105598382731415	6.9462063654479946
0.5944269769350844	7.4492722664875108	6.9432871255510182
6.6979862989795800	1.7875920894338870	6.9565698411061350
10.1820435444892716	6.7085163586129530	6.9463666773917199
10.1834890155302507	5.2746265735139515	6.9515991815105371
1.7765261625843674	5.2762800380262691	6.9514095613209745
0.5971141320847151	4.5361269534947395	6.9543787236239174
5.2636992031185326	1.7891167908819152	6.9567647647786037
4.5235414199570645	11.3766959902590905	6.9536557716925351
5.2620269526189665	20.9630693295370705	6.9494199015251459
7.1265908252697949	13.9362670076493060	6.9573036531332670
4.8365806792205461	13.9384469739995058	6.9573678733864668
3.1588445464288948	15.6161644797890524	6.9529057334661184
7.1226014943897811	19.5791891648959933	6.9453719686040793
8.7996097874436732	17.9021684680250459	6.9460527850767209
3.1566780565265393	17.9061537371130868	6.9458076557987249
6.6959309197032439	20.9616200235483490	6.9491906693423262
4.8329023478561197	19.5815380681256137	6.9455334107479185
7.4366781660778560	11.3739936124077747	6.9531031655345172
8.8019673841371660	15.6124892653999030	6.9532357972609882
1.7750032065652195	17.4775578168483392	6.9462064127174834
0.5944271134646626	18.2162689865387932	6.9432871311920215
6.6979862777932038	12.5545907792803941	6.9565698095110688
10.1820438433194198	17.4755142589813381	6.9463666990062549
10.1834893999399156	16.0416286335161509	6.9515991733824167
1.7765262626662552	16.0432815268723559	6.9514095836569769
0.5971142551886367	15.3031301603911842	6.9543787410015776
5.2636989412038995	12.5561156996244208	6.9567647803342867

15.2905469806396468	0.6097013453895687	6.9536555922208034
16.0290302157843136	10.1960683903710976	6.9494200357021878
17.8935924469084888	3.1692644486116368	6.9573035933546059
15.6035784065062231	3.1714438612358720	6.9573677608627751
13.9258403773144455	4.8491593326654732	6.9529057093327662
17.8896034443382135	8.8121924163871412	6.9453719860029430
19.5666136135548925	7.1351736410309483	6.9460527169885440
13.9236731006222758	7.1391593027890732	6.9458076115395935
17.4629276019707085	10.1946190217679789	6.9491908111189034
15.5999001265998789	8.8145412749972714	6.9455334476210746
18.2036725341835748	0.6069988059366138	6.9531030943528984
19.5689719119763730	4.8454841521125438	6.9532357683808934
12.5420011038221055	6.7105598556011579	6.9462064618391466
11.3614186984967613	7.4492722892838517	6.9432872097738851
17.4649830327456819	1.7875920555084894	6.9565696067367844
20.9490454809897066	6.7085162010026949	6.9463667202480481
20.9504911961787101	5.2746266745617572	6.9515991103731274
12.5435244140439526	5.2762796792894573	6.9514095549376504
11.3641057363283924	4.5361270748519873	6.9543787540490980
16.0307018530896244	1.7891170372024909	6.9567645396475637
15.2905471039625986	11.3766963489669504	6.9536556210577380
16.0290302438887444	20.9630696248275825	6.9494199098504534
17.8935991685079578	13.9362578266571457	6.9573037521712413
15.6035721657487763	13.9384383474228102	6.9573678638485221
13.9258352374951855	15.6161542449287616	6.9529058716978920
17.8896094130923444	19.5791981477753154	6.9453718312750885
19.5666191380845582	17.9021783812618516	6.9460526689205793
13.9236673755092468	17.9061646414837377	6.9458074842355124
17.4629277985880229	20.9616200111249249	6.9491906975102591
15.5998939184282186	19.5815475128077310	6.9455332668902132
18.2036725874709653	11.3739937032689937	6.9531031593595021
19.5689776254302004	15.6124789558602952	6.9532359204472440
12.5420009243137773	17.4775582006431414	6.9462064226844191
11.3614187552207557	18.2162691501290794	6.9432871257488058
17.4649832626174408	12.5545906124910953	6.9565696521999678
20.9490454968330155	17.4755143645247486	6.9463667491892522
20.9504914042719328	16.0416286185282999	6.9515991116328841
12.5435245193372857	16.0432816151208364	6.9514095808174616
11.3641059771632271	15.3031304203752114	6.9543787904446948
16.0307019107793209	12.5561159626591010	6.9567645453976903
0.5988228534812629	3.4457467612111725	6.9590249853995925
3.4331519536571622	0.6114381387121935	6.9540853375300005
8.5272486752743681	0.6056729502211406	6.9528405585472139
0.5931450538828386	8.5398416603153020	6.9388690488356639

0.5988227115507228	14.2127468781533324	6.9590250654128010
3.4331517513080669	11.3784403168723696	6.9540855747485608
8.5272485279930592	11.3726752931708965	6.9528405452867910
0.5931451820543177	19.3068414913900064	6.9388690421087444
11.3658263735665699	3.4457464465741068	6.9590249604875307
14.2001523568073722	0.6114379699311951	6.9540853541398215
19.2942482307831717	0.6056731228156145	6.9528405449885184
11.3601487909052246	8.5398414309695401	6.9388691512367924
11.3658263798747203	14.2127466515665191	6.9590251389117048
14.2001521487659872	11.3784402382160454	6.9540854227961146
19.2942480477054126	11.3726751803677431	6.9528406853842322
11.3601485996514207	19.3068413209687542	6.9388689913494739
5.9791566012808595	5.9917350458359238	6.9481836003165247
5.9791565990514117	16.7587350008686080	6.9481839800616987
16.7461564877024642	5.9917351812674147	6.9481842811597989
16.7461566508063697	16.7587352419894273	6.9481852210732606
8.3937839387348419	3.5780992351324779	6.9564532680939388
8.3893012083488223	8.4018660899327831	6.9447571107542192
3.9532390535316924	5.9949314176670763	6.9491283404408897
5.9769480279944052	8.0176376801780762	6.9436455459355368
3.5698813161733836	3.5824810259909929	6.9563515006601895
8.0050659249684948	5.9895184443718392	6.9495767607172754
3.5655012733088003	8.4063476525546275	6.9448244953746210
5.9823677661915040	3.9658456157552489	6.9569795651558985
8.3937874252163347	14.3450970629578389	6.9564531615171523
8.3893050566250604	19.1688679620075533	6.9447572173478971
3.9532616675498944	16.7619301020450067	6.9491282551264995
5.9769488882652793	18.7846200891513178	6.9436457418473516
3.5698774509203206	14.3494791190191080	6.9563514372594959
8.0050434253196681	16.7565190546588596	6.9495766071320944
3.5654973302334483	19.1733492107955215	6.9448244758951141
5.9823664112252342	14.7328629822654449	6.9569791651275583
19.1607864453373686	3.5780930120495640	6.9564530276580046
19.1563038362282256	8.4018720433406227	6.9447573525208188
14.7202680095921821	5.9949295412054608	6.9491282104148242
16.7439487741124999	8.0176008742520413	6.9436458336255225
14.3368786631604799	3.5824750829034451	6.9563512431391796
18.7720366463774937	5.9895196218033968	6.9495765472706559
14.3324980238800439	8.4063533646425661	6.9448246483529292
16.7493660762872096	3.9658826231779538	6.9569787305206043
19.1607900977330061	14.3450915387966411	6.9564530662484207
19.1563067608608435	19.1688729612857642	6.9447572798071029
14.7202906997593992	16.7619296605699546	6.9491281992080491
16.7439490192624092	18.7845834147745983	6.9436460151747212

14.3368759152315945	14.3494743655000256	6.9563511865431629
18.7720142757398314	16.7565195553383788	6.9495764885272600
14.3324948067814901	19.1733551709694474	6.9448243916660850
16.7493660222759821	14.7329000737853200	6.9569784897779146

(2) N₂-Mo-Pc (POSCAR)

C H Mo N

1.0000000000000000		
21.5339999999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	21.5339999999999989	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000
80	16	4 34

Cartesian

4.5239374245940205	0.6161389489173817	6.9117911568578263
5.2646148097435805	10.1878561490099848	6.9315346082378477
7.1214573458892252	3.1777774952533369	7.0020482360388510
4.8377965397911202	3.1777928864442013	7.0021935964882340
3.1653141697762592	4.8502329864360627	7.0012334147071558
7.1214670068507893	8.8063534400615247	6.9984113328956719
8.7938717146287875	7.1339035578080363	6.9984825567882227
3.1653494495752419	7.1338661404153223	6.9988407172185827
6.6946323985404907	10.1879016984064936	6.9315034668050881
4.8378328272983238	8.8063026112948783	6.9985236939131195
7.4352289054079392	0.6160435774460659	6.9117484734327057
8.7938829727360623	4.8502762558615151	7.0008546387580122
1.7838357866647305	6.7070080804984551	6.9307577107439897
0.6035879328320106	7.4476626443090419	6.9090302600766886
6.6946175482099983	1.7963073788947810	6.9334733385438891
10.1753698159867909	6.7070479421005000	6.9304402958540594
10.1753638466523046	5.2770376357291253	6.9322078469444923
1.7838069476793641	5.2770056429730205	6.9325378175966277
0.6035765312545343	4.5363796652630581	6.9128611136250253
5.2646048522487119	1.7963124175777301	6.9335346565540794
4.5239327151347375	11.3681197972885411	6.9122266705527187
5.2628276062040609	20.9696491525813542	6.9081343226297172
7.1229544325598049	13.9342423942823768	6.9326567710251972
4.8360536608228051	13.9342131077143296	6.9325515287541135
3.1596919701714286	15.6150640212165541	6.9486895605402523
7.1229781625410213	19.5839786680247094	6.9283593590375521
8.7992696315421473	17.9031393210898635	6.9463035972249605
3.1597012073128870	17.9031152390568842	6.9461027753842686
6.6962706986042777	20.9696430654001240	6.9081545618979074
4.8360809223097743	19.5839625899012653	6.9282851454801246
7.4352300369176971	11.3681571947475355	6.9122431776761069

8.7992513753752792	15.6151203387828446	6.9488921518008979
1.7756682496474776	17.4750203105214403	6.9457390249677626
0.5969544290756629	18.2158145076110323	6.9460307100230603
6.6962538710134529	12.5485912420942789	6.9110561473082814
10.1832931213941844	17.4750338647463224	6.9458876950541901
10.1832665680241270	16.0432138042820469	6.9477956062667525
1.7756520987491955	16.0431920726534258	6.9476580008746591
0.5969769036571601	15.3024093115659046	6.9501629938222607
5.2628227363210822	12.5485609771733291	6.9110022963407358
15.2898368091255996	0.6096004391938534	6.9494591750067123
16.0306732103075831	10.1958545620922223	6.9465638264629863
17.8905845579211018	3.1722877997960115	6.9503617030538747
15.6025446180780154	3.1723066018211021	6.9503380024992545
13.9217006770924314	4.8486225045277092	6.9312283623522433
17.8906443202848209	8.8118614764305327	6.9457396112698406
19.5714857223130814	7.1355263783760128	6.9286597959631768
13.9216999740646106	7.1355137188493680	6.9285934746416196
17.4625082622152199	10.1958914029633743	6.9465573777262213
15.6025928809918639	8.8118193440096917	6.9457359984278417
18.2032279725448944	0.6095337310850995	6.9494461162120214
19.5714322199143389	4.8486342644357903	6.9313240291459293
12.5360498753318534	6.7087742142865272	6.9075304823646455
11.3555707344140231	7.4476890934948488	6.9088052114719654
17.4624667279270369	1.7882621954140707	6.9494165961896890
20.9571352077715822	6.7087702926514643	6.9076571026791251
20.9571098360937214	5.2753344164379348	6.9095124913013661
12.5360489257466536	5.2753449338790475	6.9093638497878977
11.3556403528920722	4.5363909227736965	6.9126163550009991
16.0306556178753574	1.7882594889115193	6.9494249321170320
15.2898522793672580	11.3745474962745714	6.9494768641038478
16.0305505652717848	20.9649171933776408	6.9499630800340064
17.8897895877645290	13.9376763571278257	6.9539838323383307
15.6031614375510426	13.9376523317739220	6.9539303016304048
13.9250436156974011	15.6157499107314113	6.9523433567206130
17.8898096382687406	19.5804813059230653	6.9492898996938361
19.5678877471287436	17.9024045023538427	6.9497718028796820
13.9250634344437820	17.9023688733790856	6.9495790646063789
17.4624687977214030	20.9649271857148030	6.9499718244893929
15.6031999560261152	19.5804566851142994	6.9492367280245739
18.2032428498604446	11.3745862105687259	6.9494604563791933
19.5678686034697513	15.6158110000783896	6.9525247554755136
12.5406087098859995	17.4750420011931773	6.9491457530175316
11.3619684558687677	18.2158142591900756	6.9460399858650490
17.4624606191734095	12.5532162245023287	6.9528728984340633

20.9523386164310494	17.4750694501605750	6.9492838122780478
20.9523187020879931	16.0431612076341317	6.9512509798418227
12.5405857637932012	16.0431273300656940	6.9511236246743051
11.3619607135793199	15.3023990455559833	6.9501680154589831
16.0305566320996711	12.5531831334638078	6.9528715828395935
0.6043431489226341	3.4461401188402205	6.9202153453285637
3.4336914924946229	0.6169967823697451	6.9176108221235264
8.5254585858911689	0.6168752076927666	6.9175712144537282
0.6044779578798211	8.5379019081808512	6.9132510974921697
0.5972532265356478	14.2120762402052332	6.9520866673491604
3.4336898940811711	11.3672837177094088	6.9180156633347929
8.5254696641256658	11.3674458269162368	6.9180622918222276
0.5972721286353524	19.3061390996888740	6.9445144252820237
11.3548856917216696	3.4461562661125948	6.9199908237975265
14.1995005145962132	0.6099464965187039	6.9496977423835773
19.2935459112362189	0.6098449033923210	6.9496274437999830
11.3547890874898361	8.5379383092745247	6.9130277073960160
11.3616459445763702	14.2120711189493321	6.9520882413203982
14.1995256234665490	11.3742397931550538	6.9497073576327022
19.2935578300989974	11.3743902041987059	6.9496373728799563
11.3617307145070399	19.3061410148898212	6.9445299389869257
5.9796503660834652	5.9923432809691821	7.3935834314600024
5.9794512218170714	16.7591304215322729	6.9892704859618346
16.7465586231391654	5.9920777988586851	6.9889954065883115
16.7464393731746952	16.7590427525865451	6.9491263370918670
8.3862697958899322	3.5854408429939704	6.9854128814826320
8.3862453289588235	8.3986872723553549	6.9817121482126314
3.9618946040808152	5.9921154613255991	7.0808945332529687
5.9796843783034621	8.0097398357145462	7.0787316230299444
3.5729989413258170	3.5854544429395188	6.9857080854925142
7.9973210666822103	5.9921790156158723	7.0804505065346550
3.5729877964987891	8.3986778904507577	6.9819578632385353
5.9796392330070116	3.9743532284700231	7.0829279226405344
8.3898811875528878	14.3470802384862051	6.9381567105138284
8.3898679831457237	19.1711155042682329	6.9339278807720266
3.9494231461161267	16.7591015851638119	6.9565605186469437
5.9795601740496975	18.7919830292028927	6.9459388662942523
3.5691276984450599	14.3470542292367735	6.9379674147082735
8.0094995331369994	16.7591569531699101	6.9567619908034919
3.5691264186455283	19.1711305798949070	6.9337634173295353
5.9795040215935389	14.7261965217443702	6.9506102764552171
19.1586045199935633	3.5816876900811989	6.9382409242668102
19.1586208945142928	8.4024154479138566	6.9338069675998923
14.7136565247203155	5.9920883552089306	6.9479276197711375

16.7466479995035940	8.0220850505073980	6.9542443711405904
14.3345346155275717	3.5817047678266549	6.9381638895297550
18.7794766553751451	5.9921323201304357	6.9479786015295755
14.3345521343016493	8.4024305063669864	6.933766488276525
16.7465783008807279	3.9620435609668241	6.9594756947919345
19.1572148692174302	14.3483679699156141	6.9537547120646863
19.1572070023861869	19.1697967263297748	6.9492281809379328
14.7149832104641405	16.7590570178446256	6.9507768815479078
16.7465293456808730	18.7905106946402256	6.9484744336074158
14.3357327225836020	14.3483303486500038	6.9536237017628926
18.7779159878912871	16.7591235855609959	6.9509788797456604
14.3357505611365728	19.1697932948277021	6.9490853587501711
16.7464763998070225	14.7276096163631998	6.9538042301229410
5.9811654518122594	5.9971933729852145	10.4982674383474599
5.9804666232922665	5.9953491603464144	9.3530946291946027

(3) N₂H-Mo-Pc (POSCAR)

C H Mo N

1.0000000000000000

21.5339999999999989 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.5339999999999989 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

80 17 4 34

Cartesian

4.5277581320496640	0.6182147847221552	7.0136233481167505
5.2659017612243595	10.1791100163330377	7.1215568551449033
7.1204728365480170	3.1833540354418957	7.2388060750547210
4.8416044657642265	3.1833501420931087	7.2394290620521060
3.1599171846830778	4.8520027780627917	7.2717815516335618
7.1203010057149934	8.7956923686875204	7.2400228605449177
8.8017384297992507	7.1276650872269709	7.2666564719640387
3.1604813735126589	7.1274208866576672	7.2681211930100753
6.6959008136096152	10.1792725796602515	7.1218052405465482
4.8418750576588785	8.7955265169963877	7.2400178863464344
7.4339905664704888	0.6180673307129714	7.0132949943297254
8.8022256177011755	4.8521188578044532	7.2697621535430796
1.7767240468573529	6.7038179725079123	7.1019039755999414
0.6034273217076270	7.4424324166104467	6.9597482348005233
6.6961726878752845	1.7998065617404244	7.1189793975414091
10.1854034789124821	6.7039368916127353	7.1000110746436906
10.1856951090023831	5.2759563522347754	7.1021244090352820
1.7763663777666632	5.2758108159666994	7.1043434907093630
0.6028281966762226	4.5375918145620071	6.9627876981973422
5.2657550256282670	1.7998969429758143	7.1191753310091110

4.5276842514191147	11.3602455643636162	7.0165005762206549
5.2637769424013472	20.9727084886400270	6.9098760026199102
7.1239381954481464	13.9270584248673881	6.8038082148718217
4.8372572365570266	13.9269795460640200	6.8044361685467178
3.1610319622508412	15.6121457513209911	6.7873693331508980
7.1241306940894420	19.5858052205206974	6.7971004265787709
8.8005313529273561	17.9010319375320179	6.7797509968108187
3.1607550085704981	17.9010301655729869	6.7837942576424997
6.6977361383890699	20.9727192239338081	6.9095250266498347
4.8372893193960484	19.5858234500687090	6.7981154598704121
7.4339263200287933	11.3605188635245504	7.0169525982069132
8.8001135146667622	15.6121596140342351	6.7836922176314935
1.7767728051448195	17.4728200286121016	6.8591626787917335
0.5972767730647075	18.2116717240343178	6.9250476029665453
6.6975205219005325	12.5400473980291913	6.9151705798503942
10.1846774490330816	17.4727655361411642	6.8509708848255793
10.1844320492884144	16.0401924256520161	6.8542711369955569
1.7769524708406637	16.0402705015861216	6.8621643546429869
0.5976266670294625	15.3014319148608688	6.9324663240107132
5.2638584887832378	12.5399615714255148	6.9151892840732208
15.2934423120662650	0.6077162273743562	6.8680397901226646
16.0324512534162444	10.1927988510172955	6.7903686088324484
17.8915772494528049	3.1711780175678390	6.6898326482015644
15.6043631081194203	3.1710606549526372	6.6869935276374211
13.9214554641587327	4.8482261162154066	6.6964138483430098
17.8916514217292395	8.8091441169590787	6.6915526609698617
19.5746260243800663	7.1321306251065248	6.6992555117662889
13.9214336852655691	7.1321637196328522	6.6959216066955820
17.4635623566648484	10.1927524962612512	6.7925781885936480
15.6045147017466590	8.8092360777507608	6.6890279206661942
18.2023968369108786	0.6081092026115621	6.8740114625197828
19.5745318793014782	4.8481761476164715	6.6999786662934842
12.5384788491081451	6.7056541893645720	6.8283060011151280
11.3587783945327434	7.4425449378504993	6.9579055069511071
17.4635319377669127	1.7870765837243354	6.7855357956865960
20.9576034719994944	6.7055115608579765	6.8310493566616257
20.9573680653049585	5.2746866574944260	6.8320209442037534
12.5386468441316481	5.2747399482949779	6.8291156810722455
11.3592717144793145	4.5377035791810423	6.9605090545144677
16.0322370940501813	1.7869919724421146	6.7830727562459865
15.2935620792854241	11.3717136558946983	6.8796727297393589
16.0322989125486046	20.9630188901472252	6.9557554318938219
17.8905669717046933	13.9344393755801157	7.0744133659509707
15.6051457592805658	13.9344895556750004	7.0692888157966429

13.9270675263928414 15.6136506408468367 7.0701199842229432
17.8905101818543848 19.5789560322692751 7.0606462590687720
19.5683667879196044 17.8997729951735600 7.0757547338294744
13.9272530245654131 17.8995822536829259 7.0637487004080031
17.4635587595165731 20.9631996774676779 6.9589559073631335
15.6051140474131813 19.5787607510592885 7.0553948469772969
18.2024651571422744 11.3714210008289669 6.8851737526984520
19.5685123963347607 15.6137985042417711 7.0819466827401767
12.5436002334529917 17.4723704347983073 6.9830472577996590
11.3643914151602967 18.2115380208867172 6.9135324493542258
17.4636649341475554 12.5499949538581692 6.9737050704818824
20.9521065438115670 17.4725741559221674 6.9963115637588134
20.9522361970123434 16.0406337003319628 7.0002193538036401
12.5434073643882833 16.0404465287647184 6.9871780562506896
11.3639015309872153 15.3012566795917557 6.9215856836549587
16.0323244412729764 12.5501240317617881 6.9706577839692923
0.6032462245468204 3.4471785833732538 6.9629028048547035
3.4371944415993538 0.6184298503978439 7.0144030792358887
8.5244614469968312 0.6179989519294576 7.0141825926675523
0.6043420407682906 8.5328073741287920 6.9586823527840407
0.5973750062393263 14.2110554134341402 6.9353858077638115
3.4372094114483853 11.3596530592337359 7.0155887046091694
8.5243336509650067 11.3600139895621304 7.0168416791637576
0.5967969934629533 19.3019333437925269 6.9216211827281127
11.3585858599181098 3.4472871744183333 6.9611267408937243
14.2026671809923393 0.6067754150318968 6.8667281777576292
19.2931365619114494 0.6077741354893930 6.8775669794357635
11.3575666910063138 8.5329252140281930 6.9577036931862661
11.3640981705396431 14.2108903182194393 6.9248327729340495
14.2028059440904944 11.3716573160753569 6.8778265911632106
19.2931650783563526 11.3709382420304177 6.8878465026913887
11.3650187705240313 19.3018096195929658 6.9098125978253986
5.9959098457313305 5.2349228626863615 11.3472558358815512
5.9815215668371584 5.9906647642550848 7.8044765991551825
5.9804479704461100 16.7560954996409777 6.5426047980317765
16.7481879439009091 5.9902117794244321 6.3968160541011763
16.7472455853135429 16.7572910092230245 7.3324357050948148
8.3902938001785472 3.5904257151967993 7.2277016005164798
8.3896751089593700 8.3890423027149819 7.2235714717011064
3.9469749714498423 5.9898118595004286 7.4272581551543144
5.9811080349067831 8.0042846705343660 7.3246756870403456
3.5717180557846784 3.5903315327074266 7.2293111018736926
8.0152740860325746 5.9899549340006821 7.4251856369041427
3.5724478722379343 8.3887793759234714 7.2241914808812968

5.9810686022695023	3.9743534053948535	7.3228577793862888
8.3889301874799553	14.3442230856239306	6.8152376991377794
8.3893691798851684	19.1690358051737419	6.8089950906329140
3.9494030328400931	16.7565707954032668	6.7115280988442665
5.9806785127911910	18.7977976384023719	6.7067065676462683
3.5722527947852480	14.3441616196255097	6.8176291765368724
8.0115801641040889	16.7566264606301338	6.7098358328111622
3.5720927484364049	19.1690202419157671	6.8119718090990187
5.9805462670259804	14.7151846733560614	6.7137023606100446
19.1586133277712598	3.5819282791168119	6.7223127920189114
19.1586849369964263	8.3982544327864641	6.7226006151849207
14.7098862855064230	5.9901658554179589	6.5870069857002029
16.7481660215858419	8.0207509335955383	6.5964625150478744
14.3372596053799413	3.5818947661546705	6.7181083580148329
18.7861415546549431	5.9901435683820088	6.5903980727316389
14.3373985133527206	8.3983249518530521	6.7188538502647326
16.7480578675570051	3.9597887999991133	6.5971443439400570
19.1567418202689410	14.3464144965663678	7.0574774430715301
19.1567512832508520	19.1670268391383090	7.0455615478449136
14.7160006694597385	16.7567955263646304	7.1471535003102540
16.7476813193802130	18.7902368752017850	7.1471873284499612
14.3389627035805329	14.3462950089325627	7.0473280083844951
18.7794167128460110	16.7569854175958817	7.1579055386840116
14.3389484182021363	19.1668244608072413	7.0352127673607416
16.7476583255635170	14.7232910599894549	7.1597651008618914
5.9922260867814439	6.1407094239958466	10.8368256798948490
5.9868153443406831	5.9983212940001609	9.6092095568124325

(4) NNH₂-Mo-Pc (POSCAR)

C H Mo N

1.0000000000000000

21.5339999999999989 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.5339999999999989 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

80 18 4 34

Cartesian

4.5176915181505741 0.6540294914008321 6.9771295001297595

5.2579952023722187 10.2156353650738616 6.9196376274684805

7.1089226976962339 3.2145346532211172 7.1550702620686790

4.8370624423975341 3.2154531831803483 7.1435658692587687

3.1778974856568314 4.8867613905491032 7.0908051592928194

7.1078907185042857 8.8364799807999752 7.0433111005570073

8.7676571088606021 7.1646240253962317 7.0634743848361889

3.1768235745361708 7.1670278075235840 7.0438329992238655

6.6882615687283353	10.2148842735180594	6.9267352213136268
4.8357729413818946	8.8372813789635813	7.0342184605067501
7.4278063197508981	0.6534509219585001	6.9925012843024055
8.7680939540405873	4.8842294186594604	7.1127270864729084
1.7967934793771974	6.7388406694489005	6.9639203182285891
0.6120776090713426	7.4756059622920832	6.8816636392292345
6.6875944652034587	1.8342114331032775	7.0629596191441397
10.1480482644761398	6.7379470880121435	6.9937073229058608
10.1487484935173402	5.3085966553840880	7.0248035356854119
1.7977779335318693	5.3096103321743957	6.9950338348247847
0.6130567506905020	4.5689650832894779	6.9455251521150716
5.2576633128971801	1.8351181702103450	7.0557447118897594
4.5185187323585732	11.3961985147414246	6.8373342806149005
5.2542306343237666	21.0063018316598118	6.9153135058195669
7.1183144455669547	13.9636444295583395	6.7403367892735666
4.8305296308327721	13.9635630436333908	6.7284827187122671
3.1549336573342748	15.6470834286785774	6.7530896794717368
7.1170954305941105	19.6214699951468425	6.8497564309702641
8.7926990311235684	17.9377412785875343	6.8288420693768881
3.1543711870081235	17.9376381437738104	6.8006713605428022
6.6914366889342913	21.0057545695964656	6.9231558571399203
4.8290255155493806	19.6215506445763914	6.8374029562843939
7.4287403212611647	11.3960364774044560	6.8522755759336853
8.7929522791471229	15.6472123657203532	6.7809889748942309
1.7706888643287217	17.5065898104142796	6.8445673271921574
0.5914114050874073	18.2441381972821617	6.9074599882754759
6.6926580686865345	12.5777672120251403	6.7865098267557675
10.1763042131775752	17.5068738158493282	6.8814616400185109
10.1762587243085658	16.0753556011961081	6.8505026856392233
1.7709740322313070	16.0750603839513886	6.8137182930345555
0.5921110057132207	15.3346998691540239	6.8429507943335039
5.2554047439460989	12.5781583927338048	6.7790363490046142
15.2854866511628540	0.6386511615733799	6.9889332328853415
16.0236658671346568	10.2220179197107566	6.7855874682106094
17.8863979685342898	3.2013815080466772	6.8666439897509060
15.5934898619150086	3.2016804297993855	6.8787340582770247
13.9052739696914553	4.8756311293477612	6.8555907827346356
17.8858517518650331	8.8372150653176114	6.7471870388272244
19.5741674405265123	7.1632265379152367	6.7775156055347310
13.9051556768301978	7.1640776839715681	6.8048564919021857
17.4557138241636594	10.2219228306507208	6.7778219266558297
15.5930443802231888	8.8375165549784889	6.7590479760323880
18.1952803761781290	0.6385822144495720	6.9722734687425527
19.5744836880820579	4.8747584855311112	6.8277115198154688

12.5172416956249908	6.7400959611844051	6.8749823148843978
11.3332176645996601	7.4754030908406488	6.9148932522874427
17.4561649738817586	1.8180628164241319	6.9323209827778109
20.9620685170952292	6.7397005848044360	6.8406696764544312
20.9627511025374460	5.3014052938132199	6.8722714868377244
12.5177164135201870	5.3017710543601009	6.9070785684012312
11.3334448753674781	4.5686881926145251	6.9793491287609042
16.0240942649431197	1.8181469015752718	6.9402070276514261
15.2850225585631740	11.4017573007347899	6.8278311013452626
16.0246292904879013	20.9924743141455750	7.0263326796238603
17.8841739513790436	13.9651634320914013	6.9236514585367859
15.5967707152410568	13.9651802134780585	6.9370361800640250
13.9188314429091360	15.6432582775808129	6.9827260805531015
17.8844952516004945	19.6080249361721464	7.0502259484435124
19.5623607407824593	17.9299912887966322	7.0039976495429528
13.9190457152187008	17.9299476925758299	7.0357203951185250
17.4566353989191967	20.9924563478700676	7.0178798573588441
15.5972799501155119	19.6080409339278248	7.0638414743426914
18.1947064422887088	11.4016890867636906	6.8114350904587901
19.5624181055921085	15.6432718569252600	6.9512023792523427
12.5353743307436822	17.5039669037236827	6.9766937475151236
11.3556101900685587	18.2442514365094155	6.9461509520740687
17.4561557922130746	12.5818813777079299	6.8588055861846904
20.9456942821535712	17.5039302510237178	6.9375231348339668
20.9458210388244979	16.0720675100192381	6.9050052519776743
12.5351913537784121	16.0721067318421902	6.9440799914889419
11.3549515413302959	15.3348385847606448	6.8814886960468415
16.0240581926791670	12.5819039705662856	6.8670939475064641
0.6138558956456238	3.4787407802119263	6.9712086445803587
3.4272257582223191	0.6539879332748483	6.9703358619919173
8.5182793149933858	0.6530197635272255	6.9973605165018613
0.6119694012858133	8.5659195807650423	6.8585613346788286
0.5925494161491693	14.2447777252686869	6.8192754690296091
3.4280038864025939	11.3967152076476328	6.8339329539781177
8.5192407298408188	11.3968205509173810	6.8604733315329129
0.5910110158068547	19.3340178823027493	6.9326114527491960
11.3329351305250903	3.4784216484129504	7.0038024029169366
14.1952968921865832	0.6386446296541927	6.9921408940717340
19.2854098870096387	0.6385733031344355	6.9628514925486460
11.3327546406199371	8.5656885118235397	6.8901074991745226
11.3544117857969020	14.2449705182133286	6.8553901078379287
14.1948559708832125	11.4014101047653345	6.8370818232460691
19.2848657406625001	11.4012875618861642	6.8081546506801347
11.3560611425527256	19.3341967418698140	6.9689065019622953

6.8714463594739801	6.1570164121658655	11.2510604681572524
5.2332424667594051	6.6402725871431780	11.2397333496796286
5.9705604853279137	6.0389920826395214	7.7403849482989093
5.9745796563829767	16.7958640891485338	6.6239857237542115
16.7390979647329594	6.0164562843533860	6.6755521731217264
16.7415388633725364	16.7831451600186341	7.1460868020941533
8.3754164346238493	3.6169786443006382	7.1297207963339186
8.3738471438457900	8.4312302060261857	7.0321838364380156
3.9884703672613564	6.0298613860162797	7.1362882519029283
5.9700733254397846	8.0364640455750642	7.1438729753674748
3.5719120836493725	3.6202068152076179	7.1067613526478173
7.9565384965767638	6.0245222131392033	7.1505555474504963
3.5689047964571854	8.4344353310150701	7.0163902245766065
5.9738520118808509	4.0178898642628562	7.2390432492735295
8.3854824920448756	14.3799075515626456	6.7695050066197142
8.3844842059563902	19.2042879929099826	6.8643552357315274
3.9476037260872920	16.7937138784063080	6.7258538138610611
5.9732414496588140	18.8325243698018490	6.7787767092487741
3.5630208886460362	14.3800863325473127	6.7454160197914987
8.0003066900966235	16.7933560816002689	6.7478970145849697
3.5617203846559580	19.2045145790319296	6.8395724321329938
5.9748238698033260	14.7540655871474762	6.6883210918388265
19.1546148034858419	3.6087393104837333	6.8663290492286366
19.1538179798408486	8.4297840704735663	6.7643194659669330
14.6951155871676900	6.0189678479725899	6.7788181216032903
16.7390254689836269	8.0442681070770483	6.7198676954813195
14.3255888558380704	3.6094821557949959	6.8904525200731168
18.7840605185586078	6.0177209215278804	6.7562283947164907
14.3249622024148096	8.4306060837064507	6.7878786027231204
16.7399041417358028	3.9932219397337221	6.8165185346810233
19.1513970635896236	14.3762376761073654	6.9133246530748949
19.1515438238212035	19.1975071506338111	7.0207205549315237
14.7099911910437644	16.7853992524311266	7.0556808945677281
16.7411483400604979	18.8162742675450900	7.0951306977282798
14.3294534913680582	14.3762001978790508	6.9403075662223035
18.7716857868971871	16.7854644419114294	7.0292039255062706
14.3300351300162649	19.1974288715850712	7.0480400172515818
16.7407895312425836	14.7553854166406868	6.9897708234945073
5.9489239814055459	6.0380619235065582	10.8217569895111083
5.9717074117836857	6.0847723655868720	9.4924375416816638

(5) $\text{NNH}_3\text{-Mo-Pc}$ (POSCAR)

C H Mo N

1.0000000000000000

21.5339999999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	21.5339999999999989	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

80 19 4 34

Cartesian

4.5386812559032634	0.6191336621281399	6.9864604501743717
5.2804253108792372	10.1788109043228427	7.0956669308886040
7.1289389940329517	3.1832080374445821	7.1920481141113903
4.8635244179922132	3.1843120687163378	7.2148231412134800
3.1947402560752085	4.8566307780389710	7.2340818227620964
7.1288341848654007	8.7917168883403036	7.2027011563045784
8.7992585616219685	7.1203019985610858	7.1852168490168182
3.1944661683646451	7.1184998105349573	7.2396809879102966
6.7079802480470345	10.1794862098737386	7.0817087746547855
4.8633354264506021	8.7904794762707645	7.2257131848114620
7.4467830143258391	0.6177301406966290	6.9598830442804172
8.7992611372038301	4.8547656152327674	7.1809868105261163
1.8051724594296328	6.7003499303789456	7.1325085004556970
0.6287433681079596	7.4415086369184236	7.0444512377957755
6.7081160949334331	1.7956281010140165	7.0678778687196440
10.1863424858017950	6.7016181392120151	7.0527636221903549
10.1863361719629335	5.2739926897417542	7.0502637659770508
1.8052996346898533	5.2751537509286797	7.1295248255513410
0.6284307441089174	4.5341779076667938	7.0396979804650233
5.2805892320729573	1.7962213250112620	7.0818522291037089
4.5385101261600012	11.3560241582498520	7.0006933528052864
5.2748423145490042	20.9716600134295348	6.8882155806626670
7.1327915287177222	13.9248400533907635	6.7937616970844221
4.8473023439670584	13.9244151936806233	6.8110170909031336
3.1726609747252574	15.6100098819585025	6.8103945373160464
7.1329165410258781	19.5840440079571536	6.7836664893992147
8.8076992777684637	17.8988036356207907	6.7686324267152624
3.1727613633266563	17.8989809110567855	6.8059714422479836
6.7075105930912375	20.9711951133961954	6.8762148489159589
4.8474853459720748	19.5844734253181123	6.8008884638377696
7.4466013821078159	11.3574607970558024	6.9742550023486833
8.8076756053508412	15.6100158860971252	6.7730080433437037
1.7888100750532185	17.4707212468473081	6.8748347442535556
0.6100019352211968	18.2111307240001352	6.9260716805592315
6.7074016696817083	12.5378766194333586	6.8895834269602982
10.1921738274561555	17.4705162635434874	6.8267567199323222
10.1922073637651387	16.0385445853229882	6.8296309836729243
1.7887346648853830	16.0386827377584069	6.8776874703243962
0.6097923448604288	15.2987292589964561	6.9318055124241020

5.2746766983566076	12.5374624605312217	6.9015448090662463
15.3040193644246809	0.6080078459019025	6.8955771831851509
16.0459045908762192	10.1898137357878742	6.8682634647745218
17.9075019564378231	3.1706637881683615	6.8280645997873073
15.6185302829579697	3.1708620131218304	6.7981815553396210
13.9331366453317091	4.8455706178973603	6.7876622493520511
17.9076276841097339	8.8057721651035781	6.8355614041181196
19.5935388111050059	7.1309834088864781	6.8657891458366942
13.9331393896479430	7.1309847200728997	6.7908694746664615
17.4779209089165910	10.1902287203931721	6.8856260411477805
15.6186340901587979	8.8055739592087257	6.8056117557487354
18.2164400322131108	0.6063861482640359	6.9278268143638373
19.5933574828789610	4.8454553527394548	6.8624872534130521
12.5451879758470088	6.7045757970450888	6.8676766191632854
11.3641150646865174	7.4421630528721456	6.9551379713352253
17.4778231781485758	1.7861010270197399	6.8759505624742303
20.9804523080530672	6.7040236795279906	6.9601931743079444
20.9803630714637244	5.2720586554549582	6.9580958706094682
12.5452244902916785	5.2717640049872987	6.8655496708778907
11.3641586827700749	4.5337914790428400	6.9504629723239075
16.0457980443117272	1.7865160774956241	6.8586087703316396
15.3040902911693362	11.3682568646477939	6.9058042037529299
16.0426519756590160	20.9622311786227442	6.9464951167616160
17.9011231863435931	13.9335137068923967	7.0188518294435802
15.6143473283929630	13.9329542429035023	6.9982752103537234
13.9353673636774253	15.6115739466076064	6.9825951822969250
17.9011360823652126	19.5769150110279426	7.0105902667135975
19.5798395637359945	17.8985243935705789	7.0220898430007788
13.9353368345412800	17.8985880408487290	6.9786013430837794
17.4746874909772707	20.9617279594064883	6.9608877623417253
15.6143104247407578	19.5773154542227346	6.9899412456979064
18.2165179253590814	11.3699808583836752	6.9380444011388196
19.5797550973928089	15.6120319143014878	7.0259837307568489
12.5504850585025416	17.4710409926829051	6.9240540535173842
11.3712114551409051	18.2108724849336170	6.8753274700740796
17.4747616088776354	12.5485842619790446	6.9710078891416085
20.9648591178979444	17.4711798976064294	6.9759666186180764
20.9647864746746393	16.0391070408186422	6.9786458562356772
12.5505487974423744	16.0388213237382722	6.9268199484366626
11.3713103160947373	15.2985814293024340	6.8812266537146680
16.0427216777898174	12.5480508763662062	6.9566434628818845
0.6296090819809240	3.4437607486589119	7.0384384700409814
3.4481742700626326	0.6206719156264349	6.9979186173637542
8.5372481503963709	0.6174903027146020	6.9511326487785974

0.6300944182851882 8.5318499355418265 7.0475256127964014
0.6095314637458887 14.2080548165585707 6.9327968993938081
3.4480354743218684 11.3544819578319078 7.0120657492589071
8.5371081561267186 11.3576849849254753 6.9658353763506646
0.6100644210138731 19.3017920586558773 6.9226030895781117
11.3637798315559007 3.4432918883628871 6.9518924024309294
14.2134377660711611 0.6092755161741916 6.8834911017706082
19.3070059586742353 0.6051561607649224 6.9400101643081902
11.3636660347148695 8.5326804072528883 6.9600360366461489
11.3712393920095316 14.2079096411114154 6.8851296207837605
14.2135205416716826 11.3669509180344619 6.8935405446874691
19.3070927958828733 11.3711932313785518 6.9500097940087695
11.3708751669976582 19.3015439065433547 6.8745031429853478
2.6838517548336194 7.1672301478441875 10.8808352792037137
2.5167546109635559 5.5519603220949953 11.0888729605887466
3.8867564438875521 6.1539116640028020 10.4076438138859491
6.0017315365630930 5.9860618874514158 7.9172788943235890
5.9886392250256311 16.7540197155552661 6.5709350948979912
16.7662078179765750 5.9885064168002673 6.6135711561461070
16.7562372698687057 16.7554178970090284 7.1553380606303776
8.3981643958920866 3.5846191442795727 7.1596098788804579
8.3980409116594448 8.3904250015777269 7.1684575031593596
3.9835340642755326 5.9873555049031433 7.3181950596101313
5.9970524970651269 8.0060103150165620 7.3187227480345785
3.5935439328323389 3.5862788827049821 7.2084971101819182
8.0143256995392331 5.9872977798490732 7.2919355168621722
3.5932908115557090 8.3885163118304913 7.2177530160538321
5.9972034467673128 3.9685861969918022 7.3098574787946173
8.3984228055904104 14.3419292596391923 6.7993339416736784
8.3985134342714485 19.1669697385861220 6.7906062696553509
3.9612571858776962 16.7543320768345190 6.7408099507463115
5.9895426875763560 18.7951912645639041 6.7166553139582543
3.5819315248431591 14.3417111434671725 6.8326111177357891
8.0184592384907418 16.7543183705501981 6.7107130612096650
3.5821172641640784 19.1672749787265140 6.8237449784888371
5.9893844579435962 14.7134218753022701 6.7245633182828639
19.1756578637542745 3.5799500809655362 6.8663260598855098
19.1758051208016838 8.3964399649619139 6.8728878591243232
14.7228469494345795 5.9883791333630079 6.7231194934467222
16.7639864634570301 8.0169930501071889 6.7618441386166319
14.3500990316332651 3.5800939088192862 6.8042175282878494
18.8042812322108759 5.9883499285773452 6.7863070636362659
14.3501698273781741 8.3963875338786025 6.8106057521549301
16.7638715675817451 3.9595462833995616 6.7558318961960158

19.1682637411877579	14.3449632117710717	7.0147208407737258
19.1683022031318337	19.1655411623981138	7.0073174115138075
14.7242914859726390	16.7551760030756896	7.0303429230389218
16.7572495463698381	18.7878103617341239	7.0451580218966452
14.3472594212504418	14.3444551002231631	6.9758095369954871
18.7902356523905283	16.7553791998592096	7.0672776319927442
14.3472397938613287	19.1656880278058601	6.9682909167866880
16.7572139806813958	14.7226217577044327	7.0520524541312319
6.0032439290095310	5.9833729693670650	9.6049957768141372
2.8641723956257441	6.2618049410997889	10.4382462474700048

(6) NH-Mo-Pc (POSCAR)

C H Mo N

1.0000000000000000

21.5339999999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	21.5339999999999989	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

80 17 4 33

Cartesian

4.5247034389589436	0.6234205688106006	6.8910833916386158
5.2654971293553396	10.1629330074357540	6.9644131996798011
7.1154986411460950	3.1892283066076828	6.9751658646146835
4.8438248081123216	3.1892746454257508	6.9751917875772875
3.1836511676305359	4.8494829445809389	6.9870656618281197
7.1152158846765881	8.7807110718288328	7.0180537179313580
8.7752449304797011	7.1207318867120994	7.0056306832460749
3.1841211210976246	7.1207435730374957	7.0058526535716288
6.6938516251839522	10.1629737954839428	6.9644188234591002
4.8441950270671059	8.7806761362126142	7.0180653316374890
7.4343788058084295	0.6233269317227236	6.8911399674476232
8.7756975716005083	4.8494454120344921	6.9868664919059622
1.8020759928337762	6.7002444162933719	6.9444438934587014
0.6186204626542646	7.4419329943482122	6.9266808145232686
6.6938749638956603	1.8074577689805471	6.9136130464782761
10.1572718852412276	6.7002288938579877	6.9440967936326174
10.1577081872452588	5.2718055198308340	6.9324240704407067
1.8016245226812200	5.2718313167676438	6.9327531216418992
0.6169726563645160	4.5323692949092589	6.9048731567557171
5.2653344881185458	1.8074876750255788	6.9136068354618452
4.5248200888177825	11.3469219308239939	6.9413159437877816
5.2605470082025239	20.9734620273010748	6.8872513551420900
7.1241895362978340	13.9192495250217068	6.9398355519458050
4.8347776104122078	13.9192061444990980	6.9396838176034157
3.1608227612099973	15.6063283422274477	6.9411833992029512

7.1240095174204239	19.5854361827272534	6.9059491993248256
8.7976611802191567	17.8987703727110556	6.9320609962016242
3.1612635846619366	17.8987146412491143	6.9316564233623161
6.6984361404884565	20.9734450762143112	6.8873050249606544
4.8349629914305234	19.5854238622693870	6.9058156883650526
7.4343863906913317	11.3470436130172505	6.9413459894296254
8.7980717598733893	15.6064168150527234	6.9415918796509350
1.7773038054656145	17.4692191028624180	6.9382900081060921
0.5985756260556955	18.2099934496916696	6.9425885622241497
6.6985026123010023	12.5310490225275295	6.9336556616961538
10.1816206183366500	17.4692701140382276	6.9386179873065466
10.1820378190814349	16.0368808884768228	6.9414495411066062
1.7768440425507170	16.0368139005716657	6.9411535729640130
0.5969780452653176	15.2979746975181197	6.9436707590049780
5.2605513347025550	12.5310080795440300	6.9336124209840619
15.2905762744690730	0.6069308299469598	6.9424198699491173
16.0303768015402639	10.1908809818100661	6.9432976772923833
17.8927325374174870	3.1701114698185875	6.9315794807104085
15.6005052087228488	3.1701209396927892	6.9315339256380222
13.9138054620797273	4.8439563698061789	6.9179195980487735
17.8929287597268107	8.8069626328137574	6.9420210414278403
19.5800065137761052	7.1331765133021365	6.9275538498245126
13.9133101786675688	7.1331354001669860	6.9273053445087429
17.4628501760717008	10.1909315138769312	6.9433244557116343
15.6004026011522274	8.8069040356902946	6.9419474270070429
18.2025064470429534	0.6068728336832756	6.9424271066259600
19.5794737544385242	4.8439756503188729	6.9181308325232758
12.5252330204469029	6.7070742024715164	6.9142249047914417
11.3407163979968466	7.4419218702886143	6.9263401255103911
17.4627734995366453	1.7861439838758966	6.9369127323940267
20.9680979144283341	6.7070924159169998	6.9145560526216325
20.9675895202967517	5.2691928769544090	6.9058496560785301
12.5257216296374239	5.2691844226829483	6.9055225372084408
11.3423605415688602	4.5323552422916888	6.9045287877533053
16.0304002508205485	1.7861501250042282	6.9369114598670656
15.2905278134937817	11.3701419059115860	6.9442887221084293
16.0302489273717939	20.9611066045490837	6.9477754537112251
17.8902081238010489	13.9337824647093509	6.9498712927756028
15.6026751871764233	13.9337433711803573	6.9497642343714139
13.9249321859014561	15.6115187866814313	6.9500851010054907
17.8904613536119683	19.5772286071471235	6.9521571430825979
19.5684158382969997	17.8992839228894951	6.9517266048827704
13.9245175388505835	17.8992485067371589	6.9514864919229229
17.4627589222114352	20.9611091737839317	6.9477949531544771

15.6025493442435064 19.5772079723145858 6.9520866215783315
18.2025558096627762 11.3702608797214229 6.9443258670467856
19.5679358242112009 15.6115759068585973 6.9503625335024593
12.5406568180276921 17.4711506111424235 6.9474335053780099
11.3603541594422932 18.2100217274249303 6.9427136989205058
17.4626853473379278 12.5499305601230571 6.9468962360944833
20.9522692822978129 17.4711495352878075 6.9475642596891767
20.9517951833190743 16.0387265996856669 6.9469450906797663
12.5410760847864786 16.0387093497768305 6.9467918222815008
11.3618903792078392 15.2979986160491013 6.9437245982143248
16.0302635722729221 12.5498828989734541 6.9468686705456539
0.6161824564744287 3.4417364175166876 6.8980899844881201
3.4340396733530407 0.6237802876838815 6.8937168257449342
8.5250277686930165 0.6235861322574281 6.8938227550437103
0.6200681544079558 8.5325286980310278 6.9379840026061084
0.5959168094761454 14.2074311102854889 6.9430289010545705
3.4341718400648218 11.3463576219318192 6.9433920769621453
8.5250183890624953 11.3466529813252581 6.9434241553248102
0.5997899998510857 19.3005385431831300 6.9429466459547893
11.3431720941329743 3.4417231813580833 6.8977898019500374
14.2000174214472565 0.6071907513217391 6.9429130771375815
19.2930530881312912 0.6070518408455596 6.9428645791179093
11.3393128425268213 8.5325131897398308 6.9376891279909429
11.3628469922836182 14.2074534649435567 6.9430462432896327
14.1999493542917019 11.3699954373885586 6.9434875431726093
19.2931210131587392 11.3702840351695240 6.9434897876266000
11.3591282409684755 19.3005666686425776 6.9431125598665711
5.9796717925269220 5.9233865718377672 10.4338934697816459
5.9797445910529055 5.9778384970526206 7.6807749039590183
5.9794438806390335 16.7524220573799951 6.9549901914525867
16.7466461190704550 5.9885843710154072 6.9550229790399341
16.7464393514471155 16.7556073806553556 6.9585827723925524
8.3833468454838620 3.5817389437150426 6.9680013160758030
8.3829749447717656 8.3885198662614631 7.0051420402835936
3.9941450426564540 5.9844964106327021 7.0563221141589043
5.9797178958670845 7.9701836586857704 7.0752053307377327
3.5759844155499865 3.5817873710067847 6.9681244895118866
7.9652464137207861 5.9844766837210868 7.0561470811908817
3.5764238144000280 8.3885149548777171 7.0052642943692938
5.9796825840183550 3.9992189968606153 7.0374998607601587
8.3908990766088678 14.3380417138177076 6.9409915441843184
8.3906300705118628 19.1669959468156677 6.9159934911321219
3.9533629740944018 16.7524213480958473 6.9398668587312242
5.9794979860288890 18.7950427425521553 6.9193966517345595

3.5680350732865240	14.3379556696623105	6.9406747682641008
8.0055213605033781	16.7525045107203994	6.9403247833740283
3.5683311777135973	19.1669432190161793	6.9157050547082086
5.9794774104378270	14.7095614535231771	6.9468359115927587
19.1609363678237372	3.5772669677665996	6.9220231120052471
19.1613131121269902	8.3998298762952199	6.9349160576657560
14.7039112476436884	5.9886514843856959	6.9330863391424584
16.7466903126606290	8.0146341808027994	6.9457352278007765
14.3322848665794975	3.5772433328283006	6.9218845534472839
18.7893706049768419	5.9886950257511185	6.9332643022442992
14.3320030304827259	8.3997796709759491	6.9347159479791118
16.7466254281859328	3.9624829975414251	6.9346154738129968
19.1577985081821076	14.3439608288802489	6.9493290414814011
19.1581638914215233	19.1669267641070071	6.9515673701841791
14.7158165857815693	16.7554964741077406	6.9535455483816673
16.7465218836885477	18.7861639173652719	6.9549550902150346
14.3350611483678723	14.3438932549048559	6.9491026260443478
18.7770531982516999	16.7555638827684241	6.9538497667710510
14.3348289470190391	19.1668854628136529	6.9514003925573222
16.7464375249321193	14.7249379176274342	6.9524544527557053
5.9799799932917859	5.9534119725245782	9.4145264676396785

(7) NH₂-Mo-Pc (POSCAR)

C H Mo N

1.0000000000000000		
21.5339999999999989	0.0000000000000000	0.0000000000000000
0.0000000000000000	21.5339999999999989	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.0000000000000000

80 18 4 33

Cartesian

4.5235413598656953	0.6097010852923684	6.9536556707098187
5.2620268832919610	10.1960679250272346	6.9494199933507854
7.1265849098808776	3.1692729461543485	6.9573036836542412
4.8365869620045512	3.1714531240781465	6.9573678596264203
3.1588503008905104	4.8491697082269178	6.9529056498845003
7.1225951881230358	8.8121837199423876	6.9453720246151018
8.7996045629091810	7.1351633566647186	6.9460527820053404
3.1566831092942467	7.1391492806522221	6.9458076518591954
6.6959310555715916	10.1946187665339814	6.9491907310013756
4.8329083559576445	8.8145317452117276	6.9455334917689822
7.4366781383381717	0.6069986376944241	6.9531031798863872
8.8019615695375215	4.8454942001587353	6.9532357654581940
1.7750032512426146	6.7105598382731415	6.9462063654479946
0.5944269769350844	7.4492722664875108	6.9432871255510182
6.6979862989795800	1.7875920894338870	6.9565698411061350

10.1820435444892716	6.7085163586129530	6.9463666773917199
10.1834890155302507	5.2746265735139515	6.9515991815105371
1.7765261625843674	5.2762800380262691	6.9514095613209745
0.5971141320847151	4.5361269534947395	6.9543787236239174
5.2636992031185326	1.7891167908819152	6.9567647647786037
4.5235414199570645	11.3766959902590905	6.9536557716925351
5.2620269526189665	20.9630693295370705	6.9494199015251459
7.1265908252697949	13.9362670076493060	6.9573036531332670
4.8365806792205461	13.9384469739995058	6.9573678733864668
3.1588445464288948	15.6161644797890524	6.9529057334661184
7.1226014943897811	19.5791891648959933	6.9453719686040793
8.7996097874436732	17.9021684680250459	6.9460527850767209
3.1566780565265393	17.9061537371130868	6.9458076557987249
6.6959309197032439	20.9616200235483490	6.9491906693423262
4.8329023478561197	19.5815380681256137	6.9455334107479185
7.4366781660778560	11.3739936124077747	6.9531031655345172
8.8019673841371660	15.6124892653999030	6.9532357972609882
1.7750032065652195	17.4775578168483392	6.9462064127174834
0.5944271134646626	18.2162689865387932	6.9432871311920215
6.6979862777932038	12.5545907792803941	6.9565698095110688
10.1820438433194198	17.4755142589813381	6.9463666990062549
10.1834893999399156	16.0416286335161509	6.9515991733824167
1.7765262626662552	16.0432815268723559	6.9514095836569769
0.5971142551886367	15.3031301603911842	6.9543787410015776
5.2636989412038995	12.5561156996244208	6.9567647803342867
15.2905469806396468	0.6097013453895687	6.9536555922208034
16.0290302157843136	10.1960683903710976	6.9494200357021878
17.8935924469084888	3.1692644486116368	6.9573035933546059
15.6035784065062231	3.1714438612358720	6.9573677608627751
13.9258403773144455	4.8491593326654732	6.9529057093327662
17.8896034443382135	8.8121924163871412	6.9453719860029430
19.5666136135548925	7.1351736410309483	6.9460527169885440
13.9236731006222758	7.1391593027890732	6.9458076115395935
17.4629276019707085	10.1946190217679789	6.9491908111189034
15.5999001265998789	8.8145412749972714	6.9455334476210746
18.2036725341835748	0.6069988059366138	6.9531030943528984
19.5689719119763730	4.8454841521125438	6.9532357683808934
12.5420011038221055	6.7105598556011579	6.9462064618391466
11.3614186984967613	7.4492722892838517	6.9432872097738851
17.4649830327456819	1.7875920555084894	6.9565696067367844
20.9490454809897066	6.7085162010026949	6.9463667202480481
20.9504911961787101	5.2746266745617572	6.9515991103731274
12.5435244140439526	5.2762796792894573	6.9514095549376504
11.3641057363283924	4.5361270748519873	6.9543787540490980

16.0307018530896244	1.7891170372024909	6.9567645396475637
15.2905471039625986	11.3766963489669504	6.9536556210577380
16.0290302438887444	20.9630696248275825	6.9494199098504534
17.8935991685079578	13.9362578266571457	6.9573037521712413
15.6035721657487763	13.9384383474228102	6.9573678638485221
13.9258352374951855	15.6161542449287616	6.9529058716978920
17.8896094130923444	19.5791981477753154	6.9453718312750885
19.5666191380845582	17.9021783812618516	6.9460526689205793
13.9236673755092468	17.9061646414837377	6.9458074842355124
17.4629277985880229	20.9616200111249249	6.9491906975102591
15.5998939184282186	19.5815475128077310	6.9455332668902132
18.2036725874709653	11.3739937032689937	6.9531031593595021
19.5689776254302004	15.6124789558602952	6.9532359204472440
12.5420009243137773	17.4775582006431414	6.9462064226844191
11.3614187552207557	18.2162691501290794	6.9432871257488058
17.4649832626174408	12.5545906124910953	6.9565696521999678
20.9490454968330155	17.4755143645247486	6.9463667491892522
20.9504914042719328	16.0416286185282999	6.9515991116328841
12.5435245193372857	16.0432816151208364	6.9514095808174616
11.3641059771632271	15.3031304203752114	6.9543787904446948
16.0307019107793209	12.5561159626591010	6.9567645453976903
0.5988228534812629	3.4457467612111725	6.9590249853995925
3.4331519536571622	0.6114381387121935	6.9540853375300005
8.5272486752743681	0.6056729502211406	6.9528405585472139
0.5931450538828386	8.5398416603153020	6.9388690488356639
0.5988227115507228	14.2127468781533324	6.9590250654128010
3.4331517513080669	11.3784403168723696	6.9540855747485608
8.5272485279930592	11.3726752931708965	6.9528405452867910
0.5931451820543177	19.3068414913900064	6.9388690421087444
11.3658263735665699	3.4457464465741068	6.9590249604875307
14.2001523568073722	0.6114379699311951	6.9540853541398215
19.2942482307831717	0.6056731228156145	6.9528405449885184
11.3601487909052246	8.5398414309695401	6.9388691512367924
11.3658263798747203	14.2127466515665191	6.9590251389117048
14.2001521487659872	11.3784402382160454	6.9540854227961146
19.2942480477054126	11.3726751803677431	6.9528406853842322
11.3601485996514207	19.3068413209687542	6.9388689913494739
6.7929876012808590	5.6034380458359241	9.9180486003165242
5.1653256012808599	5.6034380458359241	9.9180486003165242
5.9791566012808595	5.9917350458359238	6.9481836003165247
5.9791565990514117	16.7587350008686080	6.9481839800616987
16.7461564877024642	5.9917351812674147	6.9481842811597989
16.7461566508063697	16.7587352419894273	6.9481852210732606
8.3937839387348419	3.5780992351324779	6.9564532680939388

8.3893012083488223	8.4018660899327831	6.9447571107542192
3.9532390535316924	5.9949314176670763	6.9491283404408897
5.9769480279944052	8.0176376801780762	6.9436455459355368
3.5698813161733836	3.5824810259909929	6.9563515006601895
8.0050659249684948	5.9895184443718392	6.9495767607172754
3.5655012733088003	8.4063476525546275	6.9448244953746210
5.9823677661915040	3.9658456157552489	6.9569795651558985
8.3937874252163347	14.3450970629578389	6.9564531615171523
8.3893050566250604	19.1688679620075533	6.9447572173478971
3.9532616675498944	16.7619301020450067	6.9491282551264995
5.9769488882652793	18.7846200891513178	6.9436457418473516
3.5698774509203206	14.3494791190191080	6.9563514372594959
8.0050434253196681	16.7565190546588596	6.9495766071320944
3.5654973302334483	19.1733492107955215	6.9448244758951141
5.9823664112252342	14.7328629822654449	6.9569791651275583
19.1607864453373686	3.5780930120495640	6.9564530276580046
19.1563038362282256	8.4018720433406227	6.9447573525208188
14.7202680095921821	5.9949295412054608	6.9491282104148242
16.7439487741124999	8.0176008742520413	6.9436458336255225
14.3368786631604799	3.5824750829034451	6.9563512431391796
18.7720366463774937	5.9895196218033968	6.9495765472706559
14.3324980238800439	8.4063533646425661	6.9448246483529292
16.7493660762872096	3.9658826231779538	6.9569787305206043
19.1607900977330061	14.3450915387966411	6.9564530662484207
19.1563067608608435	19.1688729612857642	6.9447572798071029
14.7202906997593992	16.7619296605699546	6.9491281992080491
16.7439490192624092	18.7845834147745983	6.9436460151747212
14.3368759152315945	14.3494743655000256	6.9563511865431629
18.7720142757398314	16.7565195553383788	6.9495764885272600
14.3324948067814901	19.1733551709694474	6.9448243916660850
16.7493660222759821	14.7329000737853200	6.9569784897779146
5.9791566012808595	5.9917350458359238	9.4481836003165238

(8) NH₃-Mo-Pc

C H Mo N

1.0000000000000000

21.5339999999999989 0.0000000000000000 0.0000000000000000

0.0000000000000000 21.5339999999999989 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

80 19 4 33

Cartesian

4.5239502827955489 0.6114234575890269 6.9315368481467905

5.2636201503070543 10.1914294363174065 6.9469248061163098

7.1248211559564565 3.1718380737975997 6.9988052038894724

4.8343274338198681	3.1717332481216580	6.9988988241225334
3.1595031985032889	4.8468550561778150	6.9971337526475166
7.1250182154009192	8.8120749666750147	6.9926619589569388
8.7997230615108855	7.1375581649832762	6.9915837777633847
3.1595454883722804	7.1374686430142917	6.9916326085061860
6.6955537308182684	10.1913939527686193	6.9468437850641678
4.8342934351958933	8.8120208063524927	6.9927481827200495
7.4351743511059860	0.6115147379166666	6.9313270099912199
8.7996161771045145	4.8469724252734121	6.9970881216362439
1.7802053378053413	6.7078949439348792	6.9436266308207095
0.5992283615089602	7.4475804158407177	6.9240695051765035
6.6955068545616934	1.7924560914931775	6.9504538381952869
10.1789434257678781	6.7079487920543288	6.9436211038053699
10.1789972648265721	5.2760509164757181	6.9477940561155354
1.7802137775589946	5.2759391851634021	6.9478140170030311
0.5990178556523320	4.5363983585944911	6.9328234546540051
5.2635505154467435	1.7924820402726793	6.9505583280529235
4.5239605462404189	11.3724519516319198	6.9320734595122229
5.2625783647653321	20.9659655490630925	6.9283645967917620
7.1231480280311414	13.9359553905709213	6.9473959221002595
4.8359085579855750	13.9358560247896950	6.9474380486488378
3.1597529271256115	15.6146939924110715	6.9547487066471865
7.1231627770071135	19.5821524050488662	6.9387168747275156
8.7992538863904031	17.9033708916238190	6.9494260563397443
3.1598837295968134	17.9033156145713050	6.9493288469035033
6.6964970503177179	20.9659268991206496	6.9282881950487516
4.8360180779948685	19.5821321828941848	6.9387565743424906
7.4351862510453657	11.3725816218201565	6.9318758747693296
8.7992688070278042	15.6147987297153872	6.9548169445288792
1.7757754506678634	17.4747211261819402	6.9501916150556822
0.5969968841443444	18.2153954750206353	6.9457827797049783
6.6965280857476319	12.5520508728571460	6.9337685411754597
10.1832542386690346	17.4747568126820241	6.9502789400565614
10.1833094550133669	16.0433211677504275	6.9542686582351037
1.7757935964578835	16.0432158543431775	6.9541996157121355
0.5968467738042212	15.3027349794727527	6.9543583817400707
5.2624804313509861	12.5520771250126177	6.9338500422539129
15.2902163750270379	0.6095002287137803	6.9534776096317144
16.0308216238522796	10.1958751751731143	6.9523905851928554
17.8908568944181674	3.1724810049633230	6.9580425793553760
15.6022213882055834	3.1723974828721873	6.9580976817147935
13.9233735860690864	4.8484941829877615	6.9444702393568720
17.8909206570172294	8.8118279015626424	6.9488172171114488
19.5697650632132785	7.1357366946648275	6.9389445105369285

13.9234357829105573	7.1356817130286236	6.9388806046312004
17.4622692923575897	10.1958282124894506	6.9523160658605372
15.6022914741728229	8.8117970311802285	6.9488596205220423
18.2028508482516855	0.6095791616313287	6.9532803602049214
19.5697139116949046	4.8485755080783450	6.9445244993878470
12.5395765257817349	6.7090070417726198	6.9260679665426697
11.3600183296669126	7.4476062190632719	6.9240523252179873
17.4622421353830362	1.7883869249394313	6.9580308924052652
20.9535506501928417	6.7090210460709372	6.9261323316388443
20.9535902262145548	5.2750723766928296	6.9302251003843276
12.5395997094745439	5.2749956371847597	6.9301695835424804
11.3599820362600195	4.5364048955963856	6.9328183955939888
16.0307448719437176	1.7884199085619639	6.9581134157136235
15.2902211618121910	11.3746345639852358	6.9534672721305970
16.0306498752717737	20.9648243624119566	6.9495461098598819
17.8896457989172752	13.9384822880281831	6.9556664404965511
15.6033917649901426	13.9383910351513904	6.9557127436289177
13.9257970831810063	15.6159590400439505	6.9524302481353697
17.8897016825461392	19.5798407910337602	6.9464212194365995
19.5672450380231915	17.9022669532097005	6.9469746708957398
13.9258825915695041	17.9022102572151951	6.9468704674701840
17.4623925510117246	20.9647777337953976	6.9494723366949840
15.6034638718779348	19.5798136669847516	6.9464568388863075
18.2028641565506248	11.3747279352628627	6.9532696896765342
19.5672168348316902	15.6160608794830722	6.9525090826168681
12.5408558177738527	17.4749443404449885	6.9473217561290426
11.3621169729163931	18.2154036521415534	6.9457844293869107
17.4623845452351354	12.5534530217998110	6.9551752171531636
20.9521710456382806	17.4749636778766231	6.9474141729204240
20.9522057774061103	16.0432314085690990	6.9514504520153464
12.5408931486513868	16.0431416117149261	6.9513751515834903
11.3620592987687470	15.3027425470208520	6.9543576081871556
16.0305926587410674	12.5534837140880651	6.9552585071799617
0.5979470094783855	3.4462670712702157	6.9385788499623775
3.4337864057969369	0.6104870848588262	6.9340355226514951
8.5254105393241986	0.6107177268347935	6.9335956568036021
0.5985650533013164	8.5378532862086942	6.9226707050868290
0.5968028841322058	14.2125195280508478	6.9565356302293067
3.4337860066024426	11.3732841763395154	6.9340964013652133
8.5254294546602587	11.3736264320844889	6.9336782354224464
0.5972331486883786	19.3056862874787178	6.9408626634208836
11.3608828027140412	3.4462729665460197	6.9386126416033242
14.1999975982810476	0.6095510199591386	6.9522007998782627
19.2931363874319182	0.6097703756243017	6.9517666771493820

11.3609293774810975 8.5378752184267288 6.9226686673660200
11.3619291406165743 14.2125256165329272 6.9565357819825531
14.1999938184581893 11.3744861881880315 6.9521955608363806
19.2931536160109012 11.3747296264098985 6.9517697765722524
11.3620886023877095 19.3056911153859581 6.9408766733616467
5.9792617446047540 6.9522065884008679 9.7644838573936141
5.1503160037113496 5.5157613120832902 9.7670785276007859

References

1. J. Zhao and Z. Chen, *J. Am. Chem. Soc.*, 2017, **139**, 12480-12487.
2. X. Liu, Y. Jiao, Y. Zheng, M. Jaroniec and S.-Z. Qiao, *J. Am. Chem. Soc.*, 2019, **141**, 9664-9672.