

Supplementary Information

Unveiling the Key Intermediates in Electrocatalytic Synthesis of Urea with CO₂ and N₂ Coupling Reactions on Double Transition-Metal MXenes

Yufei Yang,^a Jiahe Peng,^a Zuhao Shi,^a Peng Zhang,^c Arramel Arramel,^d Neng Li^{a,b,e,*}

^a State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology, Wuhan 430070, China E-mail: lineng@whut.edu.cn

^b School of Chemistry and Environmental Engineering, Key Laboratory of Green Chemical Engineering Process of Ministry of Education, Novel Catalytic Materials of Hubei Engineering Research Center, Wuhan Institute of Technology, Wuhan 430205, China

^c State Center for International Cooperation on Designer Low-Carbon & Environmental Materials (CDLCEM), School of Materials Science and Engineering, Zhengzhou University, Zhengzhou 450001, Henan, China

^d Nano Center Indonesia, Jalan Raya PUSPIPTEK, South Tangerang, Banten 15314, Indonesia

^e Shenzhen Research Institute of Wuhan University of Technology, Shenzhen 518000, Guangdong, China

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Supplementary Notes

Reaction Gibbs Free Energy

Under the standard conditions, the activity of electrochemical urea synthesis can be evaluated by the change of the Gibbs free energy(ΔG) of each elementary step, and it can be defined as:

$$\Delta G = \Delta E + \Delta E_{ZPE} - T\Delta S \quad (1)$$

where ΔE stands for the computed reaction energy, T is the temperature, ΔE_{ZPE} and ΔS are the difference between zero-point energy and of the entropy between the adsorbed state and the gas phase. The ΔE was computed by:

$$\Delta E = E(\text{MXene} + n\text{H}) - E(\text{MXene}) - E(\text{N}_2) - E(\text{CO}_2) - n/2E(\text{H}_2) + mE(\text{H}_2\text{O}) \quad (2)$$

Where $E(\text{MXene} + n\text{H})$ refers to the total energies of MXenes with n ($n = 1, 2, \dots, 6$) adsorbed hydrogen atoms and m ($m = 0, 1$) desorbed H_2O . $E(\text{MXene})$ stands for the energy of clean MXene. $E(\text{N}_2)$, $E(\text{CO}_2)$, $E(\text{H}_2)$, refer to the energy of N_2 , CO_2 and H_2 in the gas phase.

Surface Pourbaix Diagrams

The thermal stability of MXenes could be evaluated from the surface Pourbaix diagrams¹ constructed via relevant U_{SHE} and pH. Water can be split to O_mH_n^* (a generalized representation of the adsorption of oxygenated intermediates)²⁻⁴ on the MXenes surface through:

$$m(\text{H}_2\text{O}) \rightleftharpoons (2m-n)(e^- + \text{H}^+) - \text{O}_m\text{H}_n \quad (3)$$

where m and n are the number of adsorbed oxygen and hydrogen atoms, respectively. According to the CHE model, on the standard hydrogen electrode (SHE) scale, the free energy of proton and electron pairs can be represented as $1/2 \text{H}_2$:

$$G_{e^-} + G_{\text{H}^+} = 1/2 G_{\text{H}_2} - eU_{\text{SHE}} + k_B T (\ln[a_{\text{H}^+}]) \quad (4)$$

The associated free energy change can be computed as:

$$\Delta G(U, \text{pH}) = G_{\text{MXene}} + mG_{\text{H}_2\text{O}} - G_{\text{MXene-O}_m\text{H}_n} - (2m - n)(G_{e^-} + G_{\text{H}^+}) \quad (5)$$

Then the free-energy change for adsorption of O_mH_n^* intermediates can be written as:

$$\Delta G(U, \text{pH}) = G_{\text{MXene}} + mG_{\text{H}_2\text{O}} - G_{\text{MXene-O}_m\text{H}_n} - (2m - n)(1/2 G_{\text{H}_2} - U_{\text{SHE}} - k_B T \text{pH} \ln 10) \quad (6)$$

According to equation (6), we can derive a relation between potential and pH for a wide

variety of oxygen-containing adsorbates on MXene about standard conditions when ΔG (U, pH) = 0.

Table S1 Performance of various urea synthesis catalysts.

Catalysts	Performance	Methods	Ref.
NiF ₃ /Ni ₂ P@CC	1.36Vvs.RHE	experiment	5
NiCoP@CC	1.42Vvs.RHE	experiment	6
V–Ni ₃ N/NF	1.54Vvs.RHE	experiment	7
Ni ₂ P/C-YS	1.37Vvs.RHE	experiment	8
dual-Sidopedg-C ₆ N ₆ sheet	-0.79V	calculation	9
Ni ₂ P/Fe ₂ P	1.34Vvs.RHE	experiment	10
Mo ₂ B ₂ &Cr ₂ B ₂	-0.49V	calculation	11
Vo-CeO ₂	1.6Vvs.RHE	experiment	12
	-0.27V	calculation	12
Ni ₂ P@N-dopedcarbon	1.42Vvs.RHE	experiment	13
Mo ₂ P	-0.39V	calculation	14
Fe/p-BN&Co/p-BN	-0.63V	calculation	15
Si ₂ @C ₉ N ₄	-0.84V	calculation	16
Ni@NCNT	1.56Vvs.RHE	experiment&calculation	17

Table S2 Comparison of the adsorption energy of small molecules on Mo₂VC₂ surface at different U values.

Adsorption		Adsorption Energy (eV)				
	Site	U=0	U=1	U=2	U=3	U=4
CO ₂	bridge	-1.42	-1.40	-1.42	-1.46	-1.04
	fcc	-1.60	-1.57	-1.57	-1.54	-1.10
	hcp	-1.57	-1.54	-1.55	-1.53	-0.82
N ₂	fcc	-1.35	-1.30	-1.29	-1.28	-0.89
	hcp	-1.18	-1.15	-1.14	-1.18	-0.70
	top	-0.30	-0.30	-0.30	-0.35	+0.16
CO ₂ +N ₂	1	-2.78	-2.72	-2.69	-2.63	-2.25
	2	-2.49	-2.43	-2.39	-2.42	-2.19
	3	-2.45	-2.40	-2.37	-2.36	-2.14
	4	-2.30	-2.25	-2.23	-2.22	-2.26
	5	-3.16	-3.09	-3.05	-2.93	-2.66

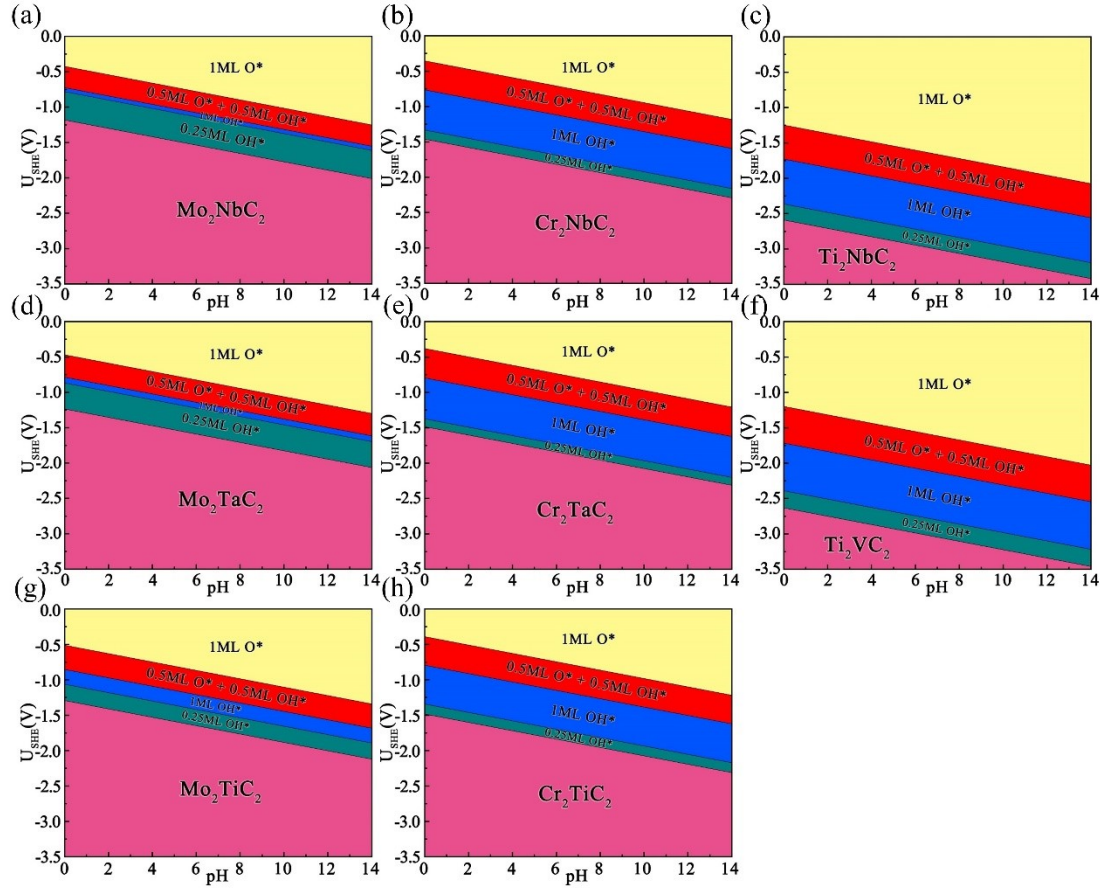


Figure S1. Surface Pourbaix diagrams of (a) Mo_2NbC_2 , (b) Cr_2NbC_2 , (c) Ti_2NbC_2 , (d) Mo_2TaC_2 , (e) Cr_2TaC_2 , (f) Ti_2VC_2 , (g) Mo_2TiC_2 and (h) Cr_2TiC_2 .

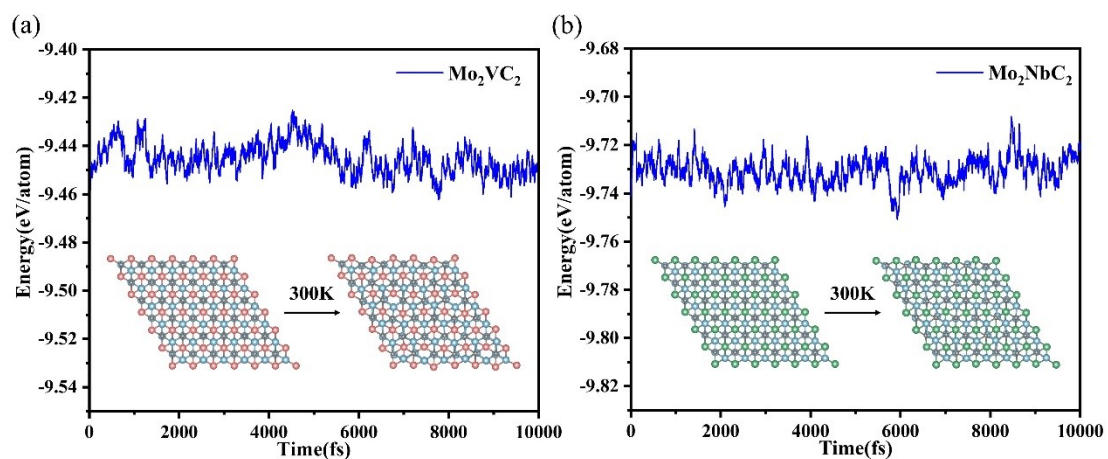


Figure S2. The evolution of the total energy of first-principles molecular dynamics (FPMD) simulations for (a) Mo_2VC_2 , (b) Mo_2NbC_2 at 300 K by AIMD.

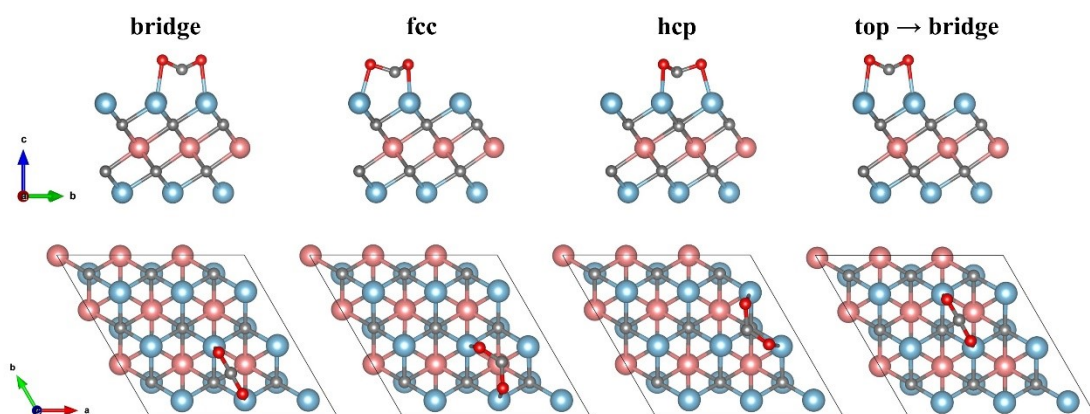


Figure S3. The optimized geometric structures of CO₂ adsorbed at different sites on Mo₂VC₂.

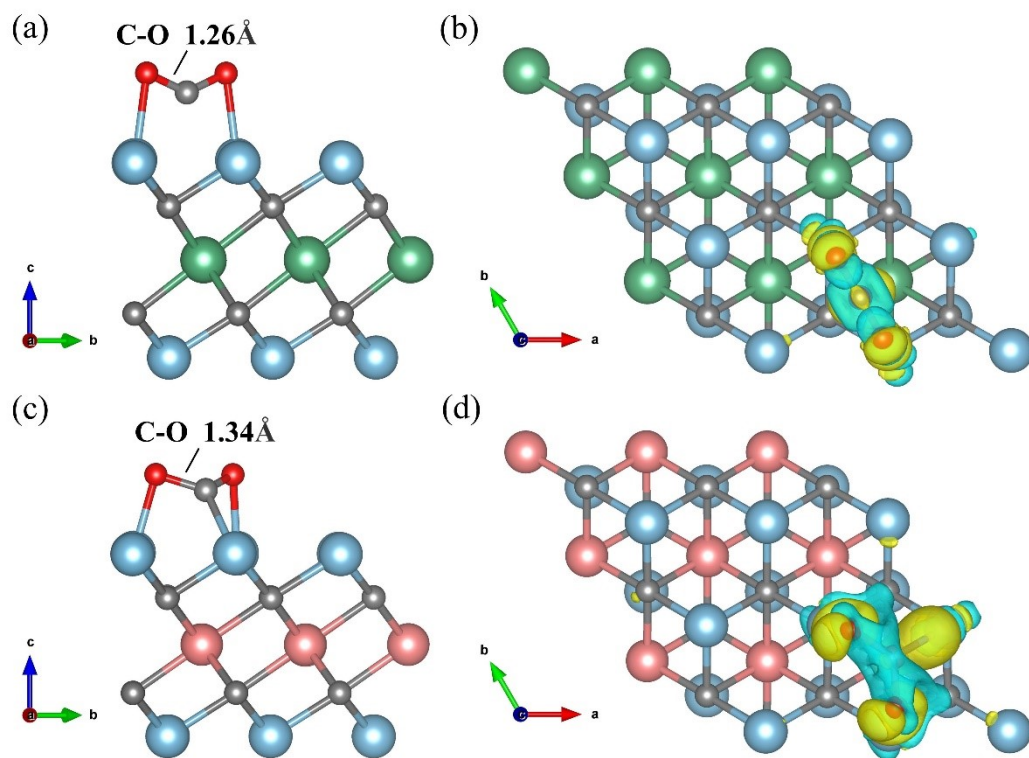


Figure S4. Charge density difference of CO_2 adsorbed on MXene. (a)the side view of CO_2 adsorbed at Mo_2NbC_2 , (b)the top view of CO_2 adsorbed at Mo_2NbC_2 , (c) the side view of CO_2 adsorbed at Mo_2VC_2 , (d)the top view of CO_2 adsorbed at Mo_2VC_2 . Blue and yellow colors represent losing and gaining electrons.

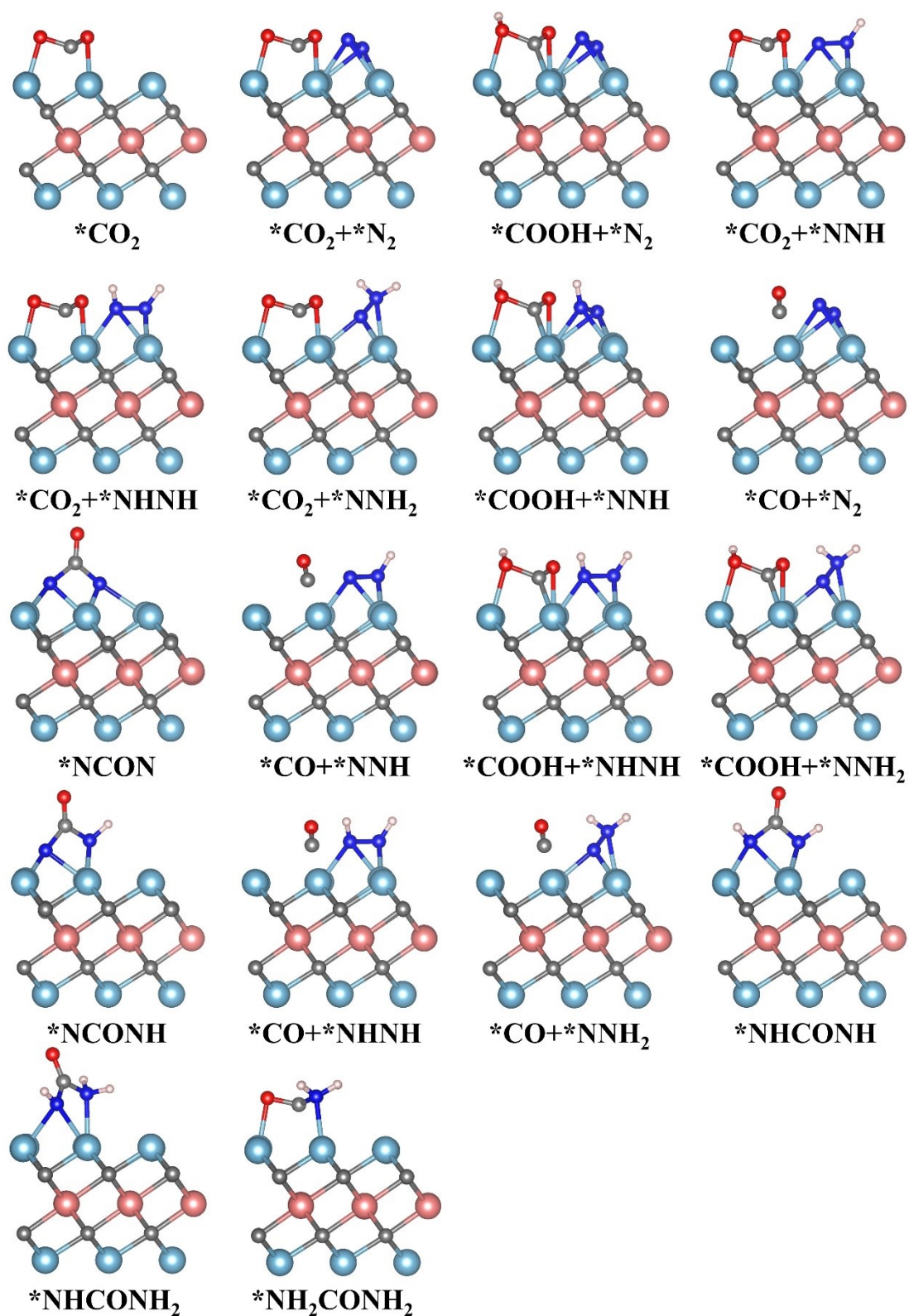


Figure S5. The optimized geometric structures of various intermediates along the reaction path of urea production on Mo_2VC_2 .

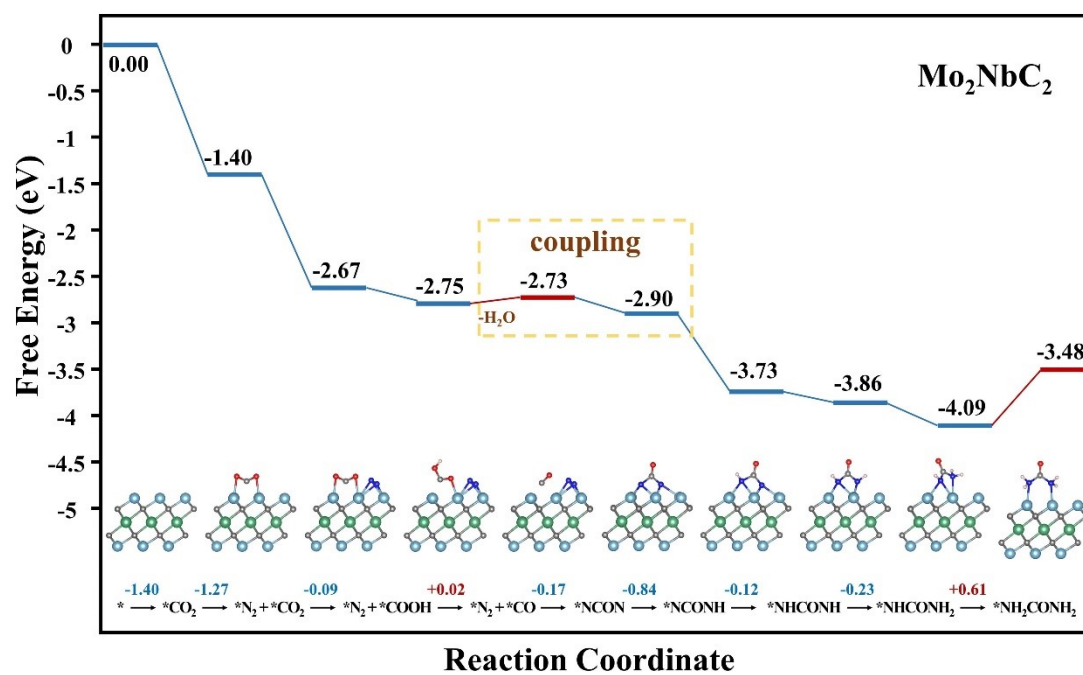


Figure S6. Free energy profiles of electrochemical urea production on Mo₂NbC₂.

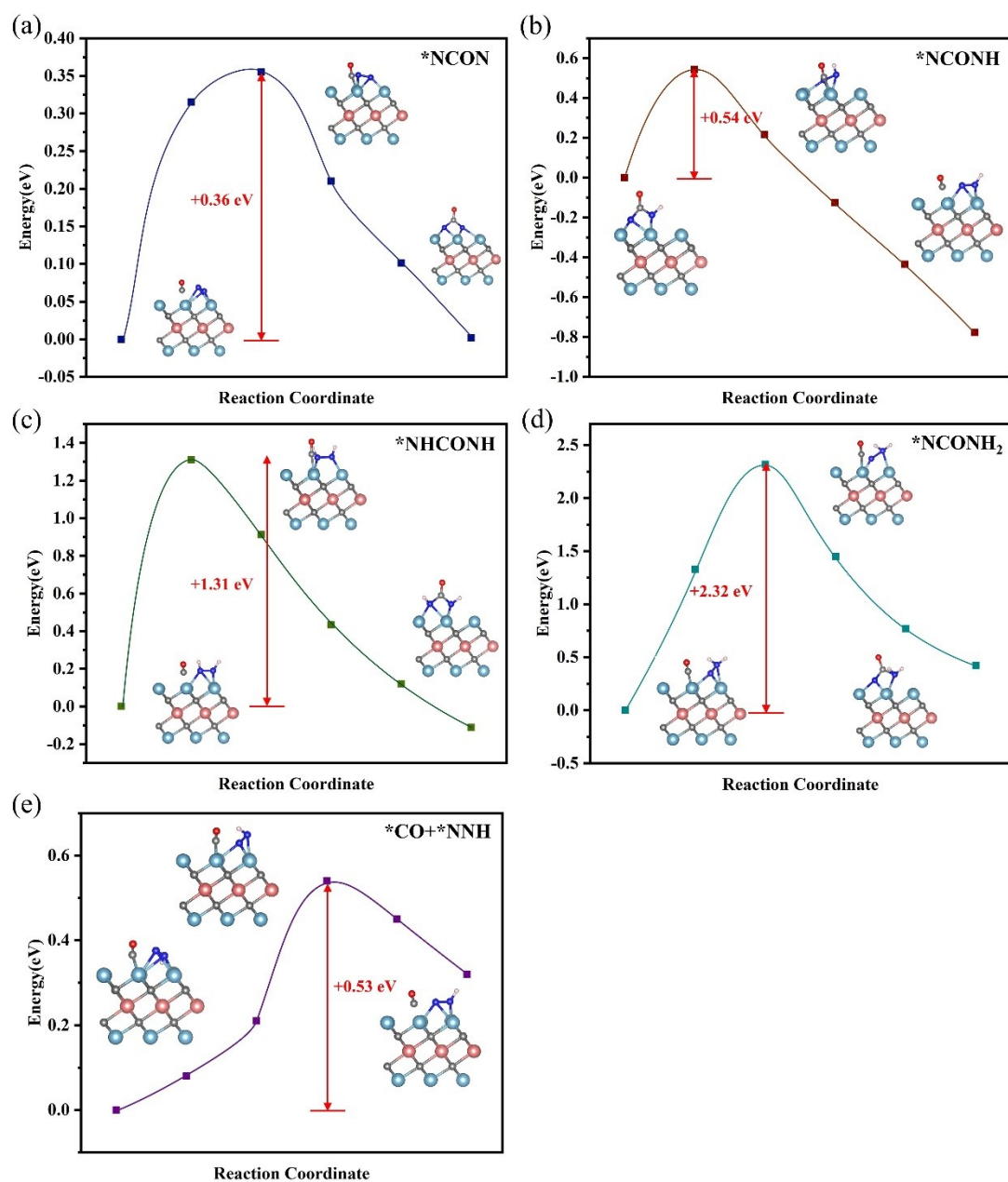


Figure S7. The transition state energy change in the synthesis of (a)*NCON, (b)*NCONH, (c)*NHCONH, (d)*NCONH₂ and (e)*CO + *NNH.

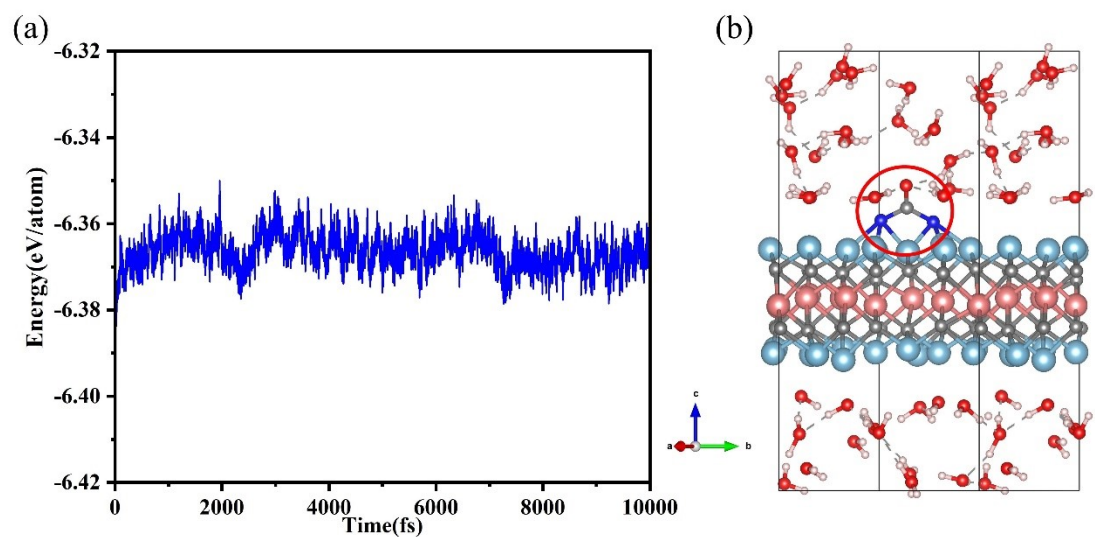


Figure S8. (a) The evolution of the total energy of first-principles molecular dynamics (FPMD) simulations for Mo_2VC_2 with *NCON covered in liquid water at 300 K for 10 ps, and (b) its structure after simulation.

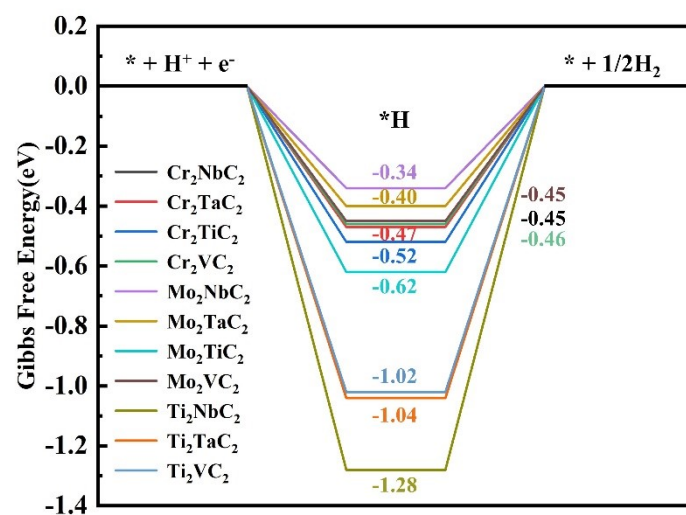
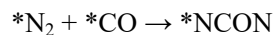


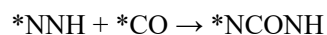
Figure S9. Gibbs free energy diagrams for HER on different MXenes.

Frequency calculation

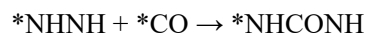
Frequency calculations were performed using VASP for transition state intermediates, where the convergence criterion was set at 10^{-6} eV in energy and 10^{-3} eV Å⁻¹ in force.



1 f	=	58.000263 THz	364.426399 2PiTHz	1934.680460 cm-1	239.869892 meV
2 f	=	35.506198 THz	223.092022 2PiTHz	1184.359246 cm-1	146.841884 meV
3 f	=	21.044866 THz	132.228793 2PiTHz	701.981146 cm-1	87.034601 meV
4 f	=	19.631235 THz	123.346687 2PiTHz	654.827494 cm-1	81.188291 meV
5 f	=	19.489523 THz	122.456287 2PiTHz	650.100503 cm-1	80.602219 meV
...					
143 f	=	2.357659 THz	14.813610 2PiTHz	78.643045 cm-1	9.750498 meV
144 f	=	1.935692 THz	12.162313 2PiTHz	64.567741 cm-1	8.005382 meV
145 f	=	1.653355 THz	10.388333 2PiTHz	55.149972 cm-1	6.837728 meV
146 f	=	0.650490 THz	4.087152 2PiTHz	21.698024 cm-1	2.690213 meV
147 f/i=	=	5.213159 THz	32.755247 2PiTHz	173.892276 cm-1	21.559902 meV



1 f	=	101.266213 THz	636.274384 2PiTHz	3377.877182 cm-1	418.803545 meV
2 f	=	50.945126 THz	320.097668 2PiTHz	1699.346439 cm-1	210.692182 meV
3 f	=	35.568898 THz	223.485978 2PiTHz	1186.450695 cm-1	147.101191 meV
4 f	=	29.471318 THz	185.173753 2PiTHz	983.057327 cm-1	121.883618 meV
5 f	=	20.600175 THz	129.434716 2PiTHz	687.147847 cm-1	85.195506 meV
...					
146 f	=	2.293878 THz	14.412861 2PiTHz	76.515534 cm-1	9.486721 meV
147 f	=	1.924720 THz	12.093373 2PiTHz	64.201751 cm-1	7.960005 meV
148 f	=	1.337828 THz	8.405822 2PiTHz	44.625141 cm-1	5.532814 meV
149 f	=	1.018488 THz	6.399352 2PiTHz	33.973118 cm-1	4.212131 meV
150 f/i=	=	4.582169 THz	28.790615 2PiTHz	152.844693 cm-1	18.950334 meV

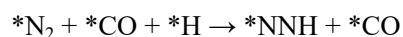


1 f	=	106.197558 THz	667.258938 2PiTHz	3542.369138 cm-1	439.197956 meV
2 f	=	102.383917 THz	643.297125 2PiTHz	3415.159772 cm-1	423.425999 meV
3 f	=	47.133206 THz	296.146666 2PiTHz	1572.194464 cm-1	194.927340 meV
4 f	=	39.920630 THz	250.828717 2PiTHz	1331.608847 cm-1	165.098515 meV
5 f	=	34.963872 THz	219.684489 2PiTHz	1166.269210 cm-1	144.599005 meV
...					
149 f	=	2.180186 THz	13.698513 2PiTHz	72.723175 cm-1	9.016528 meV
150 f	=	0.581447 THz	3.653336 2PiTHz	19.394969 cm-1	2.404671 meV
151 f	=	0.139636 THz	0.877360 2PiTHz	4.657763 cm-1	0.577489 meV
152 f/i=	=	0.253375 THz	1.592004 2PiTHz	8.451691 cm-1	1.047876 meV

153 f/i=	5.255959 THz	33.024167 2PiTHz	175.319930 cm-1	21.736909 meV
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1 f =	105.224939 THz	661.147789 2PiTHz	3509.926043 cm-1	435.175523 meV
2 f =	101.832246 THz	639.830872 2PiTHz	3396.757995 cm-1	421.144468 meV
3 f =	66.710524 THz	419.154582 2PiTHz	2225.223477 cm-1	275.892648 meV
4 f =	44.360525 THz	278.725397 2PiTHz	1479.707783 cm-1	183.460449 meV
5 f =	38.836762 THz	244.018571 2PiTHz	1295.454889 cm-1	160.615994 meV
...				
149 f =	2.293867 THz	14.412792 2PiTHz	76.515169 cm-1	9.486675 meV
150 f =	1.563709 THz	9.825071 2PiTHz	52.159702 cm-1	6.466981 meV
151 f =	1.272004 THz	7.992238 2PiTHz	42.429492 cm-1	5.260588 meV
152 f =	0.307231 THz	1.930389 2PiTHz	10.248120 cm-1	1.270605 meV
153 f/i=	5.169351 THz	32.479992 2PiTHz	172.430995 cm-1	21.378726 meV



1 f =	92.387894 THz	580.490256 2PiTHz	3081.728320 cm-1	382.085753 meV
2 f =	49.338663 THz	310.003963 2PiTHz	1645.760602 cm-1	204.048382 meV
3 f =	38.632429 THz	242.734711 2PiTHz	1288.639088 cm-1	159.770942 meV
4 f =	30.675489 THz	192.739781 2PiTHz	1023.224137 cm-1	126.863670 meV
5 f =	24.407702 THz	153.358113 2PiTHz	814.153269 cm-1	100.942177 meV
...				
146 f =	2.173661 THz	13.657517 2PiTHz	72.505537 cm-1	8.989544 meV
147 f =	1.495247 THz	9.394914 2PiTHz	49.876071 cm-1	6.183847 meV
148 f =	1.129166 THz	7.094760 2PiTHz	37.664926 cm-1	4.669857 meV
149 f =	0.494115 THz	3.104619 2PiTHz	16.481918 cm-1	2.043498 meV
150 f/i=	5.563617 THz	34.957236 2PiTHz	185.582279 cm-1	23.009278 meV

Cartesian Coordinates

The optimized geometric structures of various intermediates along the reaction path of urea production on Mo₂VC₂.

In all cases:

a	9.1323003769000000	0.0000000000000000	0.0000000000000000
b	-4.5661501884000000	7.9088041214000002	0.0000000000000000
c	0.0000000000000000	0.0000000000000000	20.0000000000000000

clean surface

Mo	V	C
18	9	18

Direct

0.1138442474728263	0.2177336327542608	0.3636154036891322
0.2249691001080378	0.1065438112127708	0.5967880418695036
0.4473011876573246	0.2179453590022644	0.3636316300416990
0.5583540164142334	0.1066371917775735	0.5967884752016825
0.7804675426706056	0.2179312680192597	0.3636166591124943
0.8916924421262559	0.1066220096531806	0.5968033793941104
0.1137493684584661	0.5510861510945301	0.3635700806320127
0.2249201751990698	0.4399579428610928	0.5967822198908150
0.4472249403596590	0.5510179026265158	0.3635697280707931
0.5583721343738856	0.4399981628369610	0.5967666822173364
0.7804700837526488	0.5512170269450098	0.3636490259197782
0.8917936794415733	0.4400009918236409	0.5967654035084863
0.1138334511446709	0.8844509934002688	0.3636113719823327
0.2249639477407997	0.7732391618050022	0.5966966773784264
0.4472579528279041	0.8845666890168860	0.3635828915858041
0.5582444449936447	0.7732957458785502	0.5967766332592057
0.7805095897389444	0.8844609775284821	0.3635925233010480
0.8918033765428195	0.7734568014259701	0.5967871406718650
0.0028776699477590	0.9956628263583188	0.4802975692688307
0.3361760864537004	0.9956806013592270	0.4802012748089671
0.6692867831705680	0.9955025283474355	0.4801991162429585
0.0027923219642990	0.3287595059535425	0.4802447283832658
0.3362400593977308	0.3291023577217830	0.4803028949744860
0.6696072171805315	0.3290701585885010	0.4803058275262766
0.0028464379205423	0.6622386011310767	0.4802160943094331
0.3360175091248819	0.6621855985048177	0.4801546623719815
0.6695655818849172	0.6623792212087464	0.4802781539945019
0.1139109952510074	0.2178112157943086	0.5413058772416126
0.2250490207764739	0.1066909822611675	0.4191871504277039
0.4472470159525805	0.2178462109022960	0.5412498135980287
0.5583421667054578	0.1067425458908536	0.4192017027169851

0.7805130773792848	0.2177671495652871	0.5412632193090694
0.8916011297801391	0.1066240283522746	0.4191786807537683
0.1139305776757230	0.5511018458159983	0.5411461438639039
0.2249299102941889	0.4399223169829993	0.4191303301948360
0.4471277409783130	0.5511683361393712	0.5412497113396944
0.5583613677535127	0.4401494155552733	0.4192424648358068
0.7806788046414019	0.5512920833886896	0.5412886481745016
0.8917257392895305	0.4400804474797840	0.4192222594465672
0.1139514256254975	0.8845647946484081	0.5412025903669243
0.2249707353727344	0.7732541631200240	0.4190883244061236
0.4471874460347435	0.8844636408902795	0.5412154806930881
0.5582701570294666	0.7732552017255947	0.4190887834974625
0.7805053861050005	0.8844827471651489	0.5412756960728252
0.8917058652866557	0.7734988244865630	0.4192487884538725

*CO₂

Mo	V	C	O
18	9	19	2

Direct

0.1159862820093122	0.2200506956155978	0.3635791681900029
0.2207564726965138	0.1045792359803007	0.5963097291520856
0.4480487064947922	0.2179512419962289	0.3636575028250343
0.5644423875914880	0.1102301179997955	0.5979526881276355
0.7815729036607179	0.2178191207252153	0.3635850921121439
0.8952391683094262	0.1053855063600543	0.5957882093085055
0.1144664760522592	0.5512200052181107	0.3636018602047802
0.2254369684246411	0.4427473011868756	0.5965273931991244
0.4480347717318263	0.5511333396281173	0.3635208889643743
0.5640968741281024	0.4424967456024466	0.5977415827977257
0.7816943546072467	0.5515715632642479	0.3635771727181693
0.8819240365680504	0.4352198011009686	0.5972280050790756
0.1160749677110592	0.8839280532316297	0.3636353887858328
0.2257553312805303	0.7712084747403516	0.5966408783853973
0.4481376038581659	0.8850365645606402	0.3635598859555020
0.5587715042858665	0.7734171440885648	0.5965553212278514
0.7806786277834847	0.8842568925703109	0.3632837938741026
0.8952664351355984	0.7781999348976535	0.5958571110968242
0.0034247758820917	0.9956905006349739	0.4802787455456741
0.3373740553250514	0.9965347536225027	0.4809727206836213
0.6709216986176737	0.9958647584830320	0.4806621678505147
0.0061648038578579	0.3297649575848324	0.4805798768394247
0.3370956584018842	0.3286249134882447	0.4807987224650480
0.6703192840732030	0.3290942531644485	0.4804943721349534
0.0065578477707706	0.6649821617839141	0.4806618236974163

0.3401011331994298	0.6641312946473853	0.4792818871191700
0.6709484691812272	0.6628059604082402	0.4805904242310673
0.1158802661579999	0.2195446708995389	0.5409012622918781
0.2256051597069507	0.1066995963786086	0.4191178353522945
0.4471445904871524	0.2175439316407183	0.5418561612189796
0.5595607082523910	0.1072927132160583	0.4191451679033649
0.7819599190185874	0.2173190845811371	0.5399955631557970
0.8933508578254103	0.1063887247125794	0.4187319928608886
0.1193075478066371	0.5539548355996138	0.5406210860375075
0.2266545650935564	0.4407186818799215	0.4192439908290655
0.4477731054108757	0.5519472467808412	0.5409914753226761
0.5595396406727039	0.4400658056490954	0.4189870153331652
0.7819585963623372	0.5530822182904236	0.5399641784570323
0.8918993227528347	0.4398262849187696	0.4190700330760616
0.1158901004156383	0.8844565630069526	0.5410271994312490
0.2267026037967109	0.7739559706974749	0.4192840359351123
0.4481967187025191	0.8842380566724436	0.5411202633750671
0.5600449121220373	0.7739695374426587	0.4188290278334322
0.7805851765094978	0.8842068295220163	0.5405153958472763
0.8933596358270217	0.7744623876007367	0.4187415127080413
0.6942345758516085	0.3419121555693851	0.6778373260844844
0.6207485456307604	0.1808806823678906	0.6976292746736735
0.6208217819585059	0.4298478789884445	0.6974176907018935

*CO₂+N₂

Mo	V	C	O	N
18	9	19	2	2

Direct

0.1169384827195220	0.2184652800301788	0.3640477870770211
0.2210879169866189	0.1027002668035831	0.5968956177713433
0.4473528596299884	0.2157519489883622	0.3636932777154613
0.5662247951418514	0.1116610761382379	0.5961661243312054
0.7829802999705073	0.2166138459896714	0.3638016843379703
0.8965396874754268	0.1044563865128387	0.5972692648270516
0.1160452696694885	0.5508596193340284	0.3640485456337280
0.2345419080186662	0.4506468724040048	0.5981127217783464
0.4492312689742649	0.5500653733668823	0.3634382560503315
0.5665687842515266	0.4394339927402963	0.5960173035227685
0.7840805661218990	0.5523603916474292	0.3636902611524986
0.8804553831266270	0.4319813664558241	0.5957074678831881
0.1163871623005810	0.8836919461125630	0.3640246007632933
0.2314068371651810	0.7667412149147922	0.5997517297324561
0.4487044815408019	0.8837378026893188	0.3639466203036358
0.5490617503080605	0.7635268234189906	0.5980768293497694

0.7822184738337935	0.8833959328324598	0.3634885818504404
0.8964536092160619	0.7770776497897590	0.5965465305485683
0.0032790907094519	0.9945194342312808	0.4811109710876288
0.3368926125996110	0.9970661119381656	0.4810753002334892
0.6737951750775656	0.9969748163296938	0.4802948719142006
0.0044191956493507	0.3260105885860615	0.4804505096785334
0.3362080450129086	0.3274376118619115	0.4815029663982331
0.6709398542389654	0.3289836236093047	0.4806766509291453
0.0052700381652312	0.6646909389154606	0.4808100821745075
0.3399909035187895	0.6634063362084845	0.4784221782284288
0.6720119255133676	0.6637386381897068	0.4810362500798393
0.1161963745544045	0.2191410251920757	0.5424783150550926
0.2254361444305619	0.1056755394023591	0.4194804019517001
0.4454787183287586	0.2152939484190987	0.5410391977130575
0.5603913249150007	0.1073516515966731	0.4188645580408319
0.7840552702605283	0.2141639153702498	0.5394702330201119
0.8940701395485469	0.1053497950481474	0.4188541086341703
0.1195243104615232	0.5532621856188870	0.5397176092289976
0.2276263882416707	0.4394804685228814	0.4189202744035980
0.4493981920401987	0.5497952044209270	0.5388277806068361
0.5608907309960304	0.4386905635867442	0.4184928307017274
0.7844518235928533	0.5545421548435340	0.5394778465222413
0.8922410430337564	0.4388840360406164	0.4188120329688510
0.1146321784948159	0.8848300655338215	0.5413624776147665
0.2272845225339243	0.7730951135395882	0.4191168697856864
0.4490508277618226	0.8847137571619963	0.5402349209398131
0.5614429045022045	0.7729741867499319	0.4183503656886943
0.7805145436337869	0.8835671930484265	0.5421599988061638
0.8940338572090230	0.7745933977320441	0.4191673711509171
0.6957910744072204	0.3408411113443646	0.6765981149298097
0.6201368080139383	0.1794353346639743	0.6960394877055726
0.6229859763559203	0.4300525864975707	0.6954071086323402
0.3942986228414431	0.6036052774971608	0.6881503175817253
0.3200215409059815	0.6796249161296555	0.6700947949642148

*N₂+*COOH

Mo	V	C	O	N	H
18	9	19	2	2	1

Direct

0.1176366476453249	0.2176940037330311	0.3637865639429207
0.2213888191341472	0.1015215401864638	0.5965887950469824
0.4484120936814541	0.2156206468174045	0.3637940687504466
0.5652643494948201	0.1101021124072410	0.5957483818694828
0.7838902407450165	0.2160904879893767	0.3639049616424147

0.8976998323173074	0.1038153764054931	0.5973932843149773
0.1162801294278880	0.5501814536880504	0.3641696852834207
0.2350567818882957	0.4504185928848290	0.5988617500957271
0.4502486573567095	0.5495003173818628	0.3637123921826816
0.5660730055918287	0.4369696536657479	0.5965389122397191
0.7845295549649121	0.5516250998312073	0.3639447440269815
0.8818959857567169	0.4315447270241063	0.5955767994051451
0.1169598208812509	0.8829928850214078	0.3636753308224162
0.2331415147061781	0.7678941644724367	0.6003044814953149
0.4501398393529790	0.8836968470443879	0.3641523385965345
0.5502099770534623	0.7643893798744120	0.5987086035085710
0.7831480325520122	0.8829305898274336	0.3635037312756275
0.8985126851983050	0.7785521873394029	0.5964579092025707
0.0047963834072144	0.9949499461932014	0.4806461686639295
0.3384474484254256	0.9976592754387096	0.4810895093752245
0.6746338106340685	0.9968803446454672	0.4804544297826771
0.0060603662029652	0.3260692883286826	0.4801804348640412
0.3378581561372390	0.3283741440937972	0.4820602194780264
0.6721079033792090	0.3291385617423200	0.4806341823702003
0.0059639740782909	0.6642886992256486	0.4806190221548474
0.3399916340876150	0.6629406805141489	0.4788180304404085
0.6716883664011030	0.6630600417296106	0.4812928487576057
0.1168599959545475	0.2192525077181819	0.5421619481205885
0.2267137644923706	0.1053816931067945	0.4192095189867172
0.4462512292302626	0.2152821190258183	0.5410611987681579
0.5615314838683240	0.1070708363003155	0.4189625781825464
0.7855708602105715	0.2134235375069801	0.5396268942791537
0.8950766253433711	0.1050856195482220	0.4186845101341494
0.1200979816771207	0.5531970902434580	0.5399656016332631
0.2286674231728034	0.4392900820257060	0.4189594222740837
0.4505311284900738	0.5496175324979755	0.5396287707654006
0.5613079895984914	0.4383577464970242	0.4188783839234879
0.7852063406397962	0.5549275241973647	0.5399353678914781
0.8933355243115483	0.4384510555086201	0.4188128195616350
0.1154601016898840	0.8844296648961703	0.5406432783451347
0.2284898434233044	0.7727883711610860	0.4190119467093744
0.4496423348813656	0.8843706982361409	0.5405175769597481
0.5618716596683553	0.7723233624903202	0.4185443809333957
0.7813811419360254	0.8834979606069835	0.5419062868585219
0.8949428592094143	0.7741376281568211	0.4190283213898662
0.7083557244654795	0.3558292217754254	0.6775123399149450
0.6366113345831940	0.1849891440609514	0.7043788415385224
0.6274947747595450	0.4297536128962587	0.6996986965129968
0.3960192754935819	0.6047814890198858	0.6887912279106779

0.3206297642856805	0.6798258290416908	0.6703258665963499
0.5419143351131330	0.1659540919759500	0.7338863612209162

*N₂+*CO

Mo	V	C	O	N
18	9	19	1	2

Direct

0.1183606633965438	0.2211424564657473	0.3636358141286894
0.2261955172269882	0.1063705185629582	0.5958424188721991
0.4498655890589179	0.2192202509654507	0.3632790298371444
0.5655186593366504	0.1138361253105215	0.5958411086250229
0.7854812992579820	0.2205092298559735	0.3639261163513450
0.8955984735458768	0.1068301174431539	0.5971613066856646
0.1176001073047960	0.5528598304398401	0.3640791286216886
0.2390549226635404	0.4550892559875113	0.5983942827788331
0.4515866259527272	0.5527585372181146	0.3634136321341853
0.5652829451432685	0.4381657426464812	0.5969410899683469
0.7855002955233907	0.5547177098909778	0.3639905189808929
0.8841151168263921	0.4385630096706383	0.5975082095049715
0.1182936055601335	0.8867591363750130	0.3632936685927518
0.2378828361372243	0.7739843664435243	0.5998011204800437
0.4513807415063824	0.8875781196911028	0.3633850420127563
0.5540782497531748	0.7700478001962200	0.5990541415597762
0.7850623685625957	0.8865873741829785	0.3632823744972546
0.9005857026735395	0.7812778376477061	0.5960947646897206
0.0068291966209901	0.9984721912673857	0.4812390346814634
0.3405493387471066	0.0020272841843347	0.4798734508531253
0.6757609639097786	0.9994436218382867	0.4791012676841195
0.0080913066773380	0.3294857411931118	0.4802942310493670
0.3411463071993138	0.3328980558161478	0.4816546085157233
0.6742050959733339	0.3325777365156366	0.4806137099636834
0.0094846931884304	0.6685309201592923	0.4800205404177246
0.3416936803339389	0.6659596440051274	0.4787439313925715
0.6731922012768152	0.6661240845338032	0.4806627205001516
0.1180207206424897	0.2229618561688090	0.5426611049515048
0.2286385576081877	0.1095834068132442	0.4187293854145822
0.4490286835003530	0.2196389301632706	0.5403225817244229
0.5628401935248346	0.1101844617183981	0.4187738294672881
0.7853697254578984	0.2174252878404569	0.5403619155254116
0.8964000687923359	0.1088238776381691	0.4186434866765075
0.1223928856800032	0.5573280659810458	0.5400799131181846
0.2304093475923175	0.4428884915208247	0.4189531630909348
0.4537789618828615	0.5549343755563303	0.5395011383395840
0.5625387177751042	0.4422710656364953	0.4187006521377733

0.7861802916839197	0.5580870562028524	0.5393535494850250
0.8954463779778437	0.4425888573807750	0.4188669990824390
0.1180759386950919	0.8883849112737986	0.5401439356232710
0.2302444507872091	0.7766230801115271	0.4184458080013690
0.4533572170811894	0.8883856109237009	0.5398020128216379
0.5633798914140122	0.7763935292552341	0.4179410117178052
0.7834040023674934	0.8869825292517715	0.5414950519276749
0.8967035774369000	0.7776895643863789	0.4189954025019456
0.7299382697905845	0.3982692187555992	0.6743994977044583
0.6252838095949728	0.3947284745401058	0.7135615359470459
0.3990201540007297	0.6094469236188674	0.6888961470917785
0.3252009813564921	0.6856131027553052	0.6702446362701586

*NCON

Mo	V	C	O	N
18	9	19	1	2

Direct

0.1187409750133235	0.2210094626586497	0.3642807236154217
0.2350737492947101	0.1190682758001334	0.5994252658009559
0.4535899691911007	0.2200019253194112	0.3644976524568553
0.5577028727588047	0.1247757729335428	0.6007691843788340
0.7852109842249949	0.2198711474800814	0.3650972776781676
0.9010168451893412	0.1125613543675744	0.5976357225256455
0.1194086696449007	0.5545943195604225	0.3642925593089745
0.2352119956855900	0.4413058685913159	0.5990863352210605
0.4537191773601003	0.5571007108964741	0.3644144256409610
0.5597108105398121	0.4423117956507225	0.5954714108372517
0.7857822688556574	0.5545659161446752	0.3642592825431410
0.9021194103943565	0.4469046134396200	0.5968066716758945
0.1192816571386712	0.8882134514578884	0.3643422378817811
0.2276731512612048	0.7758713525787079	0.5988334503416812
0.4522925564456883	0.8879976860679801	0.3654044412354435
0.5576814393078241	0.7574658084908170	0.6006666590715365
0.7852545512505906	0.8887072134237097	0.3650558313952298
0.9018911234921456	0.7791999209641044	0.5968268623042721
0.0047735060430713	0.9994184939069928	0.4809438036796084
0.3386875089438019	-0.0044998389001578	0.4823300465590525
0.6698495682761100	0.9976590252542914	0.4850547916230866
0.0051147421312072	0.3294702459314924	0.4809300566718158
0.3410941597410915	0.3324095447820192	0.4776350854970209
0.6792113460685348	0.3315577936176866	0.4796467879086599
0.0094452915179866	0.6665482217420162	0.4798616213649352
0.3394783307893085	0.6682881417513519	0.4821295211703878
0.6791852018670352	0.6716722932249350	0.4794327711144761

0.1179932956189458	0.2211516063670425	0.5408898774178484
0.2297247442868694	0.1091185888285834	0.4194922326866163
0.4501248211471988	0.2204940150679049	0.5370131843554278
0.5636233606334884	0.1087118278432524	0.4211554930422971
0.7835146785824381	0.2210234434753069	0.5443135347377571
0.8962734437176144	0.1098835201133876	0.4208881131014712
0.1213597901126909	0.5574974280532988	0.5418048337938033
0.2298717504031275	0.4441778435021510	0.4193779332613019
0.4504729767792464	0.5543747091125600	0.5366622523617707
0.5636710844349652	0.4435040532622476	0.4187812442388863
0.7935424047669362	0.5587609498690573	0.5408913927105197
0.8974988505543210	0.4432199073540243	0.4191902078211340
0.1212875377660035	0.8882096518630250	0.5421312432346524
0.2302179664789686	0.7769656999814282	0.4195129954593628
0.4537495972039752	0.8894572749844664	0.5476270663510299
0.5637751072000394	0.7789147987553534	0.4210063742580440
0.7834386608152323	0.8867974314715568	0.5442206102953816
0.8974352767903611	0.7776552741410533	0.4191924077974868
0.4418053133365606	0.3852140202223062	0.7093969800030120
0.4584045408203825	0.3947302938254047	0.7695448842230330
0.4370951482133744	0.2519289719549986	0.6666300602486402
0.4381574179102894	0.5133876928151510	0.6659662950983535

*NCONH

Mo	V	C	O	N	H
18	9	19	1	2	1

Direct

0.1195280356463501	0.2260519575734136	0.3638694538549562
0.2355631789302665	0.1168426738895060	0.5965692274465102
0.4536882179371894	0.2254005682705224	0.3641308094576731
0.5586090064085649	0.1224844696243704	0.6000035342191574
0.7870003624769212	0.2275001062010034	0.3643119059790672
0.8996574875490301	0.1164667290156764	0.5966667275041931
0.1192396721331807	0.5582154877813424	0.3640249487481927
0.2369415259978757	0.4421125888653225	0.6007924140816691
0.4529500820367461	0.5591147684399158	0.3639167261978615
0.5568678618153520	0.4444148207505758	0.5989302402986634
0.7862873346251456	0.5583795038122040	0.3639992400830687
0.9023059691796649	0.4514780442305752	0.5978907440309824
0.1200307634863167	0.8921751496137106	0.3637711207163195
0.2303325961470964	0.7795382896017434	0.5979105899934239
0.4522201078714521	0.8919072213616236	0.3642575077817737
0.5684412569772584	0.7864493412235968	0.5954471215334475
0.7863493810380274	0.8925034113923407	0.3639258536780550

0.9008647114743835	0.7845854130567095	0.5962265820266945
0.0057206489074234	0.0030756781674241	0.4791428755741195
0.3400490136210330	0.9988765065732860	0.4803226748730371
0.6748146879815978	0.0032714177376415	0.4812186567056371
0.0086313043301719	0.3376800790340521	0.4817034348354047
0.3414804439048148	0.3382884390132121	0.4794730078299890
0.6788999185060024	0.3374131677415993	0.4802643402006652
0.0082202951220878	0.6691735607592820	0.4802989072515829
0.3408176574625089	0.6700517196255613	0.4813044674586918
0.6770473287267864	0.6723717572545708	0.4792999588453445
0.1205871813083137	0.2262441495742994	0.5407735830218180
0.2305251118684697	0.1146611300729824	0.4188448692315452
0.4531922533902725	0.2258826170308321	0.5364458900418579
0.5648170962695258	0.1138791015923958	0.4196427584134983
0.7854847806871100	0.2272835874247552	0.5433366759750732
0.8968181078274245	0.1149268636802502	0.4195929641347862
0.1221552831107688	0.5585379972387577	0.5425860782999599
0.2304039634352515	0.4483485726252221	0.4195485278050140
0.4525015817491246	0.5604987140333659	0.5404728729850867
0.5641838008424604	0.4485016341776566	0.4191724845311315
0.7889519654258978	0.5604259199290013	0.5424917348260772
0.8981611278459873	0.4483700634139834	0.4198815383999611
0.1202480197714486	0.8893731763342649	0.5407658014889990
0.2301358602201792	0.7799136572518526	0.4192350545024708
0.4520984250622401	0.8941237486033098	0.5427742876121565
0.5639828271539804	0.7816046407736924	0.4195281417375665
0.7885508553916375	0.8942916702133323	0.5403588050664576
0.8976367703190408	0.7811556284369015	0.4190147234242974
0.4343925546473332	0.3304950483354220	0.7151377893131614
0.4596769004847263	0.3248769453566223	0.7745383283387605
0.4406267993510822	0.2276438109247849	0.6634884069920619
0.4087257485761557	0.4602770743280516	0.6842895442146000
0.4459939459683187	0.5569008620374983	0.7180858684374650

*NHCONH

Mo	V	C	O	N	H
18	9	19	1	2	2

Direct

0.1218299876780397	0.2233238704829984	0.3638157946201355
0.2361153250317898	0.1182037412398882	0.5986420908633739
0.4545196120944691	0.2231289592827986	0.3639902880222400
0.5687889772306846	0.1127103190073566	0.5953778728649926
0.7886957377297932	0.2244300437616165	0.3639185529774237
0.9012086480830889	0.1136664506065071	0.5963771959776059

0.1211328205755734	0.5562195852346098	0.3637918255749554
0.2353343108205243	0.4451867371890649	0.5980812417298551
0.4545756963997294	0.5563562620259873	0.3639293362879735
0.5570372000355577	0.4419595952612918	0.6011373872841537
0.7880929712960656	0.5565793015148454	0.3638705133517395
0.9015360872438287	0.4463911480879872	0.5971245446405549
0.1212118857525833	0.8900683454848295	0.3638071651341230
0.2338435602809407	0.7798641878576901	0.5974947843028159
0.4531731095334361	0.8890934765804114	0.3639355615028525
0.5681442209941677	0.7805899299212409	0.5955545965646999
0.7889224854576300	0.8892006656739898	0.3639242382399181
0.9011282535948649	0.7807400670486968	0.5973061742727912
0.0081896265253146	0.9996463975239426	0.4805029947493552
0.3420498165629238	-0.0003906011277715	0.4803231613121213
0.6761183511862130	0.0006457449738001	0.4813709278827798
0.0078303149658145	0.3335328574773614	0.4801693262736370
0.3426873626260571	0.3340099303517638	0.4806567261640615
0.6780069618386647	0.3353246074726833	0.4801445017137147
0.0091350268179658	0.6675183768115145	0.4809673474359989
0.3420912091166811	0.6683356444378468	0.4800586961437362
0.6787361342673139	0.6680005795184720	0.4800907622661106
0.1222660522859722	0.2240390305016519	0.5406626064742490
0.2322451846641382	0.1118864239870452	0.4192295177027816
0.4545225419288476	0.2228955520393851	0.5402557291848441
0.5657703014239555	0.1116837810713210	0.4191796855232989
0.7897901070533492	0.2247249437412995	0.5406975307732664
0.8984001275598967	0.1116035049509226	0.4191838174219707
0.1217006074312301	0.5585744503115500	0.5413356129135477
0.2321985711325989	0.4451762311516634	0.4191056015375393
0.4544121841376190	0.5571520988775431	0.5397636287222233
0.5657808745827813	0.4452900617010579	0.4193368665240288
0.7868858283642743	0.5562519688008077	0.5431988042015281
0.8989647305050630	0.4458486579656973	0.4194458143821201
0.1219714882571597	0.8897866240545353	0.5418547261742243
0.2311530094446004	0.7781756113484057	0.4192066340305425
0.4536119160258912	0.8894401272681454	0.5407429259978310
0.5658208710288504	0.7789961150701202	0.4191097220793797
0.7896568836005552	0.8905049532375141	0.5408792687077617
0.8992923579910078	0.7782310174415183	0.4194761909225787
0.4185536148212833	0.3775936707841618	0.7223579661152919
0.4453086809050851	0.3931653166837846	0.7823593261596471
0.4080423013376314	0.2445422805519394	0.6820968156106741
0.4090127099627565	0.4988899194724856	0.6807640446534495
0.4429005798974036	0.6038426111678017	0.7100023769725241

0.4431323509183298 0.1755982081182418 0.7119008380609633\

*NHCONH₂

Mo	V	C	O	N	H
18	9	19	1	2	3

Direct

0.1369010593835489	0.2309271517951732	0.3619407780338005
0.2554408591638350	0.1298470795545670	0.5958824826769069
0.4698854501436330	0.2311876443104357	0.3617207941562129
0.5852376931482172	0.1147600876442490	0.5924791500147224
0.8043294437057141	0.2320037706888912	0.3616162753602518
0.9108184665921288	0.1167569651680558	0.5943256193555584
0.1365246396128365	0.5644629397244628	0.3620537866484955
0.2476944625306437	0.4528035689442895	0.5949564161558213
0.4704809403563504	0.5644644316890256	0.3618810669086973
0.5705258377118269	0.4455389762153311	0.5962709083537631
0.8034441391752335	0.5642415810323479	0.3619941919059169
0.9140919189411201	0.4528498181306774	0.5949921421522443
0.1366910637295275	0.8976587258829032	0.3620846725709432
0.2473793357580166	0.7862734080049050	0.5951137385711666
0.4691347842184582	0.8969754522792762	0.3616085957102156
0.5843547479648863	0.7901431128383565	0.5936733828771529
0.8046482569610025	0.8968489582653315	0.3618230780288293
0.9140656303494625	0.7850776623464301	0.5959292064094518
0.0256201966705063	0.0077247449470773	0.4793485287718072
0.3576555462705337	0.0081200950049117	0.4786406849810866
0.6927881580402674	0.0086851272526946	0.4782871642335665
0.0250349511503587	0.3415889203748033	0.4789493052287202
0.3594454580773374	0.3420069090265806	0.4785318658675692
0.6928227447014605	0.3432161513455271	0.4787227216273916
0.0256373004617643	0.6756725658412618	0.4785316912795436
0.3587872339537424	0.6755867090623658	0.4789555219026259
0.6934776628802091	0.6756874283161155	0.4788628708137347
0.1359881014617950	0.2307061969667706	0.5391981742541931
0.2480493908318439	0.1203483914866896	0.4174331910700142
0.4717293387187713	0.2296483311738153	0.5379384977671536
0.5813516633686984	0.1200782194777121	0.4167065657061607
0.8060059572132950	0.2322452850187389	0.5382818631085392
0.9145249073485524	0.1200081140569254	0.4172009203364272
0.1361016996627769	0.5647407165687695	0.5395247740701591
0.2482544560646947	0.4535373236120659	0.4170000556790401
0.4698677745468139	0.5644793325483101	0.5390982404536346
0.5812532101740056	0.4533513016204005	0.4173997682383463
0.8022871308634130	0.5639665321706586	0.5406322560925003

0.9147356973479147	0.4539914721757075	0.4175937540496755
0.1364354468451947	0.8983805202166197	0.5409694656380123
0.2474410077077632	0.7866446466673358	0.4175803266238554
0.4675759108261479	0.8949594590157557	0.5381531894595107
0.5817454251791190	0.7874327319949239	0.4170223517232114
0.8055022466864734	0.8961656077341938	0.5387180006733224
0.9149747375390574	0.7865188148759460	0.4178749783321762
0.3287881272327074	0.3272738551485377	0.7314484007800480
0.2903310659570230	0.2701321341052186	0.7878997208256325
0.4200817218271324	0.2921559977447963	0.6852561962567763
0.2791600717290260	0.4486406547660606	0.7064925183667679
0.1782643645176286	0.4319441939278985	0.7346855897008810
0.4670040312847153	0.2271828274276013	0.7108286314117858
0.3769680954128056	0.5689267598125197	0.7161155967859628

*NH₂CONH₂

Mo	V	C	O	N	H
18	9	19	1	2	4

Direct

0.1337731327276192	0.2285339301678070	0.3634849856262552
0.2452785371343868	0.1187882335469465	0.5989066365436015
0.4657994193948689	0.2284789875085967	0.3634527452609000
0.5807526090537437	0.1140575136270134	0.5948057879689245
0.8002037522843595	0.2294331732354247	0.3627364411963696
0.9046577667904838	0.1144611070188904	0.5948397205694721
0.1333101390100208	0.5613525229253795	0.3628412517622526
0.2437271409754660	0.4512016083448330	0.5971383796431252
0.4660968675642041	0.5610389332863466	0.3634386072185753
0.5786407459526826	0.4513080920276436	0.5971918753720675
0.7991005714463337	0.5615157429699458	0.3628623316290623
0.9112355053639196	0.4513348173084765	0.5957789994692398
0.1334149111668383	0.8960135805799065	0.3629110685637850
0.2428173478311675	0.7823824485493870	0.5962452377523815
0.4654041585106701	0.8947130544801740	0.3627701659662669
0.5797933236220225	0.7888051339662113	0.5947298676944125
0.8004856495836336	0.8947457673705810	0.3628093690116415
0.9105447263848366	0.7825604978995131	0.5962685268235219
0.0230202169618756	0.0057409376552356	0.4806024845088799
0.3540705189434810	0.0055428299414240	0.4803736839406514
0.6885419780274802	0.0058594341010353	0.4790822120563665
0.0220469980404027	0.3399992801033648	0.4801541930665868
0.3551984562957987	0.3390143892724667	0.4822364109915847
0.6890797238517680	0.3401155747872161	0.4801816715392109
0.0219209561725802	0.6729704725115974	0.4787345383124032

0.3545711928883684	0.6730712664021672	0.4797683331989404
0.6897443672441153	0.6732829260145990	0.4799114318709273
0.1321141894916780	0.2269044288699348	0.5412004278552300
0.2444304293808593	0.1177567037158316	0.4190518165312552
0.4664975784708917	0.2268214397220725	0.5411691597850432
0.5777999475364680	0.1176179482886141	0.4181495792772731
0.8001688092528766	0.2295852637747625	0.5393086126708514
0.9109811627187204	0.1176457572536291	0.4181870872299945
0.1322070309463512	0.5627872056403246	0.5396462854548003
0.2443531487707937	0.4505071627966746	0.4188732052080339
0.4669635898914321	0.5629916605019093	0.5405643232617833
0.5773775468903418	0.4505423973160083	0.4188654105538115
0.8017436049833638	0.5630283121082833	0.5397164612015120
0.9112026700696547	0.4512764705010505	0.4184445493053311
0.1327699678467666	0.8944343779868577	0.5406622209480951
0.2439024876328577	0.7842745372409672	0.4182597205384911
0.4635044619508288	0.8934842748354569	0.5394309772378323
0.5779246271796373	0.7845112594064529	0.4179463673968579
0.8009847397198563	0.8938466780619562	0.5395717583763520
0.9114709047699313	0.7844029194282955	0.4183796660107716
0.3511604103795876	0.3287828473864660	0.6897744677330175
0.2690243844791098	0.1648031482989875	0.7030178888489569
0.5305715151729290	0.4192189640553036	0.7061950796260733
0.2631127989324673	0.4202304038755605	0.7061069129782550
0.1517651393984023	0.3430546593784817	0.7302901985582240
0.5644657223065227	0.3404158127465809	0.7292175402714337
0.3326392282585320	0.5332093781317960	0.7302784466953531
0.5745226673460027	0.5307931380755554	0.7315048708879527

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