Supporting Information

Nitrogen Allotrope N_6 Enables Electrocatalytic Ammonia Synthesis under Anodic Polarization

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Nitrogen allotrope; nitrogen reduction reaction; anodic polarization; reaction mechanism; single-atom center; MXene

S1 Derivation of Equilibrium Potentials for Electrochemical N_6 Reduction

To evaluate the electrochemical feasibility of electrochemical nitrogen reduction using the nitrogen allotrope N_6, we consider three different reaction stoichiometries corresponding to different conversion degrees of N_6 to ammonia (NH_3). For each case, the standard equilibrium potential U_{eq} is derived based on the total Gibbs free energy change (ΔG_{rxn}) and the number of electrons transferred (n), following the thermodynamic relation:

$$U_{eq} = -\frac{\Delta G_{rxn}}{ne} \quad (1)$$

Here, e is the elementary charge, and the free energies are expressed in electron volts (eV). The energy required to dissociate N_6 into $3N_2$ molecules ($N_6 \rightarrow 3N_2$) is taken from high-level quantum chemical calculations at the CCSD(T)/cc-pVTZ level theory, yielding $\Delta G_x = -8.86$ eV.[1] The hydrogenation of molecular nitrogen (N_2) to ammonia is referenced from experimental thermodynamic data[2], where the standard Gibbs free energy for $N_2 + 3H_2 \rightarrow 2\ NH_3$ is $\Delta G_y = -0.38$ eV under ambient conditions.

S1.1 First Reaction: $N_6 + 18\ H^+ + 18\ e^- \rightarrow 6\ NH_3$

The first pathway involves full conversion of all nitrogen atoms in N_6 into NH_3, requiring 18 proton-coupled electron transfer (PCET) steps in total. The reaction is decomposed as:

Step 1: $N_6 \rightarrow 3N_2$, $\Delta G_x = -8.86$ eV (2)

Step 2: $3(N_2 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3)$, $\Delta G_y = 3 \times (-0.38) = -1.14$ eV (3)

Step 3: $\Delta G_{rxn} = \Delta G_x + \Delta G_y = -8.86$ eV -1.14 eV $= -10.00$ eV (4)

$U_{eq} = 0.56$ V vs. RHE (5)

S1.2 Second Reaction: $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

Here, four nitrogen atoms are reduced to four NH_3 while two nitrogen atoms retain as N_2, which requires 12 PCET steps. The reaction is decomposed as:

Step 1: $N_6 \rightarrow 3N_2$, $\Delta G_x = -8.86$ eV (6)

Step 2: $2(N_2 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3)$, $\Delta G_y = 2 \times (-0.38) = -0.76$ eV (7)

Step 3: $\Delta G_{rxn} = \Delta G_x + \Delta G_y = -8.86$ eV -0.76 eV $= -9.62$ eV (8)

$U_{eq} = 0.80$ V vs. RHE (9)

S1.3 Third Reaction: $N_6 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3 + 2\ N_2$

In this pathway, only two nitrogen atoms are reduced to two NH_3, while four nitrogen atoms retain as 2 N_2, which requires 6 PCET steps. The reaction is decomposed as:

Step 1: $N_6 \rightarrow 3N_2$, $\Delta G_x = -8.86$ eV (10)

Step 2: $N_2 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3$, $\Delta G_y = -0.38$ eV (11)

Step 3: $\Delta G_{rxn} = \Delta G_x + \Delta G_y = -8.86$ eV -0.38 eV $= -9.24$ eV (12)

$U_{eq} = 1.54$ V vs. RHE (13)

S2 Reaction Mechanisms for Electrochemical N_6 Reduction

Nitrogen reduction of the nitrogen allotrope N_6 can proceed via two primary mechanisms, namely associative (cf. **Figure S1**) or dissociative pathways (cf. **Figure S2-S3**). In the associative description, the reduction of nitrogen atoms occurs sequentially without breaking the N_6 bonds at the initial stage, with hydrogenation taking place stepwise on the intact N_6 molecule (cf. eqs. (14)-(32)). In contrast, the dissociative pathway involves the initial cleavage of the N_6 molecule, generating two adsorbed nitrogen species of the same chain length ($*N_3$ – $*N_3$, cf. eqs. (53)-(91)) or forming adsorbed $*N_4$ due to direct cleavage of N_2 (cf. eqs. (33)-(52)). The adsorbed nitrogen species are then sequentially hydrogenated to form ammonia. In the mechanistic description underneath, p, d, and m indicate proximal, distal, and medial sites with respect to the nitrogen fragment adsorbed to the single-atom center (SAC) of Mo_2C MXene.

S2.1 Associative Pathway

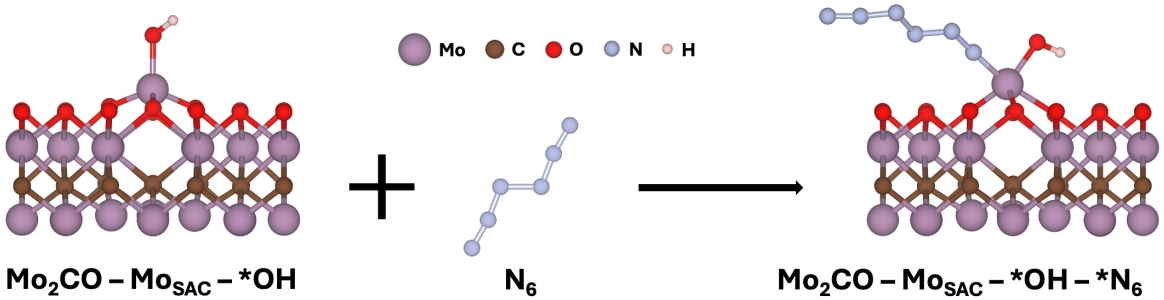

Figure S1. Adsorption configurations of N_6 at Mo-based active sites.
Associative N_6 adsorption on the model electrocatalyst $Mo_2CO - Mo_{SAC} - *OH$.

S2.1.1 $N_6 + 18\ H^+ + 18\ e^- \rightarrow 6\ NH_3$

$M_{SAC} - *OH + N_6 \rightarrow M_{SAC} - *OH - *N_6$ $\Delta G_{Chem}^{N_6}$ (14)

$M_{SAC} - *OH - *N_6 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_6H_d$ ΔG_1 (15)

$M_{SAC} - *OH - *N_6H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_6H_dH_d$ ΔG_2 (16)

$M_{SAC} - *OH - *N_6H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_5 + NH_3$ ΔG_3 (17)

$M_{SAC} - *OH - *N_5 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_5H_d$ ΔG_4 (18)

$M_{SAC} - *OH - *N_5H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_5H_dH_d$ ΔG_5 (19)

$M_{SAC} - *OH - *N_5H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4 + NH_3$ ΔG_6 (20)

$M_{SAC} - *OH - *N_4 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_d$ ΔG_7 (21)

$M_{SAC} - *OH - *N_4H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_dH_d$ ΔG_8 (22)

$M_{SAC} - *OH - *N_4H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 + NH_3$ ΔG_9 (23)

$M_{SAC} - *OH - *N_3 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_d$ ΔG_{10} (24)

$M_{SAC} - *OH - *N_3H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_dH_d$ ΔG_{11} (25)

$M_{SAC} - *OH - *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2 + NH_3$ ΔG_{12} (26)

$M_{SAC} - *OH - *N_2 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2H_d$ ΔG_{13} (27)

$M_{SAC} - *OH - *N_2H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2H_dH_d$ ΔG_{14} (28)

$M_{SAC} - *OH - *N_2H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N + NH_3$ ΔG_{15} (29)

$M_{SAC} - *OH - *N + H^+ + e^- \rightarrow M_{SAC} - *OH - *NH_p$ ΔG_{16} (30)

$M_{SAC} - *OH - *NH_p + H^+ + e^- \rightarrow M_{SAC} - *OH - *NH_pH_p$ ΔG_{17} (31)

$M_{SAC} - *OH - *NH_pH_p + H^+ + e^- \rightarrow M_{SAC} - *OH + NH_3$ ΔG_{18} (32)

S2.2 Symmetric Dissociative Pathway

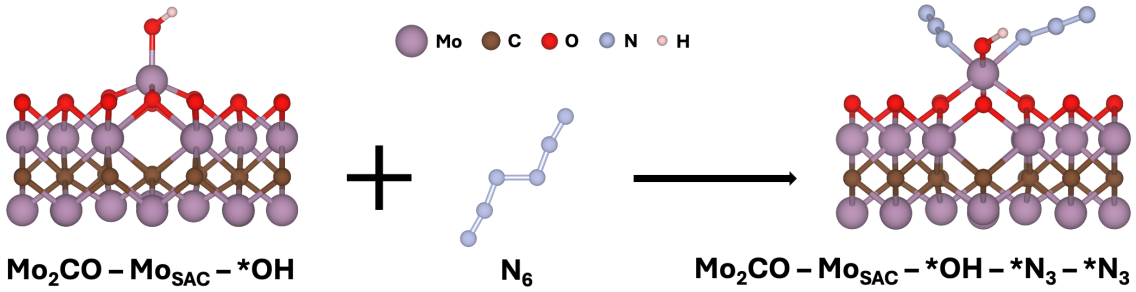

Figure S2. Adsorption configurations of N_6 at Mo-based active sites.
Dissociative N_6 adsorption on the model electrocatalyst $Mo_2CO - Mo_{SAC} - *OH$ in a symmetrical form, where N_6 decomposes into two adsorbed $*N_3$ species.

S2.2.1 $N_6 + 18\ H^+ + 18\ e^- \rightarrow 6\ NH_3$

$M_{SAC} - *OH + N_6 \rightarrow M_{SAC} - *OH - *N_3 - *N_3$ $\Delta G_{Che,1}^{N_3-}$ (33)

$M_{SAC} - *OH - *N_3 - *N_3 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N_3H_d$ ΔG_{37} (34)

$M_{SAC} - *OH - *N_3 - *N_3H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N_3H_dH_d$ ΔG_{38} (35)

$M_{SAC} - *OH - *N_3 - *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N_3H_dH_dH_m$ ΔG_{39} (36)

$M_{SAC} - *OH - *N_3 - *N_3H_dH_dH_m + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N_2H_d + NH_3$ ΔG_{40} (37)

$M_{SAC} - *OH - *N_3 - *N_2H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N_2H_dH_d$ ΔG_{41} (38)

$M_{SAC} - *OH - *N_3 - *N_2H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *N + NH_3$ ΔG_{42} (39)

$M_{SAC} - *OH - *N_3 - *N + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *NH_p$ ΔG_{43} (40)

$M_{SAC} - *OH - *N_3 - *NH_p + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 - *NH_pH_p$ ΔG_{44} (41)

$M_{SAC} - *OH - *N_3 - *NH_pH_p + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 + NH_3$ ΔG_{45} (42)

$M_{SAC} - *OH - *N_3 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_d$ ΔG_{46} (43)

$M_{SAC} – *OH – *N_3H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3H_dH_d$ ΔG_{47} (44)

$M_{SAC} – *OH – *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2 + NH_3$ ΔG_{48} (45)

$M_{SAC} – *OH – *N_2 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2H_d$ ΔG_{49} (46)

$M_{SAC} – *OH – *N_2H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2H_dH_d$ ΔG_{50} (47)

$M_{SAC} – *OH – *N_2H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N + NH_3$ ΔG_{51} (48)

$M_{SAC} – *OH – *N + H^+ + e^- \rightarrow M_{SAC} – *OH – *NH_p$ ΔG_{52} (49)

$M_{SAC} – *OH – *NH_p + H^+ + e^- \rightarrow M_{SAC} – *OH – *NH_pH_p$ ΔG_{53} (50)

$M_{SAC} – *OH – *NH_pH_p + H^+ + e^- \rightarrow M_{SAC} – *OH + NH_3$ ΔG_{54} (51)

S2.2.2 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

$M_{SAC} – *OH + N_6 \rightarrow M_{SAC} – *OH – *N_3 – *N_3$ $\Delta G_{\mathrm{Chem}}^{N_3-N_3}$ (52)

$M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 – *N_3H_d$ ΔG_{55} (53)

$M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 – *N_3H_dH_d$ ΔG_{56} (54)

$M_{SAC} – *OH – *N_3 – *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 + N_2 + NH_3$ ΔG_{57} (55)

$M_{SAC} – *OH – *N_3 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3H_d$ ΔG_{58} (56)

$M_{SAC} – *OH – *N_3H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3H_dH_d$ ΔG_{59} (57)

$M_{SAC} – *OH – *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2 + NH_3$ ΔG_{60} (58)

$M_{SAC} – *OH – *N_2 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2H_d$ ΔG_{61} (59)

$M_{SAC} – *OH – *N_2H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_2H_dH_d$ ΔG_{62} (60)

$M_{SAC} – *OH – *N_2H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N + NH_3$ ΔG_{63} (61)

$M_{SAC} – *OH – *N + H^+ + e^- \rightarrow M_{SAC} – *OH – *NH_p$ ΔG_{64} (62)

$M_{SAC} – *OH – *NH_p + H^+ + e^- \rightarrow M_{SAC} – *OH – *NH_pH_p$ ΔG_{65} (63)

$M_{SAC} – *OH – *NH_pH_p + H^+ + e^- \rightarrow M_{SAC} – *OH + NH_3$ ΔG_{66} (64)

S2.2.3 $N_6 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3 + 2\ N_2$

$M_{SAC} – *OH + N_6 \rightarrow M_{SAC} – *OH – *N_3 – *N_3$ $\Delta G_{\mathrm{Chem}}^{N_3-N_3}$ (65)

$M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 – *N_3H_d$ ΔG_{67} (66)

$M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 – *N_3H_dH_d$ ΔG_{68} (67)

$M_{SAC} – *OH – *N_3 – *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3 + N_2 + NH_3$ ΔG_{69} (68)

$M_{SAC} – *OH – *N_3 + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3H_d$ ΔG_{70} (69)

$M_{SAC} – *OH – *N_3H_d + H^+ + e^- \rightarrow M_{SAC} – *OH – *N_3H_dH_d$ ΔG_{71} (70)

$M_{SAC} – *OH – *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} – *OH + N_2 + NH_3$ ΔG_{72} (71)

S2.3 Asymmetric Dissociative Pathway

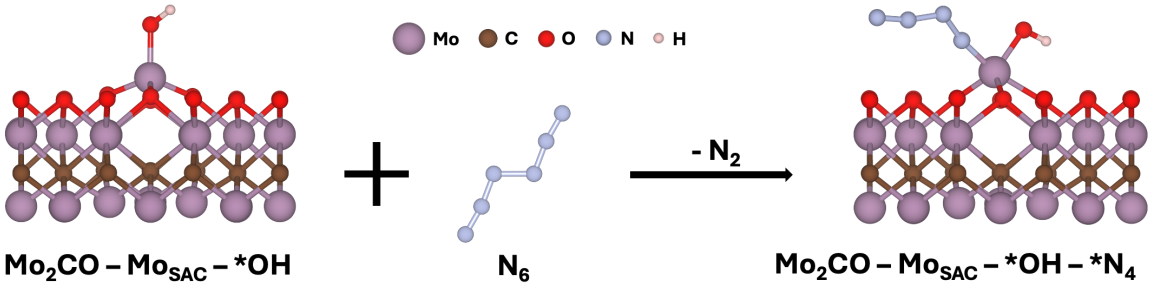

Figure S3. Adsorption configurations of N_6 at Mo-based active sites.
Dissociative N_6 adsorption on the model electrocatalyst $Mo_2CO - Mo_{SAC} - *OH$ in an asymmetrical form, where N_6 is decomposed into adsorbed $*N_4$ and N_2, which readily desorbs.

S2.3.1 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

$$M_{SAC} - *OH + N_6 \rightarrow M_{SAC} - *OH - *N_4 + N_2 \qquad \Delta G_{Chem}^{N_4+N_2} \qquad (72)$$

$$M_{SAC} - *OH - *N_4 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_d \qquad \Delta G_{19} \qquad (73)$$

$$M_{SAC} - *OH - *N_4H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_dH_d \qquad \Delta G_{20} \qquad (74)$$

$$M_{SAC} - *OH - *N_4H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 + NH_3 \qquad \Delta G_{21} \qquad (75)$$

$$M_{SAC} - *OH - *N_3 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_d \qquad \Delta G_{22} \qquad (76)$$

$$M_{SAC} - *OH - *N_3H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_dH_d \qquad \Delta G_{23} \qquad (77)$$

$$M_{SAC} - *OH - *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2 + NH_3 \qquad \Delta G_{24} \qquad (78)$$

$$M_{SAC} - *OH - *N_2 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2H_d \qquad \Delta G_{25} \qquad (79)$$

$$M_{SAC} - *OH - *N_2H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_2H_dH_d \qquad \Delta G_{26} \qquad (80)$$

$$M_{SAC} - *OH - *N_2H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N + NH_3 \qquad \Delta G_{27} \qquad (81)$$

$$M_{SAC} - *OH - *N + H^+ + e^- \rightarrow M_{SAC} - *OH - *NH_p \qquad \Delta G_{28} \qquad (82)$$

$$M_{SAC} - *OH - *NH_p + H^+ + e^- \rightarrow M_{SAC} - *OH - *NH_pH_p \qquad \Delta G_{29} \qquad (83)$$

$$M_{SAC} - *OH - *NH_pH_p + H^+ + e^- \rightarrow M_{SAC} - *OH + NH_3 \qquad \Delta G_{30} \qquad (84)$$

S2.3.2 $N_6 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3 + 2\ N_2$

$$M_{SAC} - *OH + N_6 \rightarrow M_{SAC} - *OH - *N_4 + N_2 \qquad \Delta G_{Chem}^{N_4+N_2} \qquad (85)$$

$$M_{SAC} - *OH - *N_4 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_d \qquad \Delta G_{31} \qquad (86)$$

$$M_{SAC} - *OH - *N_4H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_4H_dH_d \qquad \Delta G_{32} \qquad (87)$$

$$M_{SAC} - *OH - *N_4H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3 + NH_3 \qquad \Delta G_{33} \qquad (88)$$

$$M_{SAC} - *OH - *N_3 + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_d \qquad \Delta G_{34} \qquad (89)$$

$$M_{SAC} - *OH - *N_3H_d + H^+ + e^- \rightarrow M_{SAC} - *OH - *N_3H_dH_d \qquad \Delta G_{35} \qquad (90)$$

$$M_{SAC} - *OH - *N_3H_dH_d + H^+ + e^- \rightarrow M_{SAC} - *OH + N_2 + NH_3 \qquad \Delta G_{36} \qquad (91)$$

S3 Gas–Phase Error Corrections

We apply electronic structure theory calculations in the density functional theory framework[3–5] combined with the computational hydrogen electrode (CHE) approach[6] to determine the free-energy changes of eqs. (14) – (91). Note that the determination of the ΔG values is prone to errors due to the application of plane-wave DFT for the description of molecular species as reference states in the underlying equations. These errors have to be corrected using gas-phase error correction schemes,[7] as discussed below.

The Gibbs free energy of formation for the N_6 molecule, based on the reaction $3\ N_2 \rightarrow N_6$, was computed using coupled-cluster theory with single, double, and perturbative triple excitations [CCSD(T)], combined with the correlation-consistent polarized valence triple-zeta basis set (cc-pVTZ) in the previous work by Qian et al.[1]. The reported value is:

$$\Delta G_{\mathrm{CCSD(T)}} = 8.86 \text{ eV} \quad (92)$$

This formation energy can also be estimated using density functional theory (DFT) within the generalized gradient approximation (GGA), specifically using the PBE functional with Grimme's D3 dispersion correction (PBE-D3)[8]:

$$\Delta G_{\mathrm{PBE\text{-}D3}} = 6.71 \text{ eV} \quad (93)$$

The intrinsic gas-phase error δ associated with the DFT calculation is then determined as:

$$\delta = \Delta G_{\mathrm{CCSD(T)}} - \Delta G_{\mathrm{PBE\text{-}D3}} \quad (93)$$

$$\delta = 8.86 - 6.71 \quad (94)$$

$$\delta = 2.15 \text{ eV} \quad (95)$$

This correction term is used to adjust the DFT-derived Gibbs free energy of formation involving the N_6 molecule to improve thermodynamic accuracy and consistency with high-level theoretical benchmarks.

S3.1 Error Minimization Approach through Basis Set Method

While we discussed in the previous section a simple correction for the N_6 molecule, recent work in the field has shown that the energetics of all elementary steps of the free-energy landscape need to be corrected. This can be achieved by using the error minimization schemes developed by Exner and coworkers.[9–11]

The basis set used in the error minimization scheme comprises a set of gas-phase molecules related to the electrochemical reduction of the nitrogen allotrope N_6. This basis set serves as the reference to correct DFT-derived free energies in a statistically optimized least-squares framework. **Table S1** provides the calculated Gibbs free energies of formation using the PBE-D3 functional, while **Table S2** lists the corresponding experimental values.

Table S1. Gibbs free energies of reference molecules based on DFT.

Gibbs free energy of formation derived from DFT calculations using the PBE-D3 functional. All values are given in eV.

Molecule	ΔG
N_2H_2	1.91
N_2H_4	1.11
NH_3	–0.39
N_6	6.71
N_2	0
H_2	0

Table S2. Experimental Gibbs free energies of reference molecules.

Gibbs free energy of formation derived from experimental data or high-level quantum chemical calculations. All values are given in eV.

Molecule	ΔG
N_2H_2	2.52
N_2H_4	1.64
NH_3	–0.19

N_6	8.86 [CCSD(T)/cc-pVTZ]
N_2	0
H_2	0

To systematically address gas-phase error corrections, the atomization energy of $H_xN_\gamma O_z$-type molecules is employed, as previously described in the work by Exner and coworkers.[9–11]:

$$H_xN_yO_z(g) \rightarrow xH(g) + yN(g) + zO(g) \tag{96}$$

Therein, the authors introduced a general basis set for the Gibbs free energy of formation as given below:

$$\left(\frac{x-3y-2z}{2}\right)H_2(g) + yNH_3(g) + zH_2O \rightarrow H_xN_yO_z(g) \tag{97}$$

With the help of eq. (97) and the experimental basis set reported in **Table S2**, the experimental Gibbs free energy of formation for the $H_xN_yO_z$ molecule can be expressed as:

$$\Delta G_f^{exp} = \Delta G_{f_{H_xN_yO_z}}^{exp} + 0.19y \tag{98}$$

By using theoretical basis set values, the theoretical Gibbs free energy of formation for the $H_xN_yO_z$ molecule is:

$$\Delta G_f^{theo} = \Delta G_{f_{H_xN_yO_z}}^{theo} + 0.39y \tag{99}$$

When the basis set errors are included in the Gibbs free change given in eq. (99), this expression translates to:

$$\Delta G_f^{theo-basis} = \Delta G_{f_{H_xN_yO_z}}^{theo} - \left(-0.39 + \in_{NH_3(g)}\right)y - \left(\frac{x-3y-2z}{2}\right)\in_{H_2(g)} \tag{100}$$

Subtracting eq. (98) form eq. (100) allows us to find the error in the molecule $H_xN_yO_z$ when basis set errors are included:

$$\begin{aligned}\Delta G_f^{exp} - \Delta G_f^{theo-basis} &= \Delta G_{f_{H_xN_yO_z}}^{exp} - \Delta G_{f_{H_xN_yO_z}}^{theo} + \left(-0.20 + \in_{NH_3(g)}\right)y \\ &+ \left(\frac{x-3y-2z}{2}\right)\in_{H_2(g)}\end{aligned} \tag{101}$$

Here, $\in_{NH_3(g)}$ and $\in_{H_2(g)}$ represent basis set errors for the ammonia and hydrogen molecules, respectively. Using eq. (101) and including all the free-energy changes of the reference molecules of the reduced basis set consisting of NH_3 and H_2 (cf. **Table S1-S2**), we derive the following equations:

$$-3 \in_{H_2(g)} + 2 \in_{NH_3(g)} = 0.40 \tag{102}$$

$$-2 \in_{H_2(g)} + 2 \in_{NH_3(g)} = -0.21 \tag{103}$$

$$-1 \in_{H_2(g)} + 2 \in_{NH_3(g)} = -0.13 \tag{104}$$

$$-9 \in_{H_2(g)} + 6 \in_{NH_3(g)} = -0.95 \tag{105}$$

The above equations can be written in matrix form:

$$\begin{bmatrix}-3 & 2\\ -2 & 2\\ -1 & 2\\ -9 & 6\end{bmatrix}\begin{bmatrix}\in_{H_2(g)}\\ \in_{NH_3(g)}\end{bmatrix} = \begin{bmatrix}0.40\\ -0.21\\ -0.13\\ -0.95\end{bmatrix} \tag{106}$$

The error equations associated with the reduced basis set and their respective reference molecules are summarized in **Table S3**.

Table S3. Gas-phase formation energy error corrections in dependence of reference molecules.
Equations of gas-phase formation energy errors for reference molecules using the reduced basis set approach based on eqs. (102)–(105).

Molecule	$\Delta G_f^{exp} - \Delta G_f^{theo-basis} / eV$
$N_2(g)$	$-3 \in_{H_2(g)} + 2 \in_{NH_3(g)} - 0.40$
$N_2H_2(g)$	$-2 \in_{H_2(g)} + 2 \in_{NH_3(g)} + 0.21$
$N_2H_4(g)$	$-1 \in_{H_2(g)} + 2 \in_{NH_3(g)} + 0.13$
$N_6(g)$	$-9 \in_{H_2(g)} + 6 \in_{NH_3(g)} + 0.95$

Here, we use the least squares method to solve the system of eqs. (102)-(105). The solution of these equations is given by eqs. (107)-(108), and the calculated gas-phase formation free energy errors for reference molecules are summarized in **Table S4**.

$$\in_{NH_3(g)} = -0.04 \text{ eV} \quad (107)$$

$$\in_{H_2(g)} = 0.05 \text{ eV} \quad (108)$$

Table S4. Calculated gas-phase formation energy error corrections.
Calculated gas-phase formation free-energy errors for reference molecules using the reduced basis set approach by implementing eqs. (107)-(108) in **Table S3**.

Molecule	$\Delta G_f^{exp} - \Delta G_f^{theo-basis} / eV$
$N_2(g)$	-0.63
$N_2H_2(g)$	0.03
$N_2H_4(g)$	0
$N_6(g)$	0.26

The values listed in **Table S4** are used to correct the free-energy changes of eqs. (14) – (91) in section S2.

S4 Gibbs Free-Energy Changes of N_6RR on Mo_2C-SAC

In this section, we compile the corrected free-energy changes of the elementary steps for N_6RR over Mo_2C-SAC based on eqs. (14) – (91) in section S2.

S4.1 Associative Pathway

S4.1.1 $N_6 + 18\ H^+ + 18\ e^- \rightarrow 6\ NH_3$

Table S5. Free-energy changes for the associative pathway of N_6RR (complete conversion) over Mo_2C.
ΔG values for the associative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_6	−1.18
M_{SAC} – *OH – *N_6 + H^+ + e^- → M_{SAC} – *OH – *N_6H_d	−0.11
M_{SAC} – *OH – *N_6H_d + H^+ + e^- → M_{SAC} – *OH – *$N_6H_dH_d$	−0.87
M_{SAC} – *OH – *$N_6H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_5 + NH_3	−0.40
M_{SAC} – *OH – *N_5 + H^+ + e^- → M_{SAC} – *OH – *N_5H_d	0.03
M_{SAC} – *OH – *N_5H_d + H^+ + e^- → M_{SAC} – *OH – *$N_5H_dH_d$	−0.97

M_{SAC} – *OH – *$N_5H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_4 + NH_3	−0.42
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.13
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.83
M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.69
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.21
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.47
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.64
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	−0.18
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.61
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.07
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−2.86

S4.2 Symmetric Dissociative Pathway

S4.2.1 N_6 + 18 H^+ + 18 e^- → 6 NH_3

Table S6. Free-energy changes for the symmetric dissociative pathway of N_6RR (complete conversion) over Mo_2C.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at U = 0 V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−2.45
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.15
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.86
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_dH_m$	0.15
M_{SAC} – *OH – *N_3 – *$N_3H_dH_dH_m$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_2H_d + NH_3	−0.80
M_{SAC} – *OH – *N_3 – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_2H_dH_d$	−0.53
M_{SAC} – *OH – *N_3 – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N + NH_3	−0.17
M_{SAC} – *OH – *N_3 – *N + H^+ + e^- → M_{SAC} – *OH – *N_3 – *NH_p	−0.47
M_{SAC} – *OH – *N_3 – *NH_p + H^+ + e^- → M_{SAC} – *OH – *N_3 – *NH_pH_p	−0.25
M_{SAC} – *OH – *N_3 – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.35
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.21
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.47
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.64
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	−0.18
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.61
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.07
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−1.87

S4.2.2 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

Table S7. Free-energy changes for the symmetric dissociative pathway of N_6RR (partial conversion) over Mo_2C.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−2.44
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.15
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.86
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + N_2 + NH_3	−2.59
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.21
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.47
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.64
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	−0.18
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.61
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.07
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−1.04

S4.2.3 $N_6 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3 + 2\ N_2$

Table S8. Free-energy changes for the symmetric dissociative pathway of N_6RR (partial conversion) over Mo_2C.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−2.44
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.15
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.86
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + N_2 + NH_3	−2.59
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH + N_2 + NH_3	−2.91

S4.3 Asymmetric Dissociative Pathway

S4.3.1 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

Table S9. Free-energy changes for the asymmetric dissociative pathway of N_6RR (partial conversion) over Mo_2C.

ΔG values for the asymmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_4 + N_2	−4.10
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.13
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.83
M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.69

M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.21
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.47
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.64
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	−0.18
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.61
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.07
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−1.04

S4.3.2 N_6 + 6 H^+ + 6 e^- → 2 NH_3 + 2 N_2

Table S10. Free-energy changes for the asymmetric dissociative pathway of N_6RR (partial conversion) over Mo_2C.

ΔG values for the asymmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2C (Mo_2CO – Mo_{SAC} – *OH) at U = 0 V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_4 + N_2	−4.10
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.13
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.83
M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.69
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	0.31
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.89
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH + N_2 + NH_3	−2.91

S5 Gibbs Free-Energy Changes of N_6RR on Mo_2N-SAC

In this section, we compile the corrected free-energy changes of the elementary steps of N_6RR over Mo_2N - SAC based on eqs. (14) – (91).

S5.1 Associative Pathway

S5.1.1 N_6 + 18 H^+ + 18 e^- → 6 NH_3

Table S11. Free-energy changes for the associative pathway of N_6RR (complete conversion) over Mo_2N.

ΔG values for the associative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mo_{SAC} – *OH) at U = 0 V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_6	−2.27
M_{SAC} – *OH – *N_6 + H^+ + e^- → M_{SAC} – *OH – *N_6H_d	0.01
M_{SAC} – *OH – *N_6H_d + H^+ + e^- → M_{SAC} – *OH – *$N_6H_dH_d$	−1.08
M_{SAC} – *OH – *$N_6H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_5 + NH_3	−0.24
M_{SAC} – *OH – *N_5 + H^+ + e^- → M_{SAC} – *OH – *N_5H_d	0.07
M_{SAC} – *OH – *N_5H_d + H^+ + e^- → M_{SAC} – *OH – *$N_5H_dH_d$	−1.07
M_{SAC} – *OH – *$N_5H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_4 + NH_3	−0.29
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.31
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.79
M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.34

M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.15
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.30
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.75
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	0.17
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.49
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.10
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−1.12

S5.2 Symmetric Dissociative Pathway

S5.2.1 N_6 + 18 H^+ + 18 e^- → 6 NH_3

Table S12. Free-energy changes for the symmetric dissociative pathway of N_6RR (complete conversion) over Mo_2N.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mo_{SAC} – *OH) at U = 0 V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−3.91
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.05
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.67
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_dH_m$	−0.15
M_{SAC} – *OH – *N_3 – *$N_3H_dH_dH_m$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_2H_d + NH_3	−0.63
M_{SAC} – *OH – *N_3 – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_2H_dH_d$	−0.78
M_{SAC} – *OH – *N_3 – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N + NH_3	0.07
M_{SAC} – *OH – *N_3 – *N + H^+ + e^- → M_{SAC} – *OH – *N_3 – *NH_p	−0.54
M_{SAC} – *OH – *N_3 – *NH_p + H^+ + e^- → M_{SAC} – *OH – *N_3 – *NH_pH_p	−0.23
M_{SAC} – *OH – *N_3 – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	0.47
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.70
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.15
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.30
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.75
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	0.17
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.50
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.10
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−1.12

S5.2.2 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

Table S13. Free-energy changes for the symmetric dissociative pathway of N_6RR (partial conversion) over Mo_2N.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−3.91
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.05
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + N_2 + NH_3	−1.96
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.15
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.29
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.75
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	0.17
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.50
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.10
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−0.29

S5.2.3 $N_6 + 6\ H^+ + 6\ e^- \rightarrow 2\ NH_3 + 2\ N_2$

Table S14. Free-energy changes for the symmetric dissociative pathway of N_6RR (partial conversion) over Mo_2N.

ΔG values for the symmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_3 – *N_3	−3.91
M_{SAC} – *OH – *N_3 – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3 – *N_3H_d	0.05
M_{SAC} – *OH – *N_3 – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *N_3 – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + N_2 + NH_3	−1.96
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH + N_2 + NH_3	−1.98

S5.3 Asymmetric Dissociative Pathway

S5.3.1 $N_6 + 12\ H^+ + 12\ e^- \rightarrow 4\ NH_3 + N_2$

Table S15. Free-energy changes for the asymmetric dissociative pathway of N_6RR (partial conversion) over Mo_2N.

ΔG values for the asymmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mo_{SAC} – *OH) at $U = 0$ V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_4 + N_2	−5.07
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.31
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.78

M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.35
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_2 + NH_3	−1.16
M_{SAC} – *OH – *N_2 + H^+ + e^- → M_{SAC} – *OH – *N_2H_d	0.30
M_{SAC} – *OH – *N_2H_d + H^+ + e^- → M_{SAC} – *OH – *$N_2H_dH_d$	−0.75
M_{SAC} – *OH – *$N_2H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N + NH_3	0.17
M_{SAC} – *OH – *N + H^+ + e^- → M_{SAC} – *OH – *NH_p	−0.49
M_{SAC} – *OH – *NH_p + H^+ + e^- → M_{SAC} – *OH – *NH_pH_p	−0.10
M_{SAC} – *OH – *NH_pH_p + H^+ + e^- → M_{SAC} – *OH + NH_3	−0.29

S5.3.2 N_6 + 6 H^+ + 6 e^- → 2 NH_3 + 2 N_2

Table S16. Free-energy changes for the asymmetric dissociative pathway of N_6RR (partial conversion) over Mo_2N.

ΔG values for the asymmetric dissociative pathway of the electrochemical N_6 reduction over the SAC motif of Mo_2N (Mo_2NO – Mos_{AC} – *OH) at U = 0 V vs. RHE. All values are given in eV.

Reaction Equations	ΔG_i
M_{SAC} – *OH + N_6 → M_{SAC} – *OH – *N_4 + N_2	−5.07
M_{SAC} – *OH – *N_4 + H^+ + e^- → M_{SAC} – *OH – *N_4H_d	−0.31
M_{SAC} – *OH – *N_4H_d + H^+ + e^- → M_{SAC} – *OH – *$N_4H_dH_d$	−0.79
M_{SAC} – *OH – *$N_4H_dH_d$ + H^+ + e^- → M_{SAC} – *OH – *N_3 + NH_3	−0.35
M_{SAC} – *OH – *N_3 + H^+ + e^- → M_{SAC} – *OH – *N_3H_d	−0.05
M_{SAC} – *OH – *N_3H_d + H^+ + e^- → M_{SAC} – *OH – *$N_3H_dH_d$	−0.69
M_{SAC} – *OH – *$N_3H_dH_d$ + H^+ + e^- → M_{SAC} – *OH + N_2 + NH_3	−1.98

S6 Supercell Size Effect on the Reaction Intermediates of N_6 Reduction

In the present work, we have used a 3×3×1 supercell to model the elementary steps of the electrochemical N_6RR to ammonia. The choice of this supercell size is based on literature[12–16] and our previous work on nitrogen reduction reaction over the SAC motif of Mo_2C and Mo_2N MXene.[17] Considering the size of the N_6 molecule, we have compared the energetics of different supercell sizes (3×3×1, 4×4×1, and 5×5×1) to benchmark the application of the 3×3×1 supercell. For this purpose, we have chosen the ΔG value for the formation of the *N_6H_d intermediate. Considering that the change of this free energy is within 0.10 eV with increasing supercell size, we conclude that the usage of the 3×3×1 supercell is sufficient for an initial screening of the general applicability of the electrochemical N_6 reduction over the SAC motif of Mo_2C and Mo_2N MXene.

Table S17. Thermodynamics of the *N_6H_d intermediate at different supercell sizes of Mo-based active sites. Free-energy change for the formation of the *N_6H_d intermediate using different supercell sizes. All values are given in eV.

Reaction Intermediates	Supercell Size		
	3×3×1	4×4×1	5×5×1
ΔG(Mo_2CO – Mos_{AC} – *OH – *N_6H_d)	−0.11	−0.02	0.01
ΔG(Mo_2NO – Mos_{AC} – *OH – *N_6H_d)	0.01	−0.04	0.04

S7 Free-energy spans of the $G_{max}(U)$ descriptor for N_6RR

$G_{max}(U)$ enables a potential-dependent assessment of the electrocatalytic activity by evaluating all possible free-energy spans between the intermediate states along the reaction pathways.[18,19] As an example, we apply this procedure to the associative pathway (cf. section S2.1.1 of the SI, eqs. (14)–(32)). The Gibbs free energies of the intermediate states are defined in eqs. (109)–(128).

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}}(U) = 0 \tag{109}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_6}} = \Delta G_{\mathrm{Chem}}^{\mathrm{N_6}} \tag{110}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_6H_d}}(U) = \Delta G_1 + 1 \times e \times U \tag{111}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_6H_dH_d}}(U) = \Delta G_1 + \Delta G_2 + 2 \times e \times U \tag{112}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_5}+\mathrm{NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + 3 \times e \times U \tag{113}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_5H_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + 4 \times e \times U \tag{114}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_5H_dH_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + 5 \times e \times U \tag{115}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_4}+\mathrm{NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + 6 \times e \times U \tag{116}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_4H_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + 7 \times e \times U \tag{117}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_4H_dH_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + 8 \times e \times U \tag{118}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_3}+\mathrm{NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + 9 \times e \times U \tag{119}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_3H_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + 10 \times e \times U \tag{120}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_3H_dH_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + 11 \times e \times U \tag{121}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_2}+\mathrm{NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + 12 \times e \times U \tag{122}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_2H_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + 13 \times e \times U \tag{123}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N_2H_dH_d}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + \Delta G_{14} + 14 \times e \times U \tag{124}$$

$$G_{\mathrm{M_{SAC}}-*\mathrm{OH}-*\mathrm{N}+\mathrm{NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + \Delta G_{14} + \Delta G_{15} + 15 \times e \times U \tag{125}$$

$$G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + \Delta G_{14} + \Delta G_{15} + \Delta G_{16} + 16 \times e \times U \quad (126)$$

$$G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + \Delta G_{14} + \Delta G_{15} + \Delta G_{16} + \Delta G_{17} + 17 \times e \times U \quad (127)$$

$$G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_4 + \Delta G_5 + \Delta G_6 + \Delta G_7 + \Delta G_8 + \Delta G_9 + \Delta G_{10} + \Delta G_{11} + \Delta G_{12} + \Delta G_{13} + \Delta G_{14} + \Delta G_{15} + \Delta G_{16} + \Delta G_{17} + \Delta G_{18} + 18 \times e \times U \quad (128)$$

Based on these free energies, we can define 189 different free energy spans, as summarized in equations (129) – (319).

Taking $G_{\mathrm{M_{SAC}-{*}OH}}(U)$ as a reference

$$G_{\mathrm{span\#1}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (129)$$

$$G_{\mathrm{span\#2}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (130)$$

$$G_{\mathrm{span\#3}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (131)$$

$$G_{\mathrm{span\#4}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (132)$$

$$G_{\mathrm{span\#5}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (133)$$

$$G_{\mathrm{span\#6}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (134)$$

$$G_{\mathrm{span\#7}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (135)$$

$$G_{\mathrm{span\#8}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (136)$$

$$G_{\mathrm{span\#9}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (137)$$

$$G_{\mathrm{span\#10}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (138)$$

$$G_{\mathrm{span\#11}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (139)$$

$$G_{\mathrm{span\#12}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (140)$$

$$G_{\mathrm{span\#13}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (141)$$

$$G_{\mathrm{span\#14}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (142)$$

$$G_{\mathrm{span\#15}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (143)$$

$$G_{\mathrm{span\#16}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (144)$$

$$G_{\mathrm{span\#17}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (145)$$

$$G_{\mathrm{span\#18}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (146)$$

$$G_{\mathrm{span\#19}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH}}(U) \quad (147)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}}$ as a reference

$$G_{\mathrm{span\#20}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (148)$$

$$G_{\mathrm{span\#21}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (149)$$

$$G_{\mathrm{span\#22}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (150)$$
$$G_{\mathrm{span\#23}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (151)$$
$$G_{\mathrm{span\#24}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (152)$$
$$G_{\mathrm{span\#25}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (153)$$
$$G_{\mathrm{span\#26}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (154)$$
$$G_{\mathrm{span\#27}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (155)$$
$$G_{\mathrm{span\#28}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (156)$$
$$G_{\mathrm{span\#29}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (157)$$
$$G_{\mathrm{span\#30}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (158)$$
$$G_{\mathrm{span\#31}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (159)$$
$$G_{\mathrm{span\#32}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (160)$$
$$G_{\mathrm{span\#33}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (161)$$
$$G_{\mathrm{span\#34}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (162)$$
$$G_{\mathrm{span\#35}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (163)$$
$$G_{\mathrm{span\#36}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (164)$$
$$G_{\mathrm{span\#37}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6}} \quad (165)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U)$ as a reference

$$G_{\mathrm{span\#38}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (166)$$
$$G_{\mathrm{span\#39}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (167)$$
$$G_{\mathrm{span\#40}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (168)$$
$$G_{\mathrm{span\#41}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (169)$$
$$G_{\mathrm{span\#42}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (170)$$
$$G_{\mathrm{span\#43}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (171)$$
$$G_{\mathrm{span\#44}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (172)$$
$$G_{\mathrm{span\#45}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (173)$$
$$G_{\mathrm{span\#46}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (174)$$
$$G_{\mathrm{span\#47}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (175)$$
$$G_{\mathrm{span\#48}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (176)$$
$$G_{\mathrm{span\#49}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (177)$$
$$G_{\mathrm{span\#50}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (178)$$
$$G_{\mathrm{span\#51}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (179)$$
$$G_{\mathrm{span\#52}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (180)$$
$$G_{\mathrm{span\#53}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (181)$$
$$G_{\mathrm{span\#54}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_d}}(U) \quad (182)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U)$ as a reference

$$G_{\mathrm{span\#55}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (183)$$
$$G_{\mathrm{span\#56}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (184)$$

$$G_{\text{span\#57}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (185)$$
$$G_{\text{span\#58}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (186)$$
$$G_{\text{span\#59}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (187)$$
$$G_{\text{span\#60}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (188)$$
$$G_{\text{span\#61}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (189)$$
$$G_{\text{span\#62}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (190)$$
$$G_{\text{span\#63}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (191)$$
$$G_{\text{span\#64}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (192)$$
$$G_{\text{span\#65}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (193)$$
$$G_{\text{span\#66}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (194)$$
$$G_{\text{span\#67}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (195)$$
$$G_{\text{span\#68}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (196)$$
$$G_{\text{span\#69}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (197)$$
$$G_{\text{span\#70}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_6H_dH_d}}(U) \quad (198)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U)$ as a reference

$$G_{\text{span\#71}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (199)$$
$$G_{\text{span\#72}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (200)$$
$$G_{\text{span\#73}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (201)$$
$$G_{\text{span\#74}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (202)$$
$$G_{\text{span\#75}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (203)$$
$$G_{\text{span\#76}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (204)$$
$$G_{\text{span\#77}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (205)$$
$$G_{\text{span\#78}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (206)$$
$$G_{\text{span\#79}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (207)$$
$$G_{\text{span\#80}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (208)$$
$$G_{\text{span\#81}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (209)$$
$$G_{\text{span\#82}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (210)$$
$$G_{\text{span\#83}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (211)$$
$$G_{\text{span\#84}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (212)$$
$$G_{\text{span\#85}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5+NH_3}}(U) \quad (213)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U)$ as a reference

$$G_{\text{span\#86}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (214)$$
$$G_{\text{span\#87}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (215)$$
$$G_{\text{span\#88}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (216)$$
$$G_{\text{span\#89}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (217)$$
$$G_{\text{span\#90}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (218)$$
$$G_{\text{span\#91}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (219)$$

$$G_{\mathrm{span\#92}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (220)$$

$$G_{\mathrm{span\#93}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (221)$$

$$G_{\mathrm{span\#94}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (222)$$

$$G_{\mathrm{span\#95}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (223)$$

$$G_{\mathrm{span\#96}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (224)$$

$$G_{\mathrm{span\#97}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (226)$$

$$G_{\mathrm{span\#98}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (227)$$

$$G_{\mathrm{span\#99}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_d}}(U) \quad (228)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U)$ as a reference

$$G_{\mathrm{span\#100}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (229)$$

$$G_{\mathrm{span\#101}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (230)$$

$$G_{\mathrm{span\#102}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (231)$$

$$G_{\mathrm{span\#103}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (232)$$

$$G_{\mathrm{span\#104}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (233)$$

$$G_{\mathrm{span\#105}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (234)$$

$$G_{\mathrm{span\#106}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (235)$$

$$G_{\mathrm{span\#107}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (236)$$

$$G_{\mathrm{span\#108}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (237)$$

$$G_{\mathrm{span\#109}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (238)$$

$$G_{\mathrm{span\#110}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (239)$$

$$G_{\mathrm{span\#111}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (240)$$

$$G_{\mathrm{span\#112}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_5H_dH_d}}(U) \quad (241)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U)$ as a reference

$$G_{\mathrm{span\#113}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (242)$$

$$G_{\mathrm{span\#114}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (243)$$

$$G_{\mathrm{span\#115}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (244)$$

$$G_{\mathrm{span\#116}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (245)$$

$$G_{\mathrm{span\#117}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (246)$$

$$G_{\mathrm{span\#118}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (247)$$

$$G_{\mathrm{span\#119}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (248)$$

$$G_{\mathrm{span\#120}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (249)$$

$$G_{\mathrm{span\#121}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (250)$$

$$G_{\mathrm{span\#122}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (251)$$

$$G_{\mathrm{span\#123}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (252)$$

$$G_{\mathrm{span\#124}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4+NH_3}}(U) \quad (253)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U)$ as a reference

$$G_{\mathrm{span\#125}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (254)$$

$$G_{\mathrm{span\#126}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (255)$$
$$G_{\mathrm{span\#127}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (256)$$
$$G_{\mathrm{span\#128}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (257)$$
$$G_{\mathrm{span\#129}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (258)$$
$$G_{\mathrm{span\#130}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (259)$$
$$G_{\mathrm{span\#131}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (260)$$
$$G_{\mathrm{span\#132}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (261)$$
$$G_{\mathrm{span\#133}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (262)$$
$$G_{\mathrm{span\#134}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (263)$$
$$G_{\mathrm{span\#135}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_d}}(U) \quad (264)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U)$ as a reference

$$G_{\mathrm{span\#136}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (265)$$
$$G_{\mathrm{span\#137}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (266)$$
$$G_{\mathrm{span\#138}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (267)$$
$$G_{\mathrm{span\#139}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (268)$$
$$G_{\mathrm{span\#140}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (269)$$
$$G_{\mathrm{span\#141}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (270)$$
$$G_{\mathrm{span\#142}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (271)$$
$$G_{\mathrm{span\#143}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (272)$$
$$G_{\mathrm{span\#144}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (273)$$
$$G_{\mathrm{span\#145}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_4H_dH_d}}(U) \quad (274)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U)$ as a reference

$$G_{\mathrm{span\#146}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (275)$$
$$G_{\mathrm{span\#147}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (276)$$
$$G_{\mathrm{span\#148}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (277)$$
$$G_{\mathrm{span\#149}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (278)$$
$$G_{\mathrm{span\#150}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (279)$$
$$G_{\mathrm{span\#151}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (280)$$
$$G_{\mathrm{span\#152}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (281)$$
$$G_{\mathrm{span\#153}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (282)$$
$$G_{\mathrm{span\#154}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3+NH_3}}(U) \quad (283)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U)$ as a reference

$$G_{\mathrm{span\#155}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (284)$$
$$G_{\mathrm{span\#156}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (285)$$
$$G_{\mathrm{span\#157}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (286)$$
$$G_{\mathrm{span\#158}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (287)$$

$$G_{\text{span\#159}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (288)$$
$$G_{\text{span\#160}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (289)$$
$$G_{\text{span\#161}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (290)$$
$$G_{\text{span\#162}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_d}}(U) \quad (291)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U)$ as a reference

$$G_{\text{span\#163}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (292)$$
$$G_{\text{span\#164}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (293)$$
$$G_{\text{span\#165}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (294)$$
$$G_{\text{span\#166}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (295)$$
$$G_{\text{span\#167}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (296)$$
$$G_{\text{span\#168}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (297)$$
$$G_{\text{span\#169}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_3H_dH_d}}(U) \quad (298)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U)$ as a reference

$$G_{\text{span\#170}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (299)$$
$$G_{\text{span\#171}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (300)$$
$$G_{\text{span\#172}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (301)$$
$$G_{\text{span\#173}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (302)$$
$$G_{\text{span\#174}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (303)$$
$$G_{\text{span\#175}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2+NH_3}}(U) \quad (304)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U)$ as a reference

$$G_{\text{span\#176}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) \quad (305)$$
$$G_{\text{span\#177}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) \quad (306)$$
$$G_{\text{span\#178}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) \quad (307)$$
$$G_{\text{span\#179}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) \quad (308)$$
$$G_{\text{span\#180}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_d}}(U) \quad (309)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U)$ as a reference

$$G_{\text{span\#181}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) \quad (310)$$
$$G_{\text{span\#182}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) \quad (311)$$
$$G_{\text{span\#183}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) \quad (312)$$
$$G_{\text{span\#184}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N_2H_dH_d}}(U) \quad (313)$$

Taking $G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U)$ as a reference

$$G_{\text{span\#185}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) \quad (314)$$
$$G_{\text{span\#186}}(U) = G_{\mathrm{M_{SAC}-{*}OH-{*}NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) \quad (315)$$
$$G_{\text{span\#187}}(U) = G_{\mathrm{M_{SAC}-{*}OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-{*}OH-{*}N+NH_3}}(U) \quad (316)$$

Taking $G_{\mathrm{M_{SAC}-*OH-*NH_p}}(U)$ as a reference

$$G_{\mathrm{span\#188}}(U) = G_{\mathrm{M_{SAC}-*OH-*NH_pH_p}}(U) - G_{\mathrm{M_{SAC}-*OH-*NH_p}}(U) \quad (317)$$

$$G_{\mathrm{span\#189}}(U) = G_{\mathrm{M_{SAC}-*OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-*OH-*NH_p}}(U) \quad (318)$$

Taking $G_{\mathrm{M_{SAC}-*OH-*NH_pH_p}}(U)$ as a reference

$$G_{\mathrm{span\#190}}(U) = G_{\mathrm{M_{SAC}-*OH+NH_3}}(U) - G_{\mathrm{M_{SAC}-*OH-*NH_pH_p}}(U) \quad (319)$$

The descriptor $G_{max}(U)$ is determined by extracting the largest free-energy span from the set of spans in equations (129) – (319), where n amounts to 189 for the chosen example.

$$G_{\max}(U) = \max\{G_{\mathrm{span\#}k}(U), k = 1, \ldots, n\} \quad (320)$$

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