Supporting Information

Investigation of the Reactions of U, U^+ and U^{2+} with Ammonia: Mechanisms and Topological Analysis

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1. Fig. S1 and Fig. S2

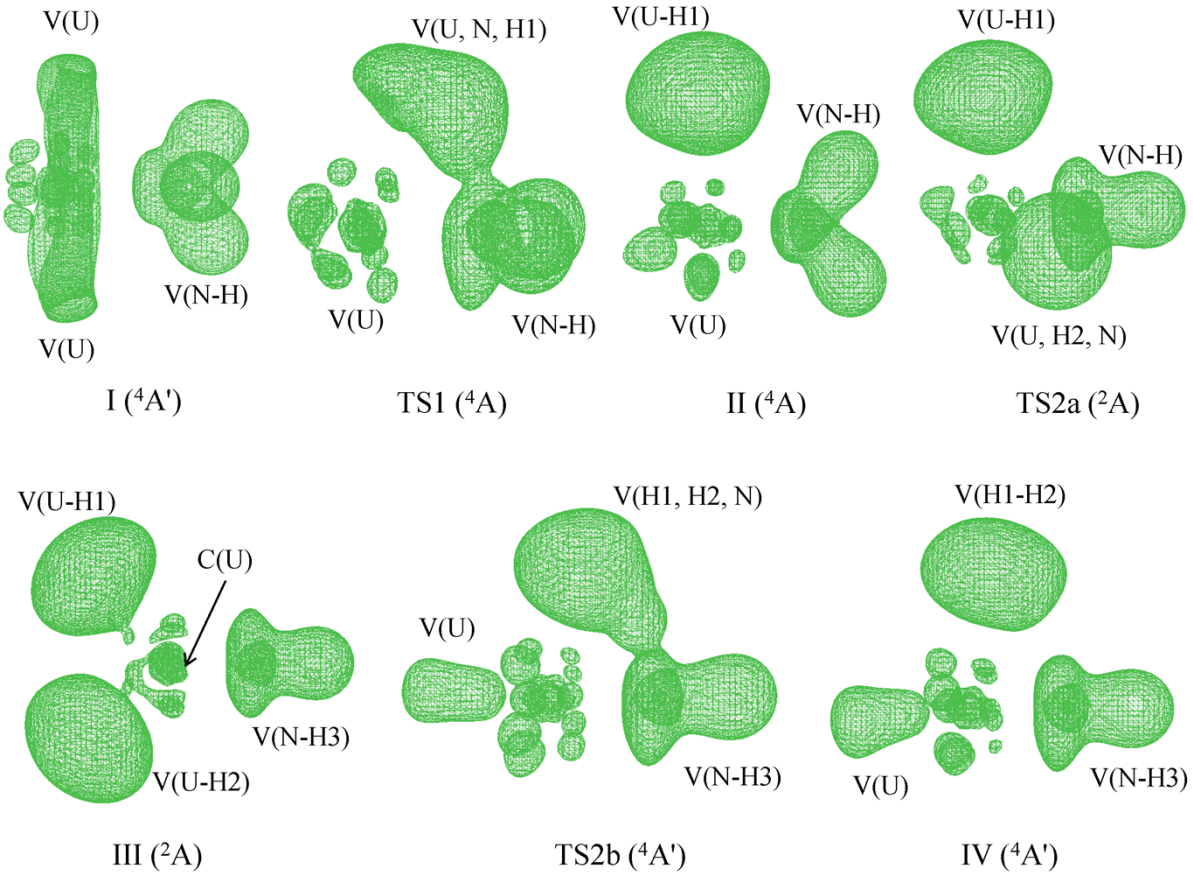

Fig. S1 ELF localization domains (η=0.70) of the lowest energy minima and transition states corresponding to the $U^+ + NH_3$ reaction pathway.

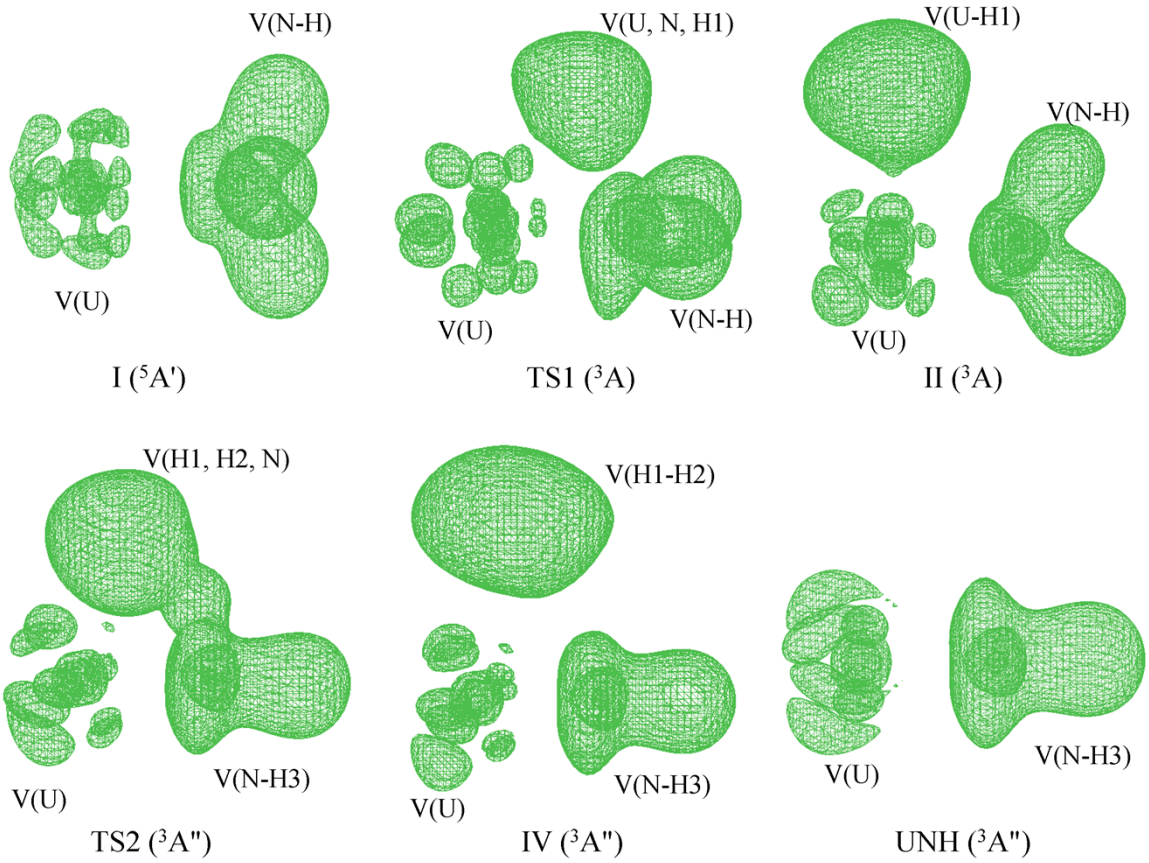

Fig. S2 ELF localization domains (η=0.70) of the lowest energy minima and transition states corresponding to the U^{2+} + NH_3 reaction pathway.

2. Fig. S3 and Fig. S4

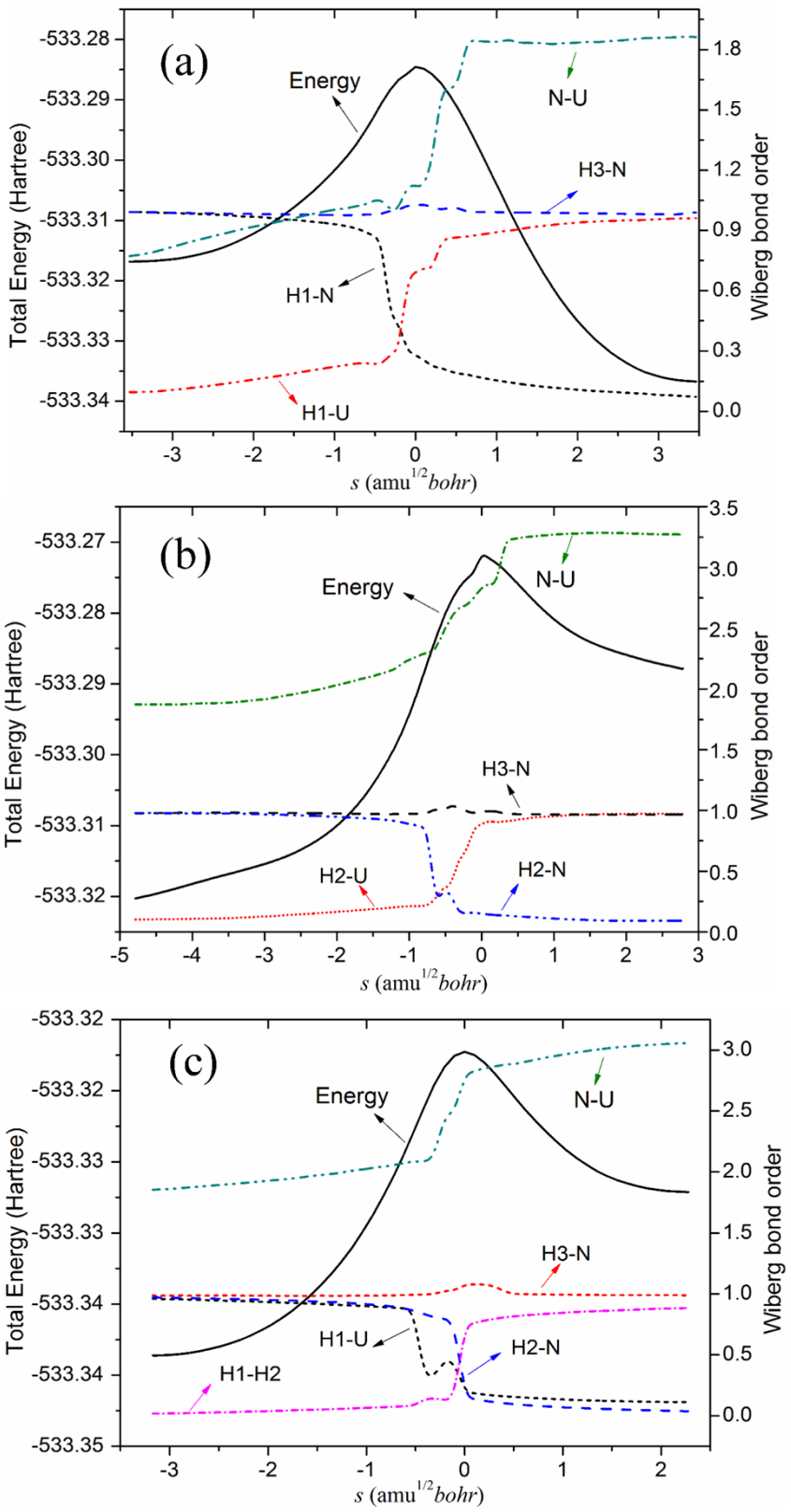

Fig. S3 IRC energy and Wiberg bond order along the reaction coordinate *s* calculated at the PW91/SDD levels corresponding to the $U^+ + NH_3$. Black solid curves are the energy and coloured curves are wiberg bond order. (a) U^+-NH_3→TS1→$HUNH_2^+$; (b) $HUNH_2^+$→TS2a→$HNUH_2^+$; (c) $HUNH_2^+$→TS2b→H_2-UNH^+.

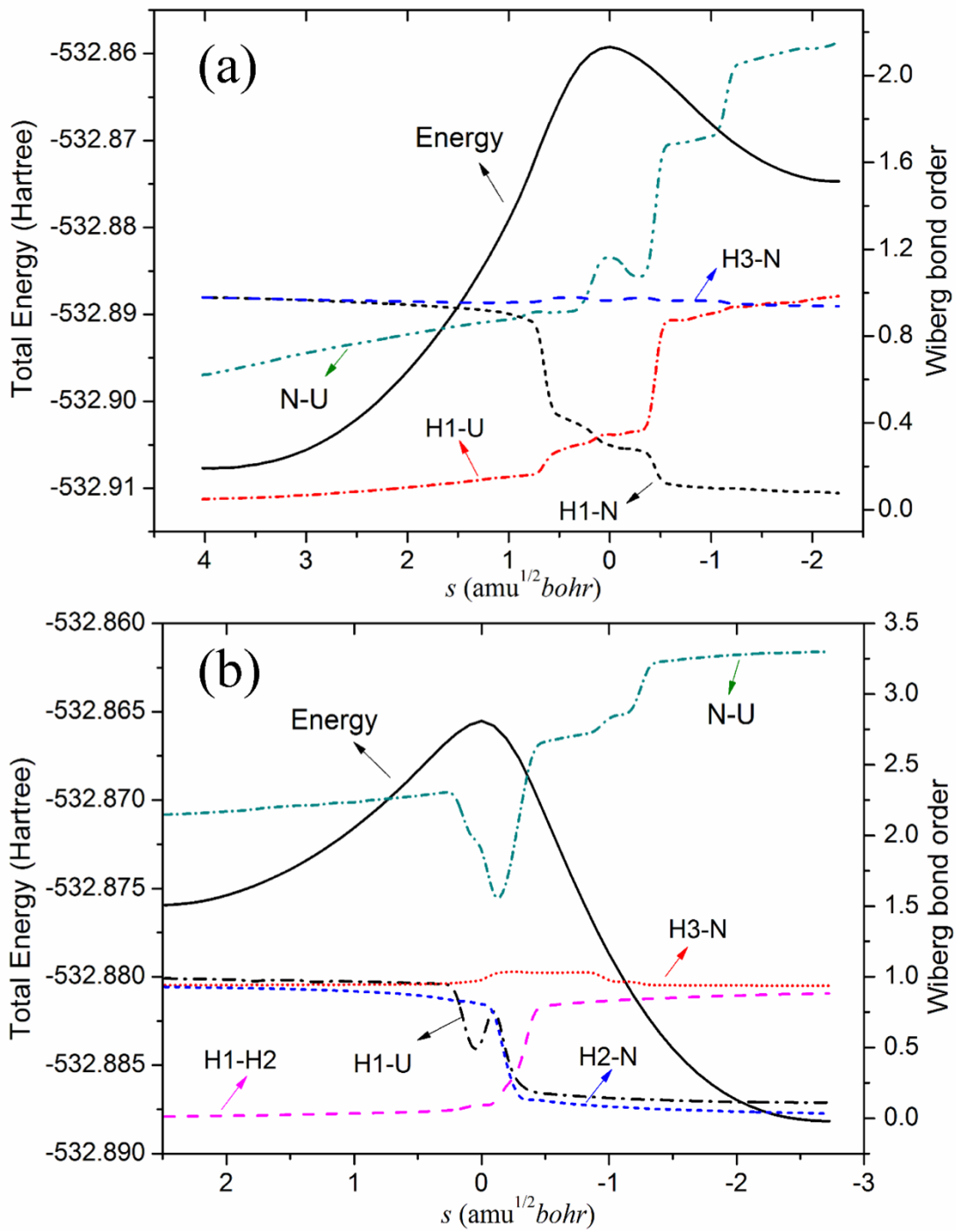

Fig. S4 IRC energy and Wiberg bond order along the reaction coordinate *s* calculated at the PW91/SDD levels corresponding to the U^{2+} + NH_3. Black solid curves are the energy and coloured curves are wiberg bond order. (a) U^{2+}-NH_3→TS1→$HUNH_2^{2+}$; (b) $HUNH_2^{2+}$→TS2→H_2-UNH^{2+}.

3. *Ab Initio* molecular dynamics simulation of the product H_2UNH.

We performed *ab Initio* molecular dynamics simulation to confirm the thermal stability of the product H_2UNH. Simulations are carried out for almost 5 ps using the BOMD method in Gaussian03. Our result indicates that the H_2UNH is stabilized. Using the dynamics simulations results, we plotted the root mean square displacement (RMSD) through time at different temperature (300 and 500K). The results are shown in the following figures. Our MD runs indicate that the H_2UNH structure keeps its identity at both room temperature (300 K) and high temperature (500 K).

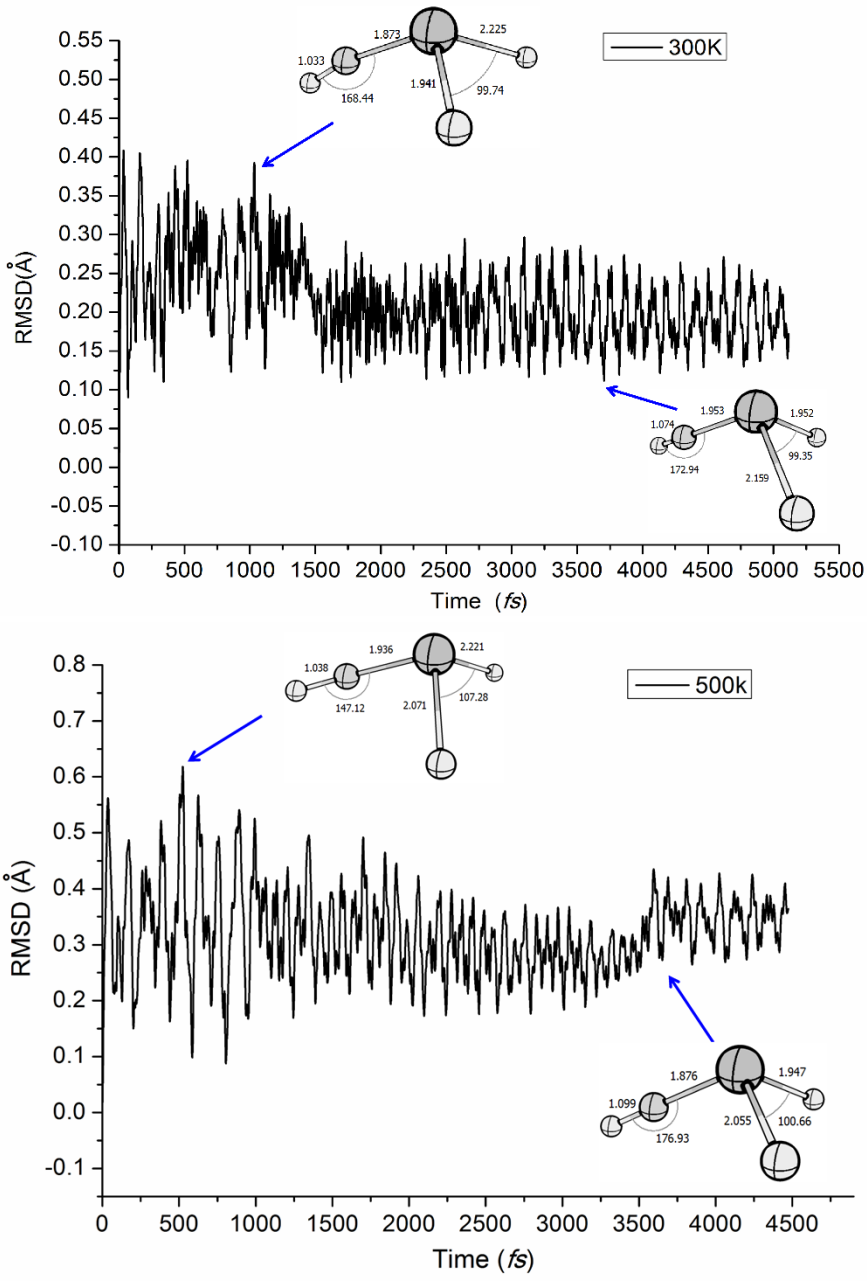

Fig. S5. The RMSD at different temperatures for the product H_2UNH.