

Hydrazine Oxidation in Aqueous Solutions II. N₄H₄ Decomposition

Martin Breza and Anton Gatial

Dept. Physical Chemistry, Slovak Technical University, Radlinskeho 9, SK-81237 Bratislava, Slovakia

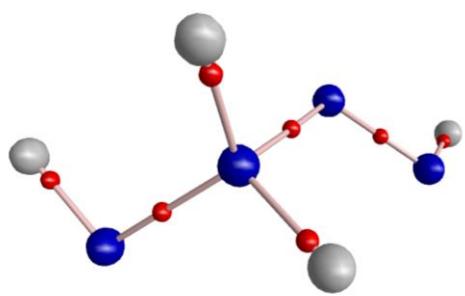
Supplementary information

Figure S1. Molecular graphs of optimized N₄H₄ structures in *anti*-conformation (N – blue, H – gray, bond critical points – red).

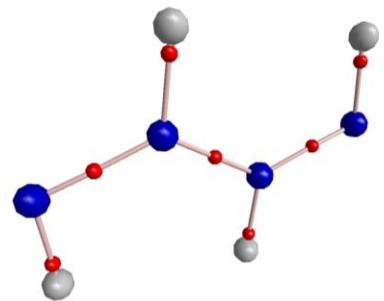
Figure S2. Molecular graphs of optimized N₄H₄ structures in *syn*-conformation (N – blue, H – gray, bond critical points – red, ring critical points - yellow).

Figure S3. Molecular graphs of optimized cyclo-N₄H₄ structures (N – blue, H – gray, bond critical points – red, ring critical points - yellow).

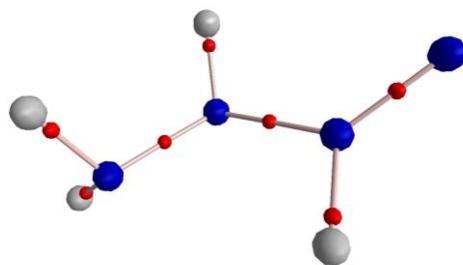
Figure S4. Molecular graphs of optimized N₄H₄ structures after N – N bond fission (N – blue, H – gray, bond critical points – red, ring critical points - yellow).



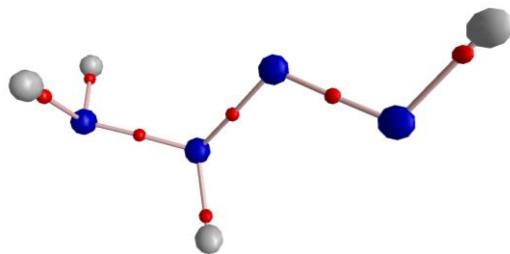
A1201



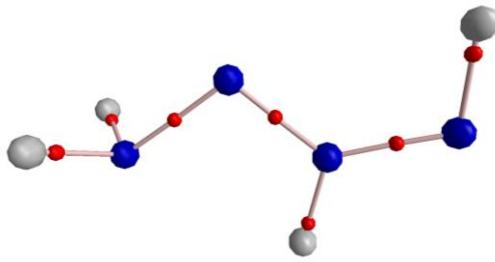
A1111



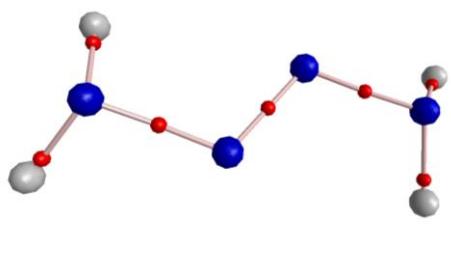
A2110



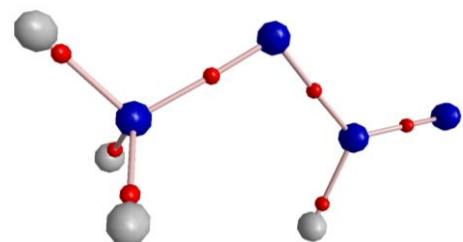
A2101



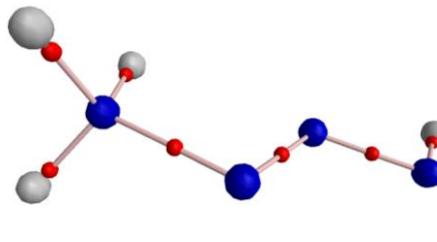
A2011



A2002



A3010



A3001

Figure S1. Molecular graphs of optimized N_4H_4 structures in *anti*-conformation (N – blue, H – gray, bond critical points – red).

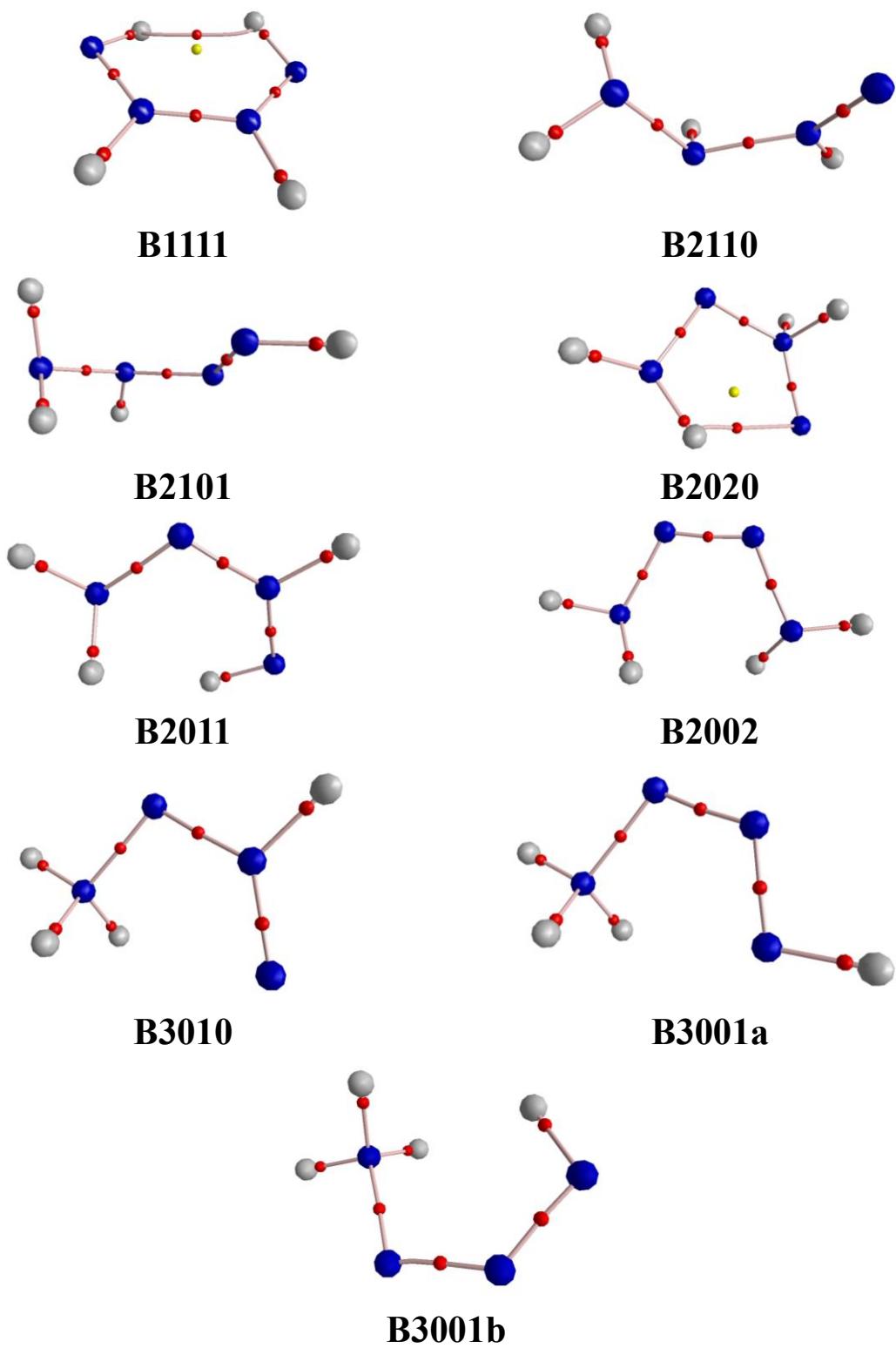


Figure S2. Molecular graphs of optimized N_4H_4 structures in *syn*-conformation (N – blue, H – gray, bond critical points – red, ring critical points - yellow).

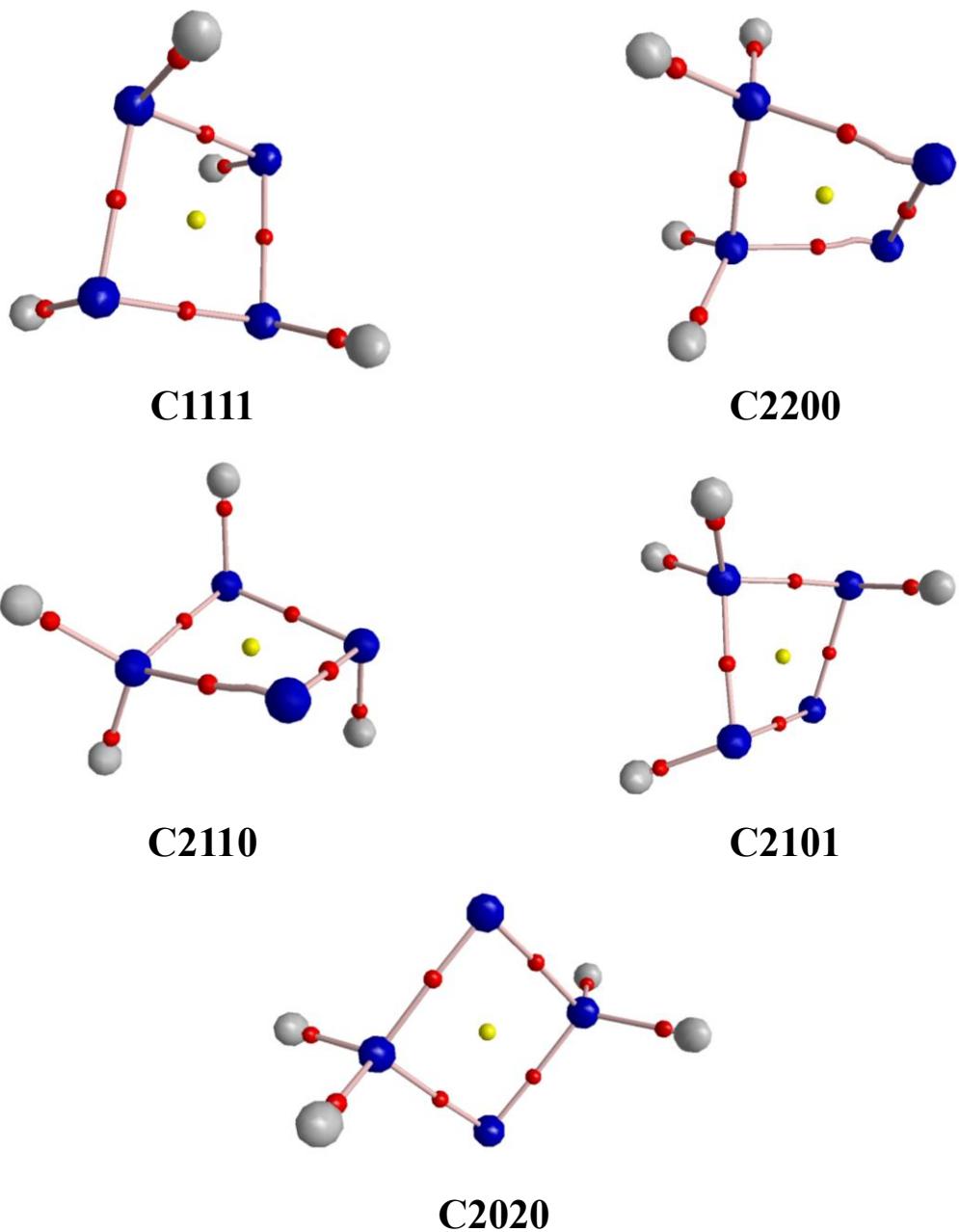


Figure S3. Molecular graphs of optimized cyclo-N₄H₄ structures (N – blue, H – gray, bond critical points – red, ring critical points - yellow).

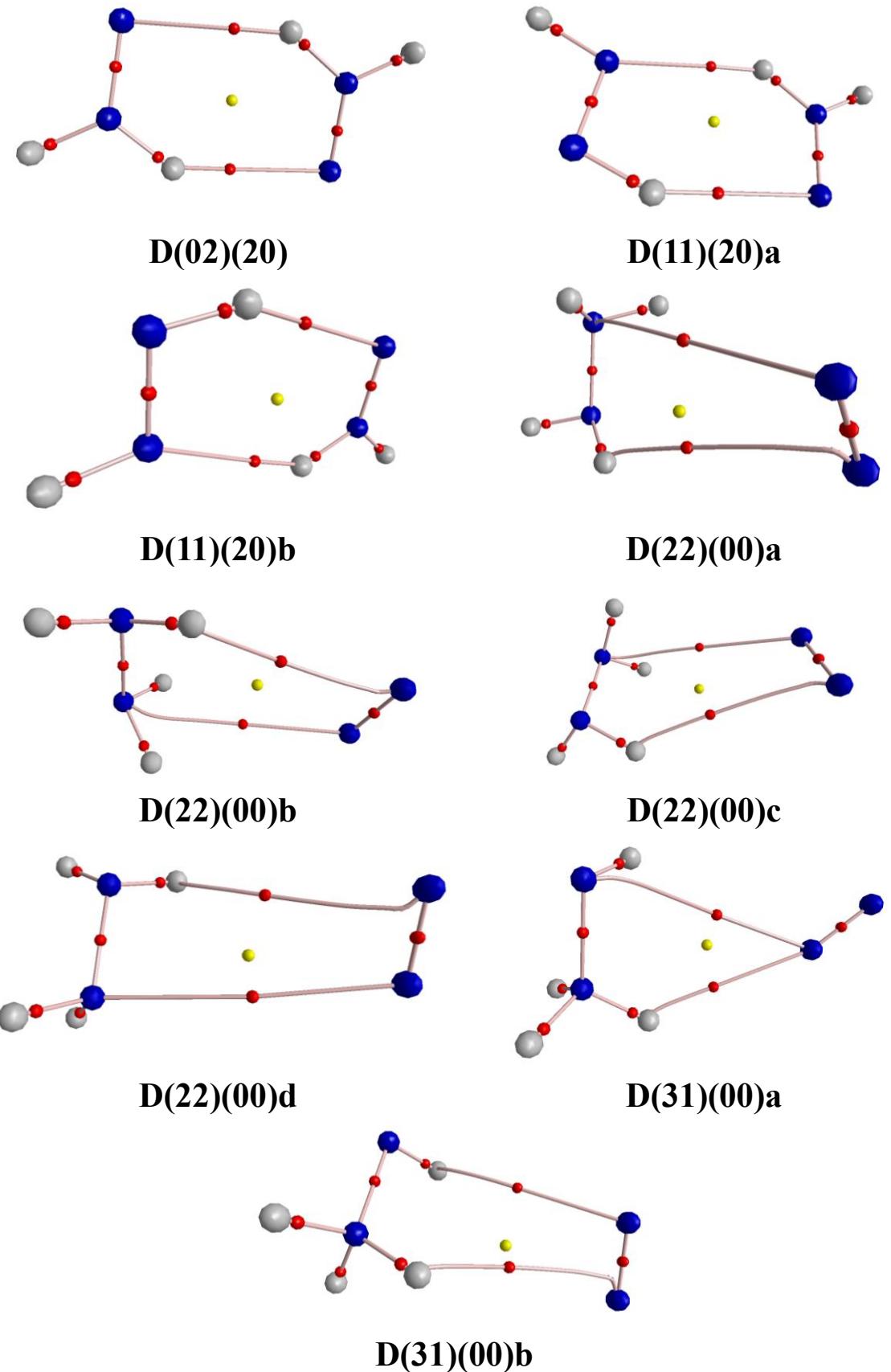


Figure S4. Molecular graphs of optimized N_4H_4 structures after $\text{N} - \text{N}$ bond fission (N – blue, H – gray, bond critical points – red, ring critical points - yellow).