

Hydrazine Oxidation in Aqueous Solutions II. N₄H₄ Decomposition

Martin Breza and Anton Gatiaľ

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

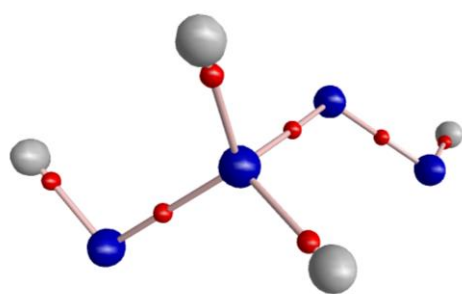
Supplementary information

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

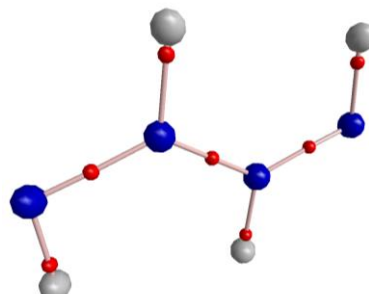
Figure S2. Molecular graphs of optimized N₄H₄ structures in *syn*-conformation (N – blue, H – gray, bond critical points – red, ring critical points - yellow).

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

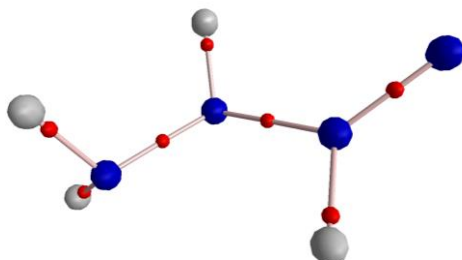
Figure S4. Molecular graphs of optimized N₄H₄ structures after N – N bond fission (N – blue, H – gray, bond critical points – red, ring critical points - yellow).



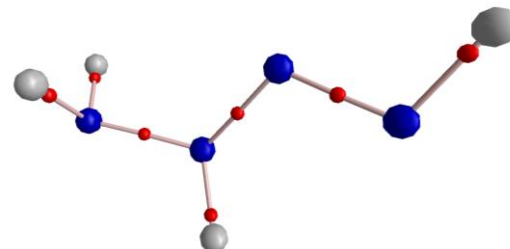
A1201



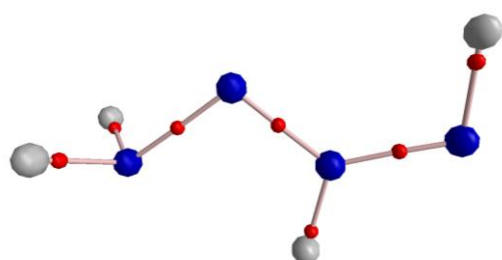
A1111



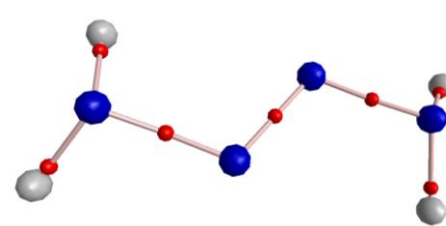
A2110



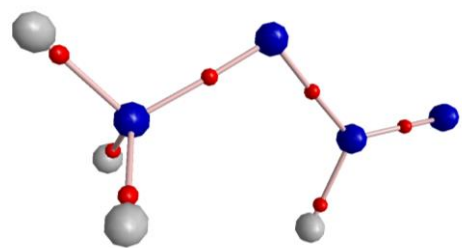
A2101



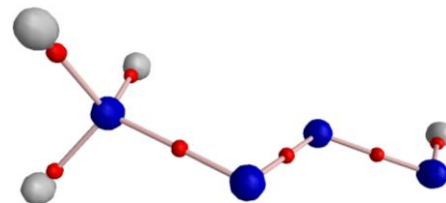
A2011



A2002



A3010



A3001

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

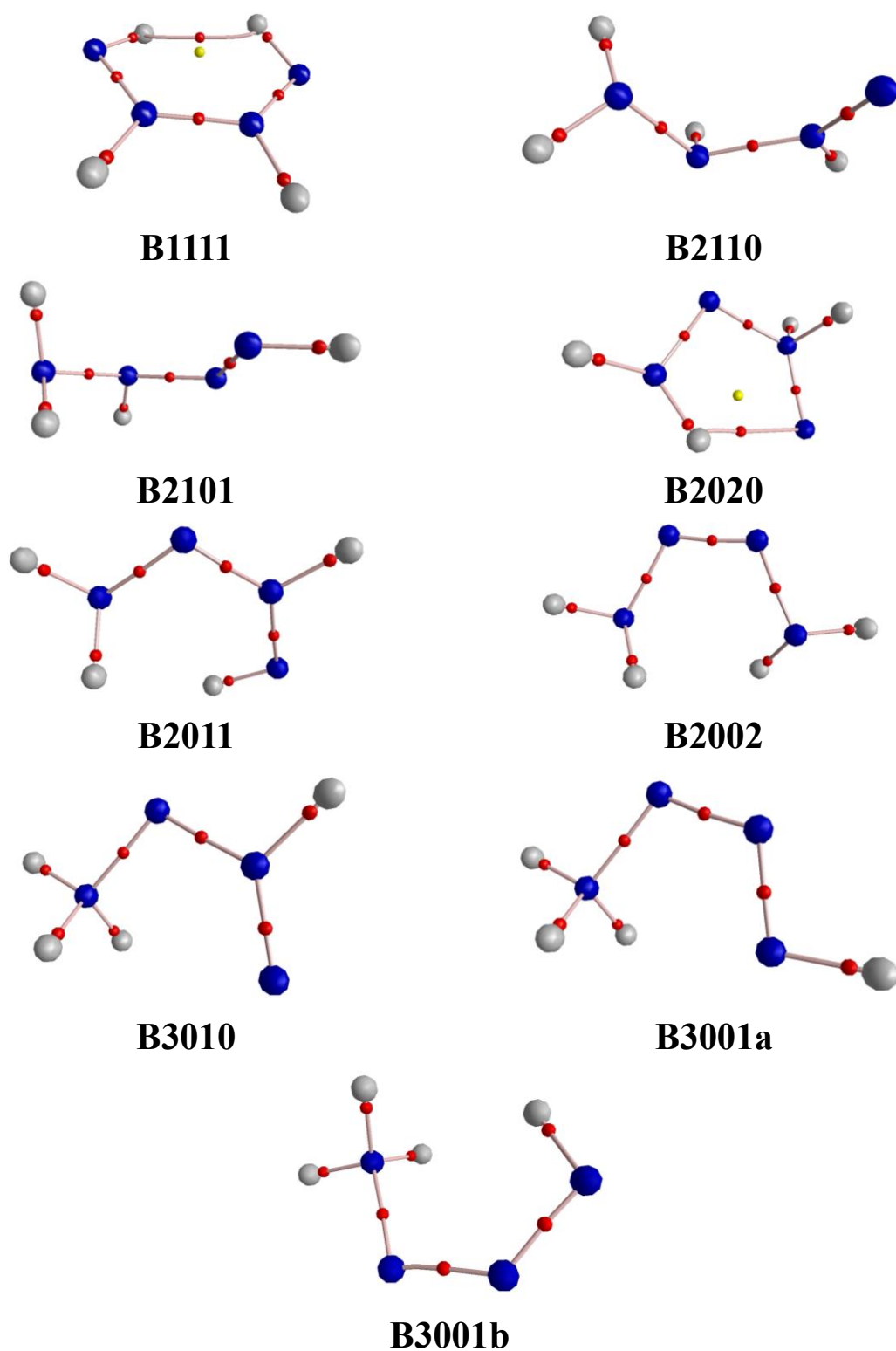
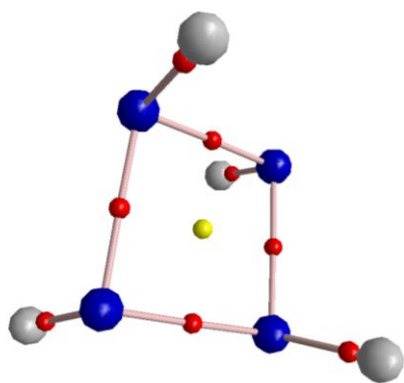
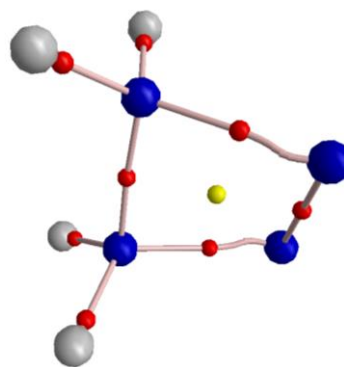


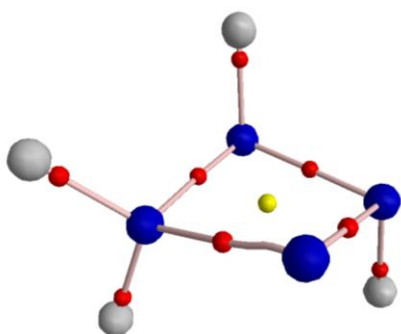
Figure S2. Molecular graphs of optimized N_4H_4 structures in *syn*-conformation (N – blue, H – gray, bond critical points – red, ring critical points - yellow).



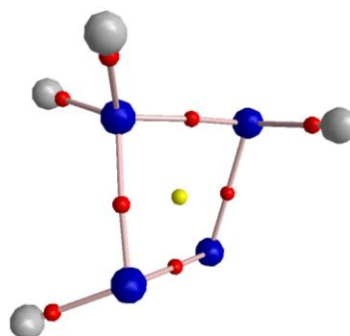
C1111



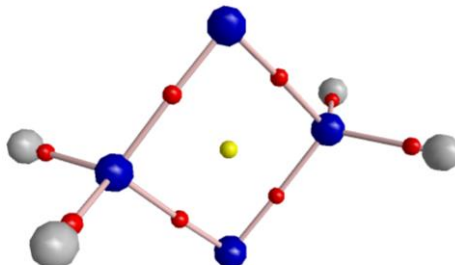
C2200



C2110

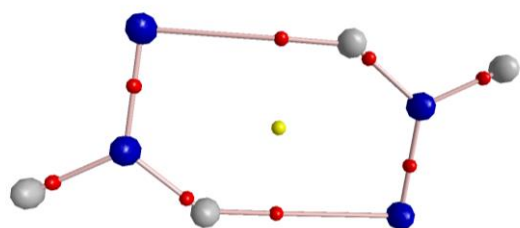


C2101

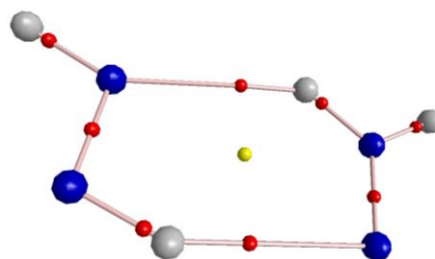


C2020

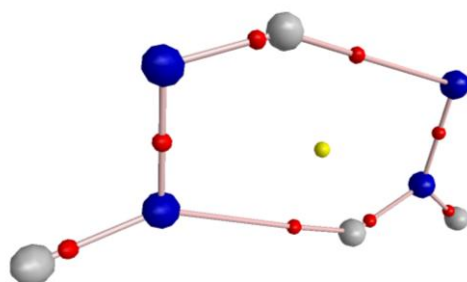
Figure S3. Molecular graphs of optimized cyclo- N_4H_4 structures (N – blue, H – gray, bond critical points – red, ring critical points – yellow).



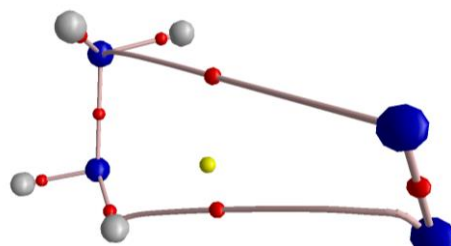
D(02)(20)



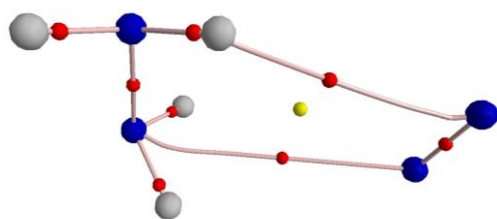
D(11)(20)a



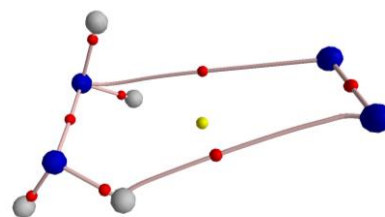
D(11)(20)b



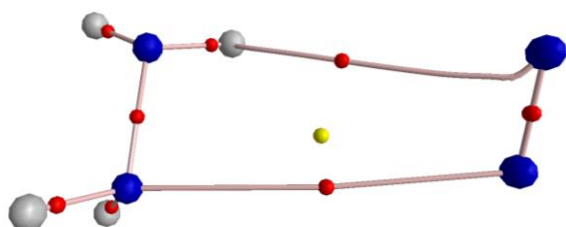
D(22)(00)a



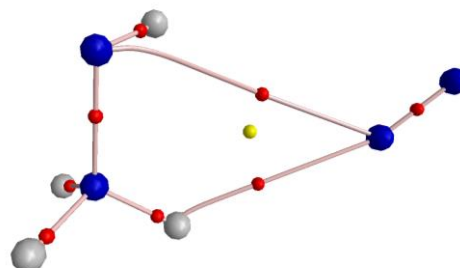
D(22)(00)b



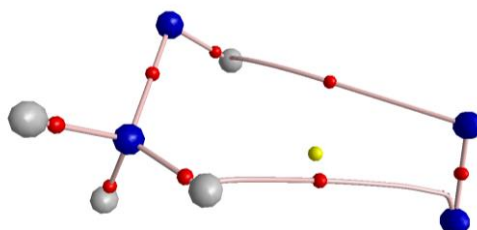
D(22)(00)c



D(22)(00)d



D(31)(00)a



D(31)(00)b

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