MILLIMETER- WAVE SPECTRUM OF CARBONYL DIAZIDE IN PURSUIT OF DIAZIRINONE

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Pyrolysis of carbonyl diazide ($CO(N_3)_2$) has been shown to give diazirinone (CON_2).[a] While diazirione decomposes over the course of a few hours under terrestrial conditions, there is the possibility for it to exist in space. In the pursuit of obtaining a rotational spectrum for diazirinone, we have started with the rotational spectroscopy of its immediate precursor, carbonyl diazide. Carbonyl diazide is highly explosive, and requires careful synthesis.[b] Spectra in the range of 260-360 GHz were collected at room temperature and at -60°C. *Ab initio* calculations at the CCSD/cc-pVDZ level predict that the conformation where both azide groups are *syn* to the carbonyl is preferred. A second conformation, where one azide is *syn* and one is *anti*, is calculated to lie about 2 kcal/ mol higher in energy. Pure rotational transitions for the ground state and multiple low-lying excited vibrational states of the *syn- syn* conformation are readily observed and assigned.

[a] X. Zeng, H. Beckers, H. Willner and J. F. Stanton, *Angew. Chem. Int. Ed.* **50** (2011), 1720-1723

[b] A. M. Nolan, B. K. Amberger, B. J. Esselman, V. S. Thimmakondu, J. F. Stanton, R. C. Woods, and R. J. McMahon, *Inorg. Chem.* **51** (2012), 9846-9851