AB INITIO INVESTIGATION OF NH_3-O_2 EXCIPLEX

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In their recent investigation of fluorescence from poly(amido amine) (PAMAM) dendrimers, Chu and Imae suggested an exciplex composed of tertiary amine and oxygen molecules might be responsible for fluorescence in PAMAM dendrimers.[a] In this work, we present an *ab initio* investigation of the electronic structure of a possible ammonia-oxygen exciplex model system using equation-of-motion coupled cluster techniques. Geometry optimization of the triplet ground state produced a weakly bound state with an equilibrium separation of ~ 3.5 Å, and an excited state geometry scan revealed a bound, excited triplet state with an equilibrium separation of 2.02 Å, consistent with results of earlier PM3 work by Juranic *et al.*[b] The energy gap between the triplet ground state and first triplet excited state of the exciplex at 2.02 Å is 412.8 nm, lending support to the exciplex hypothesis.

[a] C.-C. Chu, and T. Imae, *Macromol. Rapid. Commun.* **30**, 89-93 (2009).
[b] I. Juranic, H. S. Rzepa, and Y. MinYan, *J. Chem. Soc. Perkin Trans.* **2** (1990)