Cyanomethanimine isomers in cold interstellar clouds: insights from electronic structure and kinetic calculations

Fanny Vazart[1], Camille Latouche[1], Dimitrios Skouteris[1], Nadia Balucani[2], Vincenzo Barone[1]

The recent detection of *E*-cyanomethanimine, a species of great relevance in prebiotic chemistry, in Sgr B2(N) in the Green Bank Telescope (GBT) PRIMOS survey by Zaleski et al. [1] has raised the question of how this species is formed under the conditions of the cold interstellar medium.
Cyanomethanimine is an important species in the context of prebiotic chemistry, mostly because of its potential as an intermediate towards the formation of adenine [2]. Since its formation by HCN dimerization has already been shown to be difficult in the absence of liquid water[3], the reaction presented here is a possible shortcut for the synthesis of adenine in extraterrestrial environments that bypasses HCN dimerization.

In this contribution we demonstrate that the reaction between two widely diffuse species, that is the cyano radical and methanimine, can easily account for cyanomethanimine formation under the characteristic conditions of interstellar clouds. The interaction of the •CN radical with methanimine was already explored by Basiuk & Bogillo: [4] their B3LYP/6-31++G(d,p) calculations demonstrated that the addition of the •CN radical to the π bond of methanimine is barrierless. In the present study, one of the most reliable computational models rooted into the density functional theory (DFT) has been used, coupled to energy refinement by a coupled cluster (CC) approach in conjunction with complete basis set extrapolation (CBS-QB3). This has been done in order to reevaluate the energies obtained by Basiuk et al. [4] and to explore the exit channels that were not considered in this previous study

The CN + CH_2=NH reaction can also play a role in the chemistry of the upper atmosphere of Titan where the cyanomethanimine products can contribute to the buildup of the observed nitrogen-rich organic aerosols that cover the moon.

[1] Zaleski et al., 2013, ApJ, L10.
[2] Eschenmoser, 2007, Tetrahedron, 63, 12821.
[3] Yim et al., 2012, Chem. Phys. Lett., 538, 24.
[4] Basiuk et al. 2002, AdSpR, 30,1445.

[1] Scuola Normale Superiore, Piazza dei Cavalieri 7, 56125 Pisa, Italy
[2] Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy