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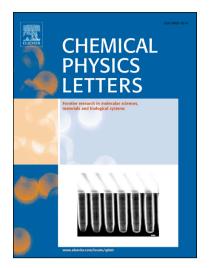
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### **ACCEPTED MANUSCRIPT**

## High-Accuracy Extrapolated Ab Initio Thermochemistry of the NCN Radical

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#### Abstract

Enthalpies of formation of the cyanonitrene radical, NCN, were calculated according to the HEAT (<u>High-accuracy Extrapolated Ab initio Thermochemistry</u>) protocol. The obtained, recommended values are  $451.7 \pm 1.0 \text{ kJ mol}^{-1}$  and  $452.2 \pm 1.0 \text{ kJ mol}^{-1}$  at 0 K and 298.15 K, respectively (gas phase, 1 bar). The calculated values are in agreement with the most recent Active Thermochemical Tables analysis and some of the previous experimental and computational results. The uncertainties associated with the HEAT values are, however, considerably smaller.

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