

Accepted Manuscript

High-Accuracy Extrapolated Ab Initio Thermochemistry of the NCN Radical

Michael E. Harding, Matthias Olzmann

PII: S0009-2614(18)30528-1
DOI: <https://doi.org/10.1016/j.cplett.2018.06.047>
Reference: CPLETT 35746

To appear in: *Chemical Physics Letters*

Received Date: 2 May 2018
Accepted Date: 22 June 2018



Please cite this article as: M.E. Harding, M. Olzmann, High-Accuracy Extrapolated Ab Initio Thermochemistry of the NCN Radical, *Chemical Physics Letters* (2018), doi: <https://doi.org/10.1016/j.cplett.2018.06.047>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

High-Accuracy Extrapolated Ab Initio Thermochemistry of the NCN Radical

Michael E. Harding^a, Matthias Olzmann^b

^a*Institut für Nanotechnologie, Karlsruher Institut für Technologie,
Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany*

^b*Institut für Physikalische Chemie, Karlsruher Institut für Technologie, Kaiserstr. 12,
76131 Karlsruhe, Germany*

Abstract

Enthalpies of formation of the cyanonitrene radical, NCN, were calculated according to the HEAT (High-accuracy Extrapolated Ab initio Thermochemistry) protocol. The obtained, recommended values are 451.7 ± 1.0 kJ mol⁻¹ and 452.2 ± 1.0 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.

Email address: michael.harding@kit.edu (Michael E. Harding)

Download English Version:

<https://daneshyari.com/en/article/7837567>

Download Persian Version:

<https://daneshyari.com/article/7837567>

[Daneshyari.com](https://daneshyari.com)