A theoretical and experimental benchmark study of core-excited states in nitrogen

vibrational structure of the core-excited states. This makes nitrogen well suited for assessing the accuracy of different electronic structure methods for core excitations. We report high resolution experimental measurements performed at the SOLEIL synchrotron facility. These are compared with theoretical spectra calculated using coupled cluster theory and algebraic diagrammatic construction theory. The coupled cluster singles and doubles with perturbative triples model known as CC3 is shown to accurately reproduce the experimental excitation energies as well as the spacing of the vibrational transitions. The computational results are also shown to be systematically improved within the coupled cluster hierarchy, with the coupled cluster singles, doubles, triples, and quadruples method faithfully reproducing the experimental vibrational structure.

General information
Publication status: Published
Organisations: Department of Chemistry, University of Oslo, Stanford University, Johns Hopkins University, Synchrotron Soleil, Norwegian University of Science and Technology
Corresponding author: Koch, H.
Number of pages: 7
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 148
Issue number: 6
Article number: 064106
ISSN (Print): 0021-9606
Ratings:
BFI (2018): BFI-level 2
Scopus rating (2018): CiteScore 2.85 SJR 1.159 SNIP 0.969
Web of Science (2018): Impact factor 2.997
Web of Science (2018): Indexed yes
Original language: English
Electronic versions:
nitro.pdf. Embargo ended: 14/02/2019
DOIs:
10.1063/1.5011148
Source: FindIt
Source ID: 2396439440
Research output: Contribution to journal › Journal article – Annual report year: 2018 › Research › peer-review