THE 67TH INTERNATIONAL

OPEN READINGS

CONFERENCE FOR STUDENTS OF PHYSICS AND NATURAL SCIENCES

BOOK OF ABSTRACTS | 2024

Vilnius University

VILNIUS UNIVERSITY PRESS

Editors:

Martynas Keršys
Rimantas Naina
Vincentas Adomaitis
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Cover and Interior Design:

Goda Grybauskaitė

Vilnius University Press
9 Saulėtekio Av., III Building, LT-10222 Vilnius
info@leidykla.vu.lt, www.leidykla.vu.lt/en/
www.knygynas.vu.lt, www.journals.vu.lt

Bibliographic information is available
on the Lithuanian Integral Library Information System (LIBIS) portal www.ibiblioteka.lt
ISBN 978-609-07-1051-7 (PDF)

DETECTING ATOMIC INTERACTIONS IN SMALL-MOLECULE CRYSTAL STRUCTURES

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Crystallography provides researchers with exact positions of atoms composing crystal structures [1], but it is unable to capture chemical bonding. Therefore, distance-based heuristics are employed to detect chemical bonds. One such heuristic is based on the sum of per-element atomic radii for each pair of atoms in a structure. However, there are several different atomic radii tables with none of them accepted universally.

The most widely used atomic radii tables [2,3,4] were derived from data from the Cambridge Structural Database [5]. This database is distributed under a proprietary license, which imposes restrictions on the usage and spread of derivative works. Therefore, a completely independent workflow is needed to produce open atomic radii tables in an unsupervised manner. In this work, we have devised a workflow to derive atomic radii tables from data in the Crystallography Open Database [6].

Our workflow identifies the lowest density region in each pairwise interatomic distance distribution as the van der Waals gap [7]. This gap separates the observations coming from covalently interacting atom pairs from those originating chiefly from the van der Waals interactions. A Gaussian distribution mixture model is fitted on the distance distribution to find the lowest density region. Finally, atomic radii are calculated by solving an equation system constructed from pairwise radii sums.

Atomic radii table derived in this work follows the typical trend of other published tables. This observation confirms that it is possible to derive usable atomic radii tables from open small-molecule data in unsupervised manner. Review of the derived results, comparison between radii in published tables and visualization of covalent bond length determination for pair of chemical elements are available online [8], as well as a tool for structure validation using derived covalent radii [9].

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