

Accepted Manuscript

Empirical Temperature-dependent Intermolecular Potentials Determined by
Data Mining from Crystal Data

D.W.M. Hofmann, L.N. Kuleshova

PII: S0009-2614(18)30237-9
DOI: <https://doi.org/10.1016/j.cplett.2018.03.053>
Reference: CPLETT 35534

To appear in: *Chemical Physics Letters*

Received Date: 12 December 2017
Accepted Date: 22 March 2018



Please cite this article as: D.W.M. Hofmann, L.N. Kuleshova, Empirical Temperature-dependent Intermolecular Potentials Determined by Data Mining from Crystal Data, *Chemical Physics Letters* (2018), doi: <https://doi.org/10.1016/j.cplett.2018.03.053>

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.

Contents

1	Introduction	2
2	Method	4
2.1	The Model	4
2.2	The Data Mining Algorithm	8
2.3	Experimental and Virtual Training Data	9
3	Results and Discussion	10
3.1	Temperature-dependent Force Field, TDFF	10
3.2	Estimation of Crystal Density with TDFF	14
3.3	Estimation of the Density Gradient Coefficient α_d	16
3.4	Phase Transition Prediction	19
3.5	Outliers	21
4	Conclusions	22
5	Supplementary	27

Download English Version:

<https://daneshyari.com/en/article/7837830>

Download Persian Version:

<https://daneshyari.com/article/7837830>

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