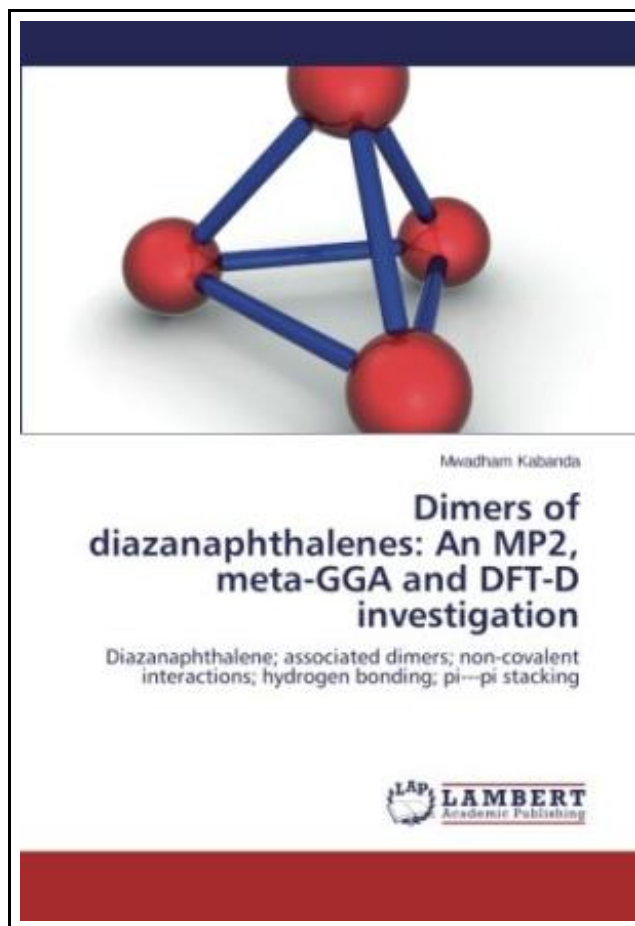


Dimers of diazanaphthalenes: An MP2, meta-GGA and DFT-D investigation



Filesize: 8.72 MB

Reviews

The ebook is simple in read easier to recognize. It is one of the most awesome book we have read through. I am happy to explain how this is basically the finest pdf we have read inside my very own lifestyle and may be he finest publication for actually.

(Jaiden Turcotte DDS)

DIMERS OF DIAZANAPHTHALENES: AN MP2, META-GGA AND DFT-D INVESTIGATION

DOWNLOAD



Book Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Diazanaphthalene; associated dimers; non-covalent interactions; hydrogen bonding; pi---pi stacking | Diazanaphthalenes are a broad class of heteroaromatic compounds with several technological and pharmacological applications. Some of these applications are attributed to the ability of diazanaphthalenes to form associated dimers through non-covalent interactions. A study of the types and strength of the interactions involved is crucial for understanding the properties of the dimers. In this study the dimers of five diazanaphthalenes, namely 1,8-naphthyridine, quinoxaline, phthalazine, quinazoline and cinnoline, are investigated by means of theoretical computational approaches. The selected computational methods include the second order Möller-Plesset perturbation theory (MP2), hybrid meta-Generalized Gradient Approximation (Meta-GGA) Density Functional Theory (DFT/MPWB1K, DFT/M05-2X and DFT/M06-2X) and DFT dispersion corrected (DFT-D/wB97XD). The objective of the study is to elucidate the dimers preferred geometries, relative energies and nature of the interactions between monomer units. A comparison across structures may also suggest the role of the position of the N atom in the ring in determining the stability of the dimers | Format: Paperback | Language/Sprache: english | 68 pp.



[Read Dimers of diazanaphthalenes: An MP2, meta-GGA and DFT-D investigation Online](#)



[Download PDF Dimers of diazanaphthalenes: An MP2, meta-GGA and DFT-D investigation](#)

Other eBooks



Read Write Inc. Phonics: Set 7 Non-Fiction 3 the Ice and Snow Book

Oxford University Press, United Kingdom, 2016. Paperback. Book Condition: New. 207 x 86 mm. Language: N/A. Brand New Book. These decodable non-fiction books provide structured practice for children learning to read. Each set of books...

[Read ePub »](#)



Serenade for Winds, Op. 44 / B. 77: Study Score

Petrucci Library Press, United States, 2013. Paperback. Book Condition: New. 240 x 166 mm. Language: English . Brand New Book ***** Print on Demand *****.Dvorak composed this deservedly popular work 1878 shortly after the premiere...

[Read ePub »](#)



Hussite Overture, Op. 67 / B. 132: Study Score

Petrucci Library Press, United States, 2013. Paperback. Book Condition: New. 244 x 170 mm. Language: English . Brand New Book ***** Print on Demand *****.Comissioned by the Committee for the Completion of the National Theatre,...

[Read ePub »](#)



The Water Goblin, Op. 107 / B. 195: Study Score

Petrucci Library Press, United States, 2013. Paperback. Book Condition: New. 238 x 170 mm. Language: English . Brand New Book ***** Print on Demand *****.The first of four late tone poems inspired by Bouquet, a...

[Read ePub »](#)



Czech Suite, Op.39 / B.93: Study Score

Petrucci Library Press, United States, 2015. Paperback. Book Condition: New. 244 x 170 mm. Language: English . Brand New Book ***** Print on Demand *****.Composed rapidly during April of 1879 in the wake of his...

[Read ePub »](#)

**ESV Study Bible, Large Print (Hardback)**

CROSSWAY BOOKS, United States, 2014. Hardback. Book Condition: New. Large Print. 249 x 178 mm. Language: English . Brand New Book. The ESV Study Bible, Large Print edition transforms the content of the award-winning ESV

[Save PDF »](#)

**Social Studies for the Preschool/Primary Child**

Book Condition: Brand New. Book Condition: Brand New.

[Save PDF »](#)

**Danses Sacree Et Profane, CD 113: Study Score**

Petrucci Library Press, United States, 2015. Paperback. Book Condition: New. 279 x 216 mm. Language: English . Brand New Book ***** Print on Demand *****.Debussy composed his concertante masterwork on commission from Pleyel for a

[Save PDF »](#)

**Variations on an Original Theme Enigma , Op. 36: Study Score**

Petrucci Library Press, United States, 2013. Paperback. Book Condition: New. 246 x 189 mm. Language: English . Brand New Book ***** Print on Demand *****.Dedicated to my friends pictured within, Elgar s orchestral showpiece started

[Save PDF »](#)

**Klara the Cow Who Knows How to Bow (Fun Rhyming Picture Book/Bedtime Story with Farm Animals about Friendships, Being Special and Loved. Ages 2-8) (Friendship Series Book 1)**

Createspace, United States, 2015. Paperback. Book Condition: New. Apoorva Dingar (illustrator). Large Print. 214 x 149 mm. Language: English . Brand New Book ***** Print on Demand *****.Klara is a little different from the other

[Save PDF »](#)