



J. Serb. Chem. Soc. 87 (12) 1439–1446 (2022)
JSCS–5605

LETTER TO THE EDITOR

25 years of NICS – much more than nothing!

RALPH PUCHTA^{1-3*}, SLAĐANA ĐORĐEVIĆ^{4#}, SLAVKO RADENKOVIĆ^{4***},
HAIJUN JIAO⁵ and NICO J. R. VAN EIKEMA HOMMES¹

¹Computer Chemistry Center, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Nägelsbachstr. 25, 91052 Erlangen, Germany, ²Inorganic Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Egerlandstr. 1, 91058 Erlangen, Germany, ³Central Institute for Scientific Computing (ZISC), University of Erlangen-Nuremberg, Martensstr. 5a, 91058 Erlangen, Germany, ⁴University of Kragujevac, Faculty of Science, Radoja Domanovića 12, 34000 Kragujevac, Serbia and ⁵Leibniz-Institut für Katalyse e.V., Albert-Einstein-Str. 29a, Rostock, 18059 Germany

(Received 3 December 2021, revised 21 June, accepted 6 July 2022)

Abstract: The famous aromaticity index NICS (nucleus independent chemical shift) was introduced 25 years ago. The authors use this anniversary for a short and to some degree personal retrospective.

Keywords: aromaticity; history; anniversary.

In 1996 Paul von Ragué Schleyer and his team published a new index for aromaticity based on gauge-independent atomic orbital (GIAO) NMR-calculations called nucleus independent chemical shift (NICS).¹ The abbreviation NICS is a pun with the colloquial German word for nothing – “Nix”, as to obtain NICS values one can calculate chemical shift at any place, in the space around a molecule, using a ghost atom – more or less nothing.

NICS values had been the enhancement of earlier NMR-calculation to evaluate aromaticity based on Li⁺ or He-atoms.^{2–6} Both nuclei interact with the system that shall be investigated. A ghost atom is not interacting and the awareness that one can calculate chemical shifts independently from a nucleus anywhere around a molecule was a milestone in investigating aromaticity. That NICS is a scientific bonanza one can easily see in the number of current citations obtained from the Web of Science database.⁷ The original NICS manuscript from 1996¹ was cited

*** Corresponding authors. E-mail: (*)ralph.puchta@fau.de; (**)slavkoradenkovic@kg.ac.rs

Serbian Chemical Society member.

• Dedicated to the memory of Paul von Ragué Schleyer (1930–2014) and all scientists who profited from the application of NICS.

<https://doi.org/10.2298/JSC211203057P>

around 4500 times in November 2021 and in the review⁸ published by Paul von Ragué Schleyer, around 10 years later, more than 2300 times. Of course, in 1996 there was only the “nativity” of NICS, before Schleyer and his team nurtured that idea. Already in summer 1995 Schleyer reported at the 8th International Symposium on Novel Aromatic Compounds (ISNA-8) in Braunschweig, Germany, about this new upcoming method. The first publication applying NICS⁹ appeared in 1996, but already in February, around half a year before the well-known method paper was published.*

What makes NICS so precious and useful? Why are scientists all over the world attracted by NICS? Surely a very striking argument is the simplicity of application. A NMR-calculation based on a structure extended by one or more ghost atoms is simple to do and the results are easy to analyze, as the resulting shielding only has to be multiplied by -1 , and with straightforward interpretation. No reference systems are necessary, one calculation can extend the knowledge of the investigated system significantly, independently if organic or inorganic. Adopting Schleyer’s color scheme a red ball shows aromaticity and a green ball anti-aromaticity. If the ball is tiny (values between -5 and 5) than one has no aromatic influences at all (Fig. 1).

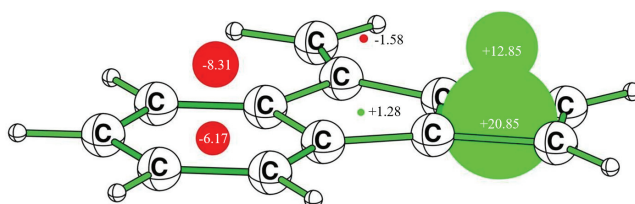


Fig. 1. 7-Methylene-7H-cyclobuta[a]indene. The NICS and geometry were calculated at the B3LYP/6-311+G** level of theory.

This simple concept allows to understand the nature of individual rings in polycyclic systems (see, *e.g.*, Fig. 1) and is therefore extremely useful in understanding fullerenes, nanotubes or graphenes. A striking example for a better understanding of graphenes, and an impressive support for Clar’s picture of aromatic π -sextets in polycyclic aromatic hydrocarbons (PAHs), is the work of Schleyer and team, demonstrating that only rings where all carbon atoms are members of a single sextet show high NICS values, compared to rings having migrating π -sextets and showing intermediate values. This leads to clearly differentiable Clar sextet ring patterns and makes the concept of Clar more concrete.¹⁰

The possibilities of NICS inspired other teams to get new, unexpected but absolutely impressive ideas in their research. Perhaps the most striking was an idea of Klod and Kleinpeter,^{11–13} they used NICS points around interesting

*The submission of the NICS-method paper was exactly 168 years after the famous letter from Friedrich Wöhler to Jens Jacob Berzelius reporting his unintentional preparation of urea.

molecules and structural motives to plot the “iso-chemical-shielding surfaces” (ICSS) investigating through space NMR shieldings and making them visible.¹⁴ It is worth mentioning that an analogous one-dimensional approach, also known as the NICS-scan method, is widely adopted.¹⁵

More straightforward was the concept of separating π - and σ -influences of the NICS values in order to get dissected NICS values. The first idea was to apply the Pipek–Mezey localization procedure (LMO-NICS)¹⁶ which was successfully applied and taught that NICS(0) shows great influences of the σ -system.^{17,18} Unluckily the formalism of Pipek and Mezey has some shortcomings, *e.g.*, that the strict σ – π separation is only applicable for planar molecules.¹⁶ Therefore, alternative methods were developed to separate the influences, like the concept of Corminboeuf *et al.*, to calculate dissected NICS of selected canonical molecular orbitals resulting in NICS $\sigma\pi$.¹⁹ An alternative dissection concept is based on individual canonical molecular orbital (CMO) contributions to the magnetic shielding of the atoms. These CMO-NICS contributions allow additional insights to the results of the localized MO based dissected NICS (LMO-NICS).²⁰ Another CMO-NICS concept utilizes natural bond orbitals (NBOs).²¹

An alternative concept to a more detailed understanding of NICS, beside σ - and π -influences, is to analyze the tensors of NICS. While by definition NICS $_{xx}$ and NICS $_{yy}$ are in the ring’s plain NICS $_{zz}$ is perpendicular and can give values unhampered by the in-plane effects easily.

While these examples show nicely why NICS is interesting for theoretical considerations, but why is NICS so fascinating for practical chemistry? The convenience while applying NICS (*vide supra*) certainly is a very big advantage, especially in combination with a probe not altering the system. The other huge plus for NICS is the wide range of application in organic,^{22–30} inorganic,^{31–35} metal clusters,^{36–38} carbon-materials,^{39–41} supramolecular chemistry,^{42–45} bio-related chemistry,^{46–49} porphyrin chemistry,^{50–53} chemistry of tailor-made properties,⁵⁴ polymer chemistry,^{55,56} *etc.* and these topics can again be divided into sub topics, *e.g.*, in organic chemistry like reaction mechanism with aromatic transition states,^{8,57,58} Möbius^{59–61} and Craig–Möbius^{62–65} aromatic systems, chelate systems⁶⁶ or to metalla aromatic systems,^{65,67–69} only to list the most prominent examples. Along these lines, it is worth mentioning that some of the present authors have been part of Schleyer’s research group when the very first papers were published on NICS, describing its definition and possibilities of its applications^{1,2,9,17} Some of the authors contributed significantly to further NICS envelopment and to its promotion among the broader chemical community.^{8,18,61} What authors of this paper have in common is that all of us actively use the NICS in our research, and the topics range from organic^{26–30,70–73} and inorganic molecules,^{33,34} metal clusters,^{37,38} supramolecular chemistry,^{44,45} mechanistic studies^{8,58} and bio-related molecules.^{46–49,74}

The simplicity of NICS-calculations can be a curse, too. Of course, NICS has also some clear shortcomings that should not be.⁷⁵ While NICS correlates very well with the other criteria for aromaticity like aromatic stabilization energy, other magnetic criteria⁷⁰ or structure,^{76,77} it is not a method applicable without critical intelligence, as impressively pointed out by recent publications.^{78–80} The reasons are manifold from conceptual shortcomings, via contribution of different effects or the tendency to overinterpretation of data, *e.g.*, to make quantitative statements about aromaticity. That NICS has restraints was obvious for Schleyer and his team and so they stated in the concluding remarks of their review from 2005⁸ “the limitations of NICS must also be appreciated.” After they had given a view sentence above some assisting hints how to handle NICS. But have all persons applying NICS read that part?

What can we expect in the next 25 years? NICS had turned out to be a Swiss army knife for investigating aromaticity. Beside its shortcomings and limitations, it will surely continue being a robust craftsman tool for exploring aromaticity abreast with structural criteria and the different ways to calculate aromatic stabilization energy. One can expect that NICS will also find additional applications, as recently demonstrated as a criterion for the design of new antifungal benzofuranones⁸¹ and in the modelling of antioxidative capacity of phenolic compounds.⁷⁴ May be NICS will one day be a common tool included in QSAR studies or any other fascinating application.

Ad multos annos, NICS!

ИЗВОД

25 ГОДИНА NICS – МНОГО ВИШЕ ОД НИЧЕГА!

RALPH PUCHTA^{1,3}, СЛАЂАНА ЂОРЂЕВИЋ⁴, СЛАВКО РАДЕНКОВИЋ⁴, HAIJUN JIAO⁵
и NICO J. R. VAN EIKEMA HOMMES¹

¹Computer Chemistry Center, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Nügelbachstr. 25, 91052 Erlangen, Germany, ²Inorganic Chemistry, Department of Chemistry and Pharmacy, University of Erlangen-Nuremberg, Egerlandstr. 1, 91058 Erlangen, Germany, ³Central Institute for Scientific Computing (ZISC), University of Erlangen-Nuremberg, Martensstr. 5a, 91058 Erlangen, Germany,

⁴Универзитет у Крагујевцу, Природно-математички факултет, 34000 Крагујевац и ⁵Leibniz-Institut für Katalyse e.V., Albert-Einstein-Str. 29a, Rostock, 18059 Germany

Познати индекс ароматичности NICS је уведен пре 25 година. Аутори користе прилику да ову годишњицу искористе за кратку и делом личну ретроспективу.

(Примљено 3. децембра 2021, ревидирано 21. јуна, прихваћено 6. јула 2022)

REFERENCES

1. P. von R. Schleyer, C. Maerker, A. Dransfeld, H. Jiao, N. J. R. van Eikema Hommes, *J. Am. Chem. Soc.* **118** (1996) 6317 (<https://doi.org/10.1021/ja960582d>)
2. H. Jiao, P. von R. Schleyer, Y. Mo, M. A. McAllister, T. T. Tidwell, *J. Am. Chem. Soc.* **119** (1997) 7075 (<https://doi.org/10.1021/ja970380x>)

3. M. Saunders, H. A. Jiménez-Vázquez, R. J. Cross, S. Mroczkowski, D. I. Freedberg, F. A. L. Anet, *Nature* **367** (1994) 256 (<https://doi.org/10.1038/367256a0>)
4. M. Buehl, W. Thiel, H. Jiao, P. v. R. Schleyer, M. Saunders, F. A. L. Anet, *J. Am. Chem. Soc.* **116** (1994) 6005 (<https://doi.org/10.1021/ja00092a076>)
5. M. Bühl, A. Hirsch, *Chem. Rev.* **101** (2001) 1153 (<https://doi.org/10.1021/cr990332q>)
6. E. Shabtai, A. Weitz, R. C. Haddon, R. E. Hoffman, M. Rabinovitz, A. Khong, R. J. Cross, M. Saunders, P.-C. Cheng, L. T. Scott, *J. Am. Chem. Soc.* **120** (1998) 6389 (<https://doi.org/10.1021/ja9805831>)
7. *Web of Science online database*, <https://www.webofscience.com>
8. Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. von R. Schleyer, *Chem. Rev.* **105** (2005) 3842 (<https://doi.org/10.1021/cr030088+>)
9. P. v. R. Schleyer, H. Jiao, H. M. Sulzbach, H. F. Schaefer, *J. Am. Chem. Soc.* **118** (1996) 2093 (<https://doi.org/10.1021/ja953126i>)
10. D. Moran, F. Stahl, H. F. Bettinger, H. F. Schaefer, P. v. R. Schleyer, *J. Am. Chem. Soc.* **125** (2003) 6746 (<https://doi.org/10.1021/ja034497z>)
11. S. Klod, E. Kleinpeter, *J. Chem. Soc., Perkin Trans. 2* (2001) 1893 (<https://doi.org/10.1039/B009809O>)
12. S. Klod, A. Koch, E. Kleinpeter, *J. Chem. Soc., Perkin Trans. 2* (2002) 1506 (<https://doi.org/10.1039/B204629F>)
13. E. Kleinpeter, S. Klod, *J. Mol. Struct.* **704** (2004) 79 (<https://doi.org/https://doi.org/10.1016/j.molstruc.2003.12.062>)
14. E. F. Kleinpeter, A. Koch, *ARKIVOC* **2012** (2011) 94 (<https://doi.org/10.3998/ark.5550190.0013.510>)
15. A. Stanger, *J. Org. Chem.* **71** (2006) 883 (<https://doi.org/10.1021/jo051746o>)
16. J. Pipek, P. G. Mezey, *J. Chem. Phys.* **90** (1989) 4916 (<https://doi.org/10.1063/1.456588>)
17. P. von R. Schleyer, H. Jiao, N. J. R. van E. Hommes, V. G. Malkin, O. L. Malkina, *J. Am. Chem. Soc.* **119** (1997) 12669 (<https://doi.org/10.1021/ja9719135>)
18. P. von R. Schleyer, M. Manoharan, Z.-X. Wang, B. Kiran, H. Jiao, R. Puchta, N. J. R. van Eikema Hommes, *Org. Lett.* **3** (2001) 2465 (<https://doi.org/10.1021/ol016217v>)
19. C. Corminboeuf, T. Heine, J. Weber, *Phys. Chem. Chem. Phys.* **5** (2003) 246 (<https://doi.org/10.1039/B209674A>)
20. T. Heine, P. v. R. Schleyer, C. Corminboeuf, G. Seifert, R. Reviakine, J. Weber, *J. Phys. Chem., A* **107** (2003) 6470 (<https://doi.org/10.1021/jp035163z>)
21. J. A. Bohmann, F. Weinhold, T. C. Farrar, *J. Chem. Phys.* **107** (1997) 1173 (<https://doi.org/10.1063/1.474464>)
22. M. Baranac-Stojanović, *J. Org. Chem.* **85** (2020) 4289 (<https://doi.org/10.1021/acs.joc.9b03472>)
23. M. Mauksch, S. B. Tsogoeva, *Chem. – A Eur. J.* **27** (2021) 14660 (<https://doi.org/https://doi.org/10.1002/chem.202102230>)
24. M. Jirásek, H. L. Anderson, M. D. Peeks, *Acc. Chem. Res.* **54** (2021) 3241 (<https://doi.org/10.1021/acs.accounts.1c00323>)
25. G. J. Richards, J. P. Hill, *Acc. Chem. Res.* **54** (2021) 3228 (<https://doi.org/10.1021/acs.accounts.1c00315>)
26. J. I. Wu, F. G. Pühlhofer, P. von R. Schleyer, R. Puchta, B. Kiran, M. Mauksch, N. J. R. van E. Hommes, I. Alkorta, J. Elguero, *J. Phys. Chem., A* **113** (2009) 6789 (<https://doi.org/10.1021/jp902983r>)

27. S. Radenković, J. Đurđević, P. Bultinck, *Phys. Chem. Chem. Phys.* **14** (2012) 14067 (<https://doi.org/10.1039/C2CP41472D>)
28. S. Radenković, I. Gutman, P. Bultinck, *J. Phys. Chem., A* **116** (2012) 9421 (<https://doi.org/10.1021/jp307281y>)
29. S. Radenković, J. Kojić, J. Petronijević, M. Antić, *J. Phys. Chem., A* **118** (2014) 11591 (<https://doi.org/10.1021/jp507309m>)
30. M. Antić, B. Furtula, S. Radenković, *J. Phys. Chem., A* **121** (2017) 3616 (<https://doi.org/10.1021/acs.jpca.7b02521>)
31. C. Riesinger, G. Balázs, M. Seidl, M. Scheer, *Chem. Sci.* **12** (2021) 13037 (<https://doi.org/10.1039/D1SC04296C>)
32. J. T. Boronski, J. A. Seed, D. Hunger, A. W. Woodward, J. van Slageren, A. J. Wooles, L. S. Natrajan, N. Kaltsoyannis, S. T. Liddle, *Nature* **598** (2021) 72 (<https://doi.org/10.1038/s41586-021-03888-3>)
33. S. Radenković, M. Antić, N. D. Savić, B. Đ. Glišić, *New J. Chem.* **41** (2017) 12407 (<https://doi.org/10.1039/C7NJ02634J>)
34. M. Walther, R. Puchta, *RSC Adv.* **2** (2012) 5815 (<https://doi.org/10.1039/C2RA20665J>)
35. R. Puchta, B. Neumüller, K. Dehnicke, *Zeitschr. Anorg. Allg. Chem.* **635** (2009) 1196 (<https://doi.org/https://doi.org/10.1002/zaac.200801360>)
36. A. I. Boldyrev, L.-S. Wang, *Chem. Rev.* **105** (2005) 3716 (<https://doi.org/10.1021/cr030091t>)
37. S. Radenković, P. Bultinck, *J. Phys. Chem., A* **115** (2011) 12493 (<https://doi.org/10.1021/jp2020947>)
38. S. Đorđević, S. Radenković, *Phys. Chem. Chem. Phys.* **21** (2019) 7105 (<https://doi.org/10.1039/c9cp00541b>)
39. M. M. Hossain, M. S. Mirzaei, S. V Lindeman, S. Mirzaei, R. Rathore, *Org. Chem. Front.* **8** (2021) 2393 (<https://doi.org/10.1039/D1QO00068C>)
40. K. Amsharov, D. I. Sharapa, O. A. Vasilyev, M. Oliver, F. Hauke, A. Goerling, H. Soni, A. Hirsch, *Carbon N. Y.* **158** (2020) 435 (<https://doi.org/https://doi.org/10.1016/j.carbon.2019.11.008>)
41. Z. Chen, J. I. Wu, C. Corminboeuf, J. Bohmann, X. Lu, A. Hirsch, P. von R. Schleyer, *Phys. Chem. Chem. Phys.* **14** (2012) 14886 (<https://doi.org/10.1039/C2CP42146A>)
42. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, F.-U. Rahman, Y. Yu, J. Rebek, *Phys. Chem. Chem. Phys.* **23** (2021) 19647 (<https://doi.org/10.1039/D1CP02277F>)
43. Y. Cohen, S. Slovak, L. Avram, *Chem. Commun.* **57** (2021) 8856 (<https://doi.org/10.1039/D1CC02906A>)
44. D. Čočić, R. Puchta, R. van Eldik, *J. Coord. Chem.* **73** (2020) 2602 (<https://doi.org/10.1080/00958972.2020.1820494>)
45. R. Puchta, R. van Eldik, *Eur. J. Inorg. Chem.* **2007** (2007) 1120 (<https://doi.org/https://doi.org/10.1002/ejic.200600715>)
46. T. V. Soldatović, E. Selimović, B. Šmit, D. Ašanin, N. S. Planojević, S. D. Marković, R. Puchta, B. M. Alzoubi, *J. Coord. Chem.* **72** (2019) 690 (<https://doi.org/10.1080/00958972.2019.1569229>)
47. S. Jovanović, R. Puchta, O. Klisurić, Ž. D. Bugarčić, *J. Coord. Chem.* **69** (2016) 735 (<https://doi.org/10.1080/00958972.2016.1146257>)

48. B. Petrović, Ž. D. Bugarčić, A. Dees, I. Ivanović-Burmazović, F. W. Heinemann, R. Puchta, S. N. Steinmann, C. Corminboeuf, R. van Eldik, *Inorg. Chem.* **51** (2012) 1516 (<https://doi.org/10.1021/ic201807a>)
49. M. D. Kostić, V. M. Divac, B. M. Alzoubi, R. Puchta, *Zeitschr. Naturforsch., B* **71** (2016) 883 (<https://doi.org/doi:10.1515/znb-2016-0055>)
50. I. Casademont-Reig, R. Guerrero-Avilés, E. Ramos-Cordoba, M. Torrent-Sucarrat, E. Matito, *Angew. Chemie Int. Ed.* **60** (2021) 24080 (<https://doi.org/https://doi.org/10.1002/anie.202108997>)
51. J. Y. M. Chan, Y. Okada, T. Kawata, N. Kobayashi, D. K. P. Ng, *Org. Lett.* **23** (2021) 5942 (<https://doi.org/10.1021/acs.orglett.1c02039>).
52. M. Rauhalhti, D. Sundholm, M. P. Johansson, *Phys. Chem. Chem. Phys.* **23** (2021) 16629 (<https://doi.org/10.1039/D1CP02381K>)
53. H. Kawashima, S. Ukai, R. Nozawa, N. Fukui, G. Fitzsimmons, T. Kowalczyk, H. Fliegl, H. Shinokubo, *J. Am. Chem. Soc.* **143** (2021) 10676 (<https://doi.org/10.1021/jacs.1c04348>)
54. F. Golpayegani, Z. Mirjafary, J. M. Aliabad, H. Saeidian, *Comput. Theor. Chem.* **1206** (2021) 113469 (<https://doi.org/https://doi.org/10.1016/j.comptc.2021.113469>)
55. M. Y. Borzehandani, E. Abdulmalek, M. B. Abdul Rahman, M. A. M. Latif, *Polymers (Basel)*. **13** (2021) (<https://doi.org/10.3390/polym13111861>)
56. C. Zeng, W. Shen, X. Xie, M. Li, *Polym. Sci., A* **52** (2010) 1355 (<https://doi.org/10.1134/S0965545X1012014X>)
57. M. Mauksch, S. B. Tsogoeva, *ChemPhysChem* **17** (2016) 963 (<https://doi.org/https://doi.org/10.1002/cphc.201600086>)
58. H. Jiao, P. von Ragué Schleyer, *J. Chem. Soc., Perkin Trans. 2* (1994) 407 (<https://doi.org/10.1039/P29940000407>)
59. M. Mauksch, V. Gogonea, H. Jiao, P. von R. Schleyer, *Angew. Chemie Int. Ed.* **37** (1998) 2395 ([https://doi.org/https://doi.org/10.1002/\(SICI\)1521-3773\(19980918\)37:17<2395::AID-ANIE2395>3.0.CO;2-W](https://doi.org/https://doi.org/10.1002/(SICI)1521-3773(19980918)37:17<2395::AID-ANIE2395>3.0.CO;2-W))
60. C. Castro, C. M. Isborn, W. L. Karney, M. Mauksch, P. von R. Schleyer, *Org. Lett.* **4** (2002) 3431 (<https://doi.org/10.1021/ol026610g>)
61. C. Castro, Z. Chen, C. S. Wannere, H. Jiao, W. L. Karney, M. Mauksch, R. Puchta, N. J. R. van E. Hommes, P. von R. Schleyer, *J. Am. Chem. Soc.* **127** (2005) 2425 (<https://doi.org/10.1021/ja0458165>)
62. Z. Huang, Y. Zhang, W.-X. Zhang, J. Wei, S. Ye, Z. Xi, *Nat. Commun.* **12** (2021) 1319 (<https://doi.org/10.1038/s41467-021-21648-9>)
63. K. An, T. Shen, J. Zhu, *Organometallics* **36** (2017) 3199 (<https://doi.org/10.1021/acs.organomet.7b00341>)
64. C. Zhu, S. Li, M. Luo, X. Zhou, Y. Niu, M. Lin, J. Zhu, Z. Cao, X. Lu, T. Wen, Z. Xie, P. v. R. Schleyer, H. Xia, *Nat. Chem.* **5** (2013) 698 (<https://doi.org/10.1038/nchem.1690>)
65. M. Mauksch, S. B. Tsogoeva, *Chem. – A Eur. J.* **16** (2010) 7843 (<https://doi.org/https://doi.org/10.1002/chem.201000396>)
66. M. K. Milčić, B. D. Ostojić, S. D. Zarić, *Inorg. Chem.* **46** (2007) 7109 (<https://doi.org/10.1021/ic062292w>)
67. M. Mauksch, S. B. Tsogoeva, *Chem. – A Eur. J.* **24** (2018) 10059 (<https://doi.org/https://doi.org/10.1002/chem.201802270>)

68. D. W. Szczepanik, M. Solà, *ChemistryOpen* **8** (2019) 219 (<https://doi.org/https://doi.org/10.1002/open.201900014>)
69. I. Fernández, G. Frenking, *Chem. – A Eur. J.* **13** (2007) 5873 (<https://doi.org/https://doi.org/10.1002/chem.200601674>)
70. S. Radenković, S. Đorđević, *Phys. Chem. Chem. Phys.* **23** (2021) 11240 (<https://doi.org/10.1039/D1CP00784J>)
71. J. Đ. Nikolić, S. Đorđević, S. Radenković, *J. Mol. Model.* **26** (2020) 275 (<https://doi.org/10.1007/s00894-020-04543-w>)
72. I. Gutman, S. Radenkovic, M. Antic, J. Djurdjevic, *J. Serb. Chem. Soc.* **78** (2013) 1539 (<https://doi.org/10.2298/JSC130520057G>)
73. S. Radenković, M. Antić, S. Đorđević, B. Braida, *Comput. Theor. Chem.* **1116** (2017) (<https://doi.org/10.1016/j.comptc.2017.01.028>)
74. S. Jeremić, S. Radenković, M. Filipović, M. Antić, A. Amić, Z. Marković, *J. Mol. Graph. Model.* **72** (2017) 240 (<https://doi.org/https://doi.org/10.1016/j.jmgm.2017.01.011>)
75. P. Lazzeretti, *Phys. Chem. Chem. Phys.* **6** (2004) 217 (<https://doi.org/10.1039/B311178D>)
76. P. von Ragué Schleyer, H. Jiao, B. Goldfuss, P. K. Freeman, *Angew. Chemie Int. Ed. English* **34** (1995) 337 (<https://doi.org/https://doi.org/10.1002/anie.199503371>)
77. L. Nyulászai, P. von R. Schleyer, *J. Am. Chem. Soc.* **121** (1999) 6872 (<https://doi.org/10.1021/ja983113f>)
78. A. Stanger, *Eur. J. Org. Chem.* **2020** (2020) 3120 (<https://doi.org/https://doi.org/10.1002/ejoc.201901829>)
79. R. Gershoni-Poranne, A. Stanger, *Chem. Soc. Rev.* **44** (2015) 6597 (<https://doi.org/10.1039/C5CS00114E>)
80. M. Solà, F. Feixas, J. O. C. Jiménez-Halla, E. Matito, J. Poater, *Symmetry* **2** (2010) (<https://doi.org/10.3390/sym2021156>)
81. M. D. Zermeño-Macías, M. M. González-Chávez, F. Méndez, A. Richaud, R. González-Chávez, L. E. Ojeda-Fuentes, P. D. Niño-Moreno, R. Martínez, *Mol.* **26** (2021) (<https://doi.org/10.3390/molecules26165078>).