

Publication Lists (2001 – present):



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Total number of publications: 119

Total number of ISI publications: 107

Total number of independent ISI citations: 1665

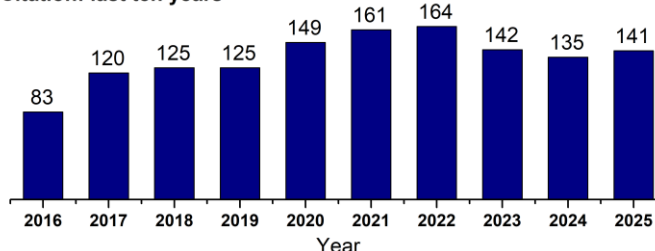
Hirsch index: 15 (WoS), 15 (Scopus)

First Author: 31

Corresponding Author: 27

[Publons](#), [Scopus](#) or [Google Scholar](#)

Citation: last ten years



Articles (ISI)

➤ 2026

1. Zs. Bálint, **A. Bende**: "A Complementary Theoretical Study on 6-Nitro BIPS Spiropyran Photoswitching Mechanism", *ChemPhotoChem*, **10**(1), e202500246 (2026). ([PDF](#)) – Quartile: Q3

➤ 2025

2. C. Berghian-Grosan, S. Varvara, **A. Bende**, R. Bostan: "A complex electrochemical, theoretical and surface analysis investigation of copper corrosion inhibition in 3.5 wt% NaCl solution. Case study: SEM images and deep learning for incipient corrosion detection", *Journal of Molecular Liquids*, **437**, 128544 (2025). ([PDF](#))

➤ 2024

3. A.-A. Farcaş and **A. Bende**: "Nature of Charge Transfer Effects in Complexes of Dopamine Derivatives Adsorbed on Graphene-Type Nanostructures", *International Journal of Molecular Sciences*, **25**(19), 10522, (2024). ([PDF](#)) – Quartile: Q1
4. A.-A. Farcaş and **A. Bende**: "Theoretical insights into dopamine photochemistry adsorbed on graphene-type nanostructures", *Physical Chemistry Chemical Physics*, **26**, 14937 – 14947 (2024). ([PDF](#)) – Quartile: Q2
5. A.-A. Farcaş, Roxana D. Paşca, Maria F. Gaele, Tonia M. Di Palma and **A. Bende**, "Rydberg-type electronic excited state dynamics in small sodium–water clusters", *Molecular Physics*, **122**, e2249133 (2024). ([PDF](#)) – Quartile: Q3
6. C. M. Muntean, R. Ştefan, A. Tăbăran, **A. Bende**, A. Fălămaş and L. E. Olar, "Characterization of the Structural Changes of the Genomic DNA of *Staphylococcus aureus* Due to Femtosecond Laser Irradiation by Fourier Transform Infrared (FT-IR) Spectroscopy", *Analytical Letters*, **57**(5), 711 – 726 (2024). ([PDF](#)) – Quartile: Q3

➤ 2023

7. C. M. Muntean, D. Cuiuş, S. Boca, A. Fălămaş, N. Toşa, I. A. Brezeştean, **A. Bende**, L. Barbu-Tudoran, R. Moldovan, E. Bodoki, C. Farcău, "Gold vs. Silver Colloidal Nanoparticle Films for Optimized SERS Detection of Propranolol and Electrochemical-SERS Analyses", *Biosensors* **13**(5), 530 (2023). ([PDF](#)) – Quartile: Q1
8. **A. Bende**, A.-A. Farcaş: „Intermolecular-Type Conical Intersections in Benzene Dimer", *International Journal of Molecular Sciences*, **24**(3), 2906 (2023). ([PDF](#)) – Quartile: Q1
9. C. C. Anghel, A. G. Mirea, C. C. Popescu, A. M. Mădălan, A. Hanganu, **A. Bende**, N. D. Hădade, M. Matache, M. Andruh: "Shifting emission of oxadiazoles via inter- or intramolecular hydrogen bonding", *Dyes & Pigments*, **210**, 111023 (2023). ([PDF](#)) – Quartile: Q1

➤ 2022

10. **A. Bende**, A.-A. Farcaş, A. Falamaş, A. Petran: "New insight into catechol photochemistry: the role of different monomer and dimer configurations in radiation-less decay of the S1 electronic excited state", *Physical Chemistry Chemical Physics*, **24**(47), 29165 – 29175 (2022). ([PDF](#)) – Quartile: Q2
11. I. A. Brezeştean, N. Toşa, A. Falamaş, D. Cuiuş, C. M. Muntean, **A. Bende**, B. Cozar, C. Berghian-Groşan, C. Farcău, "Silver Nanoparticle Films Obtained by Convective Self-Assembly for Surface-Enhanced Raman Spectroscopy Analyses of the Pesticides Thiabendazole and Endosulfan", *Frontiers in Chemistry*, **10**, 915337 (2022). ([PDF](#)) – Quartile: Q2

12. A. Falamaş, A. Petran, A.-M. Hada, **A. Bende**, "Dopamine Photochemical Behavior under UV Irradiation", *International Journal of Molecular Sciences*, **23**, 5483 (2022). ([PDF](#)) – Quartile: Q1
13. T. M. Di Palma, M. F. Gaele, **A. Bende**: "Photoionization, structures and energetics of Na-doped formic acid-water clusters", *CHEMPHYSICHEM*, **23**(5), e202100861 (2022). ([PDF](#)) – Quartile: Q3
14. **A. Bende**, A.-A. Farcaş, V. Toşa: "Theoretical study of light-induced crosslinking reaction between pyrimidine DNA bases and aromatic amino acids", *Frontiers in Bioengineering and Biotechnology*, **9**, 806415, (2022). ([PDF](#)) – Quartile: Q1

➤ **2021**

15. **A. Bende**: "The full mapping of low-lying excited state relaxation dynamic pathways for acetophenone", *Studia UBB Chemia*, **66**(3), 239 – 253 (2021). ([PDF](#))
16. C. C. Anghel, I. Stroia, A. Pop, **A. Bende**, I. Grosu, N. D. Hădade, J. Roncali: "An attempt to synthesize a terthienyl-based analog of indacenedithiophene (IDT): unexpected synthesis of a naphtho[2,3-b]thiophene derivative", *RSC Advances*, **11**(17), 9894-9900 (2021). ([PDF](#))
17. A.-A. Farcaş, **A. Bende**: "Theoretical modelling of the singlet-triplet spin transition in different Ni(II)-diketopyrpyr based metal-ligand octahedral complexes", *Physical Chemistry Chemical Physics*, **23**(8), 4784-4795 (2021). ([PDF](#))
18. C. M. Muntean, R. Ştefan, A. Tăbăran, C. Tripon, **A. Bende**, A. Fălămaş, L. M. Colobăţiu, L. E. Olar: "The Influence of UV Femtosecond Laser Pulses on Bacterial DNA Structure, as Proved by Fourier Transform Infrared (FT-IR) Spectroscopy", *ChemistrySelect*, **6**(27), 6957-6972, (2021). ([PDF](#))
19. L. Pop, I. G. Grosu, M. Miclăuş, N. D. Hădade, A. Pop, **A. Bende**, A. Terec, M. Barboiu, I. Grosu: "Halogen-Bonded Organic Frameworks of Perfluoroiodo- and Perfluorodiodobenzene with 2,2',7,7'-Tetrapyridyl-9,9'-spirobifluorene", *Crystal Growth & Design*, **21**(2), 1045-1054 (2021). ([PDF](#))

➤ **2020**

20. C. V. Crişan, A. Soran, **A. Bende**, N. D. Hădade, A. Terec, I. Grosu: "Synthesis, Structure and Supramolecular Properties of a Novel C3 Cryptand with Pyridine Units in the Bridges", *Molecules*, **25**, 3789 (2020). ([PDF](#))
21. C. Zagrean-Tuza, A. C. Moţ, T. Chmiel, **A. Bende**, I. Turcu: „Sugar matters: sugar moieties as reactivity-tuning factors in quercetin O-glycosides”, *Food & Function*, **11**, 5293-5307 (2020). ([PDF](#))
22. T.-A. Beu, **A. Bende**, A.-A. Farcaş: „Calculations of electron transfer in the tris [4-(2-thienyl) phenyl] amine–C70 donor-acceptor system”, *Chemical Physics Letters*, **754**, 137654 (2020). ([PDF](#))
23. I. G. Grosu, L. Pop, M. Miclăuş, N. D. Hădade, A. Terec, **A. Bende**, C. Socaci, M. Barboiu, I. Grosu: „Halogen Bonds (N⋯I) at Work: Supramolecular Catemeric Architectures of 2,7-Dipyridylfluorene with ortho-, meta-, or para-Diiodotetrafluorobenzene Isomers”, *Crystal Growth & Design*, **20**(5), 3429-3441 (2020). ([PDF](#))
24. Gh. Borodi, A. Turza, **A. Bende**: „Exploring the Polymorphism of Drostanolone Propionate”, *Molecules*, **25**(6), 1436 (2020). ([PDF](#))
25. T. M. Di Palma, M. F. Gaele, **A. Bende**: „Clusters tagged by alkali metals”, *AIP Conference Proceedings*, **2206**, 030002 (2020). ([PDF](#))
26. A.-A. Farcaş, **A. Bende**: „DFT study of adiabatic singlet-triplet energy gaps in Ni (II)-based macrocyclic-ligand supramolecular complexes”, *AIP Conference Proceedings*, **2206**, 030001, (2020). ([PDF](#))

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27. A.-A. Farcaş, **A. Bende**: „Improving the Light-Induced Spin Transition Efficiency in Ni(II)-Based Macrocyclic-Ligand Complexes”, *Molecules*, **24**(23), 4249 (2019). ([PDF](#))
28. C. Sacalis, C. Morar, P. Lameiras, A. Lupan, R. Silaghi-Dumitrescu, **A. Bende**, G. Katona, D. Porumb, D. Harakat, E. Gál, M. Darabantu: „Design, synthesis and structure of novel dendritic G-2 melamines comprising piperidine motifs as key linkers and 4-(n-octyloxy)aniline as a peripheral unit”, *Tetrahedron*, **75**(35), 130468 (2019). ([PDF](#))
29. L. Almásy, **A. Bende**: „Intermolecular interaction in methylene halide (CH₂F₂, CH₂Cl₂, CH₂Br₂ and CH₂I₂) dimers”, *Molecules*, **24**(9), 1810 (2019). ([PDF](#))
30. A.-A. Farcaş, T. A. Beu, **A. Bende**: „Light-induced spin transitions in Ni(II)-based macrocyclic-ligand complexes: A DFT study”, *Journal of Photochemistry and Photobiology A: Chemistry*, **376**, 316-323 (2019). ([PDF](#))
31. G. Borodi, A. Turza, O. Onija, **A. Bende**: "Succinic, fumaric, adipic and oxalic acid cocrystals of promethazine hydrochloride", *Acta Crystallographica C*, **C75**, 107–119 (2019). ([PDF](#))

➤ **2018**

32. **A. Bende**, M. F. Gaele, T. M. Di Palma: "UV Photoionization of Sodium-Doped Formic Acid Clusters", CHEMPHYSICHEM, **19**(20), 2724–2734 (2018). ([PDF](#))
33. C. Morar, P. Lameiras, **A. Bende**, G. Katona, E. Gál, M. Darabantu: "Design, synthesis and structure of novel G-2 melamine-based dendrimers incorporating 4-(n-octyloxy)aniline as a peripheral unit", Beilstein Journal of Organic Chemistry, **14**, 1704–1722 (2018). ([PDF](#))
34. C. Lar, A. Woiczehowski-Pop, **A. Bende**, I. G. Grosu, N. Miklášová, E. Bogdan, N. D. Hădade, A. Terec, I. Grosu: "A three-armed cryptand with triazine and pyridine units: synthesis, structure and complexation with polycyclic aromatic compounds", Beilstein Journal of Organic Chemistry, **14**, 1370–1377 (2018). ([PDF](#))
35. A. Petran, N. D. Hădade, C. Filip, X. Filip, **A. Bende**, A. Popa, J. Liebscher: "Poly[3,4-dihydroxybenzhydrazide]: A Polydopamine Analogue?", Macromolecular Chemistry and Physics, **219**(10), 1700564 (2018). ([PDF](#))
36. M. Coroş, F. Pogăcean, L. Măgeruşan, M.-C. Roşu, A. S. Porav, C. Socaci, **A. Bende**, R.-I. Stefan-van Staden, S. Pruneanu: "Graphene-porphyrin composite synthesis through graphite exfoliation: The electrochemical sensing of catechol", Sensors and Actuators B: Chemical, **256**, 665 – 673 (2018). ([PDF](#))
- **2017**
37. **A. Bende**: "Low-Lying Excited States and Their Relaxation Pathways of Phenothiazine", AIP Conference Proceedings, **1917**, 020002 (2017). ([PDF](#))
38. I. G. Grosu, M. I. Rednic, M. Miclăuş, I. Grosu, **A. Bende**: "The nature of intermolecular interactions in pyridinium–anion– β -hexachlorocyclohexane molecular crystals", Physical Chemistry Chemical Physics, **19**(31), 20691 – 20698 (2017). ([PDF](#))
39. C. Morar, G. L. Turdean, **A. Bende**, P. Lameiras, C. Antheaume, L. M. Muresan, M. Darabantu: "New p-aminophenol-based dendritic melamines. Iterative synthesis, structure, and electrochemical characterisation", Comptes Rendus Chimie, **20**, 402 – 414 (2017). ([PDF](#))
- **2016**
40. A. R. Deac, C. Morar, G. L. Turdean, M. Darabantu, E. Gál, **A. Bende**, L. M. Muresan: "Glassy carbon electrode modified with hemin and new melamine compounds for H₂O₂ amperometric detection", Journal of Solid State Electrochemistry, **20**(11), 3071 – 3081 (2016). ([PDF](#))
41. H. Popeneciu, D. Ristoiu, I. Bratu, G. Borodi, **A. Bende**, L. Barbu: "Inclusion compounds of β -cyclodextrin-pitofenone hydrochloride. Investigations of solid forms", Studia UBB Chemia, **61**(2), 61 – 71 (2016).
42. M. I. Rednic, R. A. Varga, **A. Bende**, I. G. Grosu, M. Miclăuş, N. D. Hădade, A. Terec, E. Bogdan, I. Grosu: "Supramolecular anion recognition by β -HCH", Chemical Communications, **52**, 12322 – 12325 (2016). ([PDF](#))
- **2015**
43. **A. Bende**, G. Perretta, P. Sementa, T. M. Di Palma: "Inception of acetic acid-water cluster growth in molecular beams", CHEMPHYSICHEM, **16**(14), 3021 – 3029 (2015). ([PDF](#))
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45. M. Vlassa and **A. Bende**: "Theoretical investigation of polymer chain stability in the metal coordinated azorubine and cyclam complex", Chemical Physics, **457**, 152–159 (2015). ([PDF](#))
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47. A. Woiczehowski-Pop, D. Gligor, **A. Bende**, C. Varodi, E. Bogdan, A. Terec, I. Grosu: "Synthesis, structure, electrochemical behaviour and electrochemical investigations on the assembling with pyrene of a novel C₃ cryptand", Supramolecular Chemistry, **27**(1-2), 52 – 58 (2015). ([PDF](#))
- **2014**
48. A. Csehi, **A. Bende**, G. J. Halász, Á. Vibók, A. Das, D. Mukhopadhyay, S. Mukherjee, S. Adhikarie, M. Baer: "Dressed Adiabatic and Diabatic Potentials to study Topological Effects for F + H₂ System", Journal of Physical Chemistry A, **118**(33), 6361 – 6366 (2014). ([PDF](#))
49. J. Ladik, **A. Bende**: "Quantum Molecular Biological Investigation of the Onset of Cancer", International Journal of Quantum Chemistry, **114**(18), 1229 – 1235 (2014). ([PDF](#))
50. T. M. Di Palma, **A. Bende**: "Tautomerism and proton transfer in photoionized acetaldehyde and acetaldehyde-water clusters", Journal of Mass Spectrometry, **49**(8), 700 – 708 (2014). ([PDF](#))
51. F. Bogár, **A. Bende**, J. Ladik: "Influence of the sequence on the ab initio band structures of single and double stranded DNA models", Physics Letters A, **378**, 2157 – 2162 (2014). ([PDF](#))

52. **A. Bende**, C. M. Muntean: "The influence of anharmonic and solvent effects on the theoretical vibrational spectra of the guanine–cytosine base pairs in Watson–Crick and Hoogsteen configurations", Journal of Molecular Modeling, **20**(3), Article №: 2113, (2014). ([PDF](#))
53. M. V. Diudea, Cs. L. Nagy, **A. Bende**: "Carbon multi-shell cages", Physical Chemistry Chemical Physics, **16**(11), 5260 - 5269 (2014). ([PDF](#))

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54. **A. Bende**: "Low-lying excited-states and relaxation pathways of acetophenone", AIP Conf. Proc., **1565**, 24 - 28 (2013). ([PDF](#))
55. A. Csehi, **A. Bende**, G. J. Halász, A. Vibók, A. Das, D. Mukhopadhyay, S. Mukherjee, S. Adhikarie, and M. Baer: "Dressed Adiabatic and Diabatic Potentials for the Renner-Teller/ Jahn-Teller F+H₂ System", Journal of Physical Chemistry A, **117**(36) 8497–8505 (2013). ([PDF](#))
56. J. Liebscher, R. Mrówczyński, H. A. Scheidt, C. Filip, N. D. Hádade, R. Turcu, **A. Bende**, S. Beck: "The Structure of Polydopamine – a Never Ending Story?", Langmuir, **29**(33), 10539–10548 (2013). ([PDF](#))
57. M. Micciarelli, C. Altucci, B. Della Ventura, R. Velotta, V. Toşa, A. B. González Pérez, M. Pérez Rodríguez, Á. R. de Lera, **A. Bende**: "Low-lying excited-states of 5-benzyluracil", Physical Chemistry Chemical Physics, **15**, 7161 - 7173 (2013). ([PDF](#))
58. **A. Bende**, F. Bogár, J. Ladik: "Hole mobilities of periodic models of DNA double helices in the nucleosomes at different temperatures", Chemical Physics Letters, **565**, 128 - 131 (2013). ([PDF](#))
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61. V. Boldescu, I. Bratu, Gh. Borodi, I. Kacsó, **A. Bende**, Gh. Duca, F. Macaev, S. Pogrebnoi, Z. Ribkovskaia: "Study of binary systems of β -cyclodextrin with a highly potential anti-mycobacterial drug", Journal of Inclusion Phenomena and Macrocyclic Chemistry, **74**, 129 – 135 (2012). ([PDF](#))
62. O. Bradea, I. Kacsó, Gh. Borodi, **A. Bende**, I. Bratu: "Complexation of Amlodipine Besylate with β -Cyclodextrin", Acta Chimica Slovenica, **59**, 18 – 23, (2012). ([PDF](#))
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64. **A. Bende**, C. M. Muntean: "Solvent effect on the anharmonic vibrational frequencies in guanine-cytosine base pair", AIP Conf. Proc., **1425**, 5 - 8 (2012). ([PDF](#))
65. S. Dreve, I. Kacsó, A. Popa, O. Raita, **A. Bende**, Gh. Borodi, I. Bratu: "Chitosan-Based Nanocarriers For Antimalarials", AIP Conf. Proc., **1425**, 17 - 21 (2012). ([PDF](#))
66. **A. Bende**, F. Bogár, J. Ladik: "Possible role of Cl⁻ ions in DNA-protein interactions in the nucleosomes", Chemical Physics Letters, **525 – 526**, 115 – 119 (2012). ([PDF](#))

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68. **A. Bende**, L. Almásy: "Weakly bonded cluster structures of N,N'-dimethylethyleneurea and water" Journal of Molecular Liquids, **162**, 45 – 49 (2011). ([PDF](#))
69. S. Dreve, I. Kacsó, A. Popa, O. Raita, F. Dragan, **A. Bende**, Gh. Borodi, I. Bratu: "Structural Investigation of Chitosan-based Microspheres with some Anti-Inflammatory Drugs", Journal of Molecular Structure, **997**(1-3), 78-86 (2011). ([PDF](#))
70. **A. Bende**, I. Turcu: "Nitrogen Substituted Phenothiazine Derivatives: Modeling of Molecular Self-Assembling", International Journal of Molecular Sciences (Special Issue "Advances in Molecular Electronic Structure Calculations"), **12**(5), 3102-3116, (2011). ([PDF](#))
71. **A. Bende**, F. Bogár, J. Ladik: "Model calculations of the energy band structures of double stranded DNA in the presence of water and Na⁺ ions", Solid State Communications, **151**(4), 301 - 305 (2011). ([PDF](#))
72. L. Almásy, **A. Bende**: "Ab initio structures of interacting methylene chloride molecules with comparison to the liquid phase", Journal of Molecular Liquids, **158**(3), 205 - 207 (2011). ([PDF](#))

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76. **A. Bende**, F. Bogár, F. Beleznay, J. Ladik: "Model calculation of the specific hole conductivities of the three homopolynucleotides, poly(guanilic acid), poly(adenilic acid) and polythymidine in presence of water and Na⁺ ions", Solid State Communications, **150**(9-10), 446 – 449 (2010). ([PDF](#))
77. **A. Bende**: "Hydrogen bonding in urea dimers and adenine-thymine DNA base pair: Anharmonic effects in intermolecular H-bond and intramolecular H-stretching vibrations", Theoretical Chemistry Accounts, **125**(3-6), 253 – 268 (2010). ([PDF](#))
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81. N. Toşa, **A. Bende**, R. A. Varga, A. Terec, I. Bratu, I. Grosu: "H-bond-Driven Supramolecular Architectures of the Syn and Anti Isomers of the Dioxime of Bicyclo[3.3.1]nonane-3,7-dione", Journal of Organic Chemistry, **74**(10), 3944 – 3947 (2009). ([PDF](#))
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➤ 2008

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84. **A. Bende**, L. Almásy: "Weak intermolecular bonding in N,N'-dimethylethyleneurea dimers and N,N'-dimethylethyleneurea - water systems: The role of the dispersion effects in intermolecular interaction", Chemical Physics, **354**(1-3), 202 – 210 (2008). ([PDF](#))
85. **A. Bende**, F. Bogár, J. Ladik: "The Role of Water and K⁺ Ion in the Charge Transfer between PO₄⁻ Groups of DNA and the Lysine⁺ and Arginine⁺ Side Chains of Histone Proteins", Chemical Physics Letters, **463**(1-3), 211 – 213 (2008). ([PDF](#))
86. J. Ladik, **A. Bende**, F. Bogár: "The electronic structure of the four nucleotide bases in DNA, of their stacks and of their homopolynucleotides in the absence and presence of water", Journal of Chemical Physics, **128**, 105101 (2008). ([PDF](#))

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88. **A. Bende**, F. Bogár, J. Ladik: "Charge Transfer between the PO₄⁻ groups of DNA and the arginine⁺ and lysine⁺ side chains of proteins", Chemical Physics Letters, **437**, 117 – 119, (2007). ([PDF](#))

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90. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "Theoretical Study of Hydrogen Bonds between Acetylene and Selected Proton Donor Systems", International Journal of Quantum Chemistry, **101**(2), 186-200 (2005). ([PDF](#))

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91. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "Ab initio Study of the Ammonia - Ammonia Dimer. BSSE-free Structures and Intermolecular Harmonic Vibrational Frequencies", International Journal of Quantum Chemistry, **99**(5), 585 - 593 (2004). ([PDF](#))

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93. **A. Bende**, Á. Vibók, G. J. Halász, S. Suhai: "*BSSE-free Description of the Formamide Dimers*", International Journal of Quantum Chemistry, **84**, 617-622 (**2001**). ([PDF](#))

Book or Book Chapters:

1. A. Bende (**2020**) Chapter 40: *Proton-Mediated Molecular Clusters*. In book: New Frontiers in Nanochemistry: Concepts, Theories, and Trends Volume 1: Structural Nanochemistry, Edited by: M. V. Putz, Vol. 1, Page 439-444, Apple Academic Press Inc., ISBN: 978-1-77188-777-9 ([WEB](#))
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