Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS

ACCEPTED MANUSCRIPT

Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS

J. Serb. Chem. Soc. **00(0)** 1-9 (2025)
JSCS–13635

Letter to the Editor
Published DD MM, 2025

Centennial of quantum theory in Belgrade: CEQPAS and the molecular excited state spectroscopy (MOLESs) initiative

FELIPE FANTUZZI[1], JELENA B. MALJKOVIĆ[2], MATIJA ZLATAR[3], CAUÊ P. SOUZA[1], HEIDY M. QUITIÁN-LARA[4], PAMIR NAG[5], BOBBY ANTONY[6], BRATISLAV P. MARINKOVIĆ[2]* AND NIGEL J. MASON[7†]

[1]School of Natural Sciences, University of Kent, Park Wood Rd, Canterbury CT2 7NH, UK, [2]Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade, Serbia, [3]Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000, Belgrade, Serbia, [4]Max Planck Institute for Extraterrestrial Physics, Gießenbachstraße 1, Garching 85748, Germany, [5]J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague, Czech Republic, [6]Department of Physics, Indian Institute of Technology (ISM), Dhanbad, 826004, Jharkhand, India, and [7]School of Engineering, Mathematics and Physics, University of Kent, Park Wood Rd, Canterbury CT2 7NH, UK.

(Received 18 November; revised 20 November; accepted 25 November 2025)

Abstract: The first week of November 2025 saw two events in Belgrade celebrating one hundred years of quantum mechanics and its impact on chemistry and molecular science. The Centennial of Quantum Theory: Progress in Atomic and Molecular Structure (CEQPAS) brought together researchers from across Europe and beyond to reflect on the scientific legacy of quantum theory and to showcase current advances in atomic and molecular spectroscopy, collision processes relevant to plasma research, chemical bonding, quantum chemistry, and the design of functional molecules, astrochemistry, the use of AI/ML for the analysis and generation of atomic and molecular data, and wider applications of quantum science. Immediately after CEQPAS, a new international initiative was launched: MOLecular Excited State spectroscopy (MOLESs), whose primary goal is to develop an atlas of molecular electronic structure and excited-state spectroscopy that rigorously integrates experiment and theory. Together, CEQPAS and MOLESs align historical perspective with future capability, positioning Belgrade as a regional hub for quantum-enabled molecular science.

Keywords: atomic and molecular spectroscopy; collision processes; plasma physics; machine learning for spectroscopy; electronic structure; quantum chemistry.

* Corresponding authors. E-mail: bratislav.marinkovic@ipb.ac.rs, † n.j.mason@kent.ac.uk
https://doi.org/10.2298/JSC251118083F

In 1925, quantum mechanics emerged from an intellectual rupture. Werner Heisenberg, then a young research assistant in Göttingen, retreated to the North Sea island of Helgoland to recover from hay fever and confront the mounting contradictions of atomic theory.[1] Working late into the night with tables of spectral lines, he set aside unobservable electron orbits and rebuilt the theory using only measurable quantities such as transition frequencies and intensities. The result was his *quantum-theoretical reinterpretation* paper.[2] Heisenberg later described the moment he realised the mathematics worked: he felt he was looking "through the surface of atomic phenomena into a strangely beautiful interior", became "far too excited to sleep", and went to the southern tip of the island where he climbed a rock and waited for the sunrise.

Within months, Born and Jordan recast Heisenberg's scheme into matrix mechanics, a formalism that recovered selection rules and line strengths drawn from spectroscopy.[3] Pauli introduced the exclusion principle,[4] and Uhlenbeck and Goudsmit proposed electron spin to explain fine structure and the anomalous Zeeman effect.[5] Early in 1926, Schrödinger formulated wave mechanics and derived the hydrogen spectrum, later showing its equivalence to matrix mechanics,[6] while Born provided the statistical interpretation that linked calculated amplitudes to observed line intensities.[7] Throughout these developments, spectroscopy supplied both the puzzles and the tests; it was spectroscopy that compelled quantum theory into being.

A century after Heisenberg's Helgoland breakthrough, the historical arc turned toward Belgrade. In the first week of November 2025, two landmark international events were organised by two institutes of national importance: the Institute of Physics Belgrade (IPB) and the Institute of Chemistry, Technology, and Metallurgy (ICTM). IPB hosted the international conference Centennial of Quantum Theory: Progress in Atomic and Molecular Structure (CEQPAS, Fig. 1).[8] Serbian-based researchers were joined by colleagues from Europe, India, New Zealand and Latin America, gathering not only to celebrate the intellectual leap of 1925 but also to examine how that leap continues to shape modern science.

Fig 1. CEQPAS conference group photo. Credits: Dušan Pantelić & Bojan Živojinović.

The opening lecture was delivered by Nigel Mason (University of Kent, UK), who reconnected the historical origin of quantum mechanics to present-day scientific challenges. Mason argued that spectroscopy was central to the birth of quantum mechanics, having first revealed the breakdown of classical physics, and remains the method most closely linked to quantum principles. He noted that major reformulations of quantum theory have often followed advances in spectroscopy, from early optical emission studies to modern free-electron lasers. Looking ahead, terahertz spectroscopy was highlighted as the next frontier for probing intermolecular forces and structural dynamics in soft matter.[9,10] Mason also warned that progress relies not only on instrumentation but on retaining expertise, as the field risks losing specialised knowledge faster than it can be renewed. He underscored that spectroscopic data underpin developments in quantum computing, astrophysics, environmental chemistry, and nanotechnology, and called for long-term stewardship through open repositories, shared protocols, and sustained training. The opening session, which included representation from the British Embassy in Belgrade and coverage by Radio Television of Serbia, marked the growing recognition of quantum science as a driver of collaboration and technological progress.

What followed during CEQPAS demonstrated this idea in concrete scientific terms, with spectroscopy and quantum theory appearing in contexts that could not have been imagined by Heisenberg in 1925. Andjelka Kovačević adapted correlation spectroscopy, originally developed for molecular systems, to analyse variability in supermassive black holes using quantum neural process models,[11] effectively treating accretion discs as spectroscopic systems and enabling tests of scenarios in which ultralight bosons form gravitationally quantised states. Larissa Lopes Cavalcante (University of Otago, New Zealand) examined cryogenic hydrocarbon and nitrogen-bearing ices relevant to Titan, showing through infrared spectroscopy and vacuum-ultraviolet photolysis that the degree of molecular ordering, crystalline or amorphous, controls both spectral signatures and photoreactivity.[12] Milan Milovanović extended the astrochemical perspective by benchmarking the vibrational and electronic spectra of fullerenes and their hydrogenated derivatives, identifying computational strategies suitable for astronomical assignments. Bratislav Marinković then led a guided tour of the IPB facilities, presenting the Omicron High-Resolution Hemispherical Analyser (OHRHA),[13] a shielded crossed-beam spectrometer capable of resolving electron-atom interactions with sub-0.1 eV precision, alongside the UGRA (UGaona RAspodela, Angular Distribution) system,[14] which measures angular-dependent differential cross sections and underpins the derivation of integral and momentum-transfer cross sections essential for plasma, atmospheric and environmental modelling. These contributions all pointed to the same realisation: spectroscopy is not only a tool for identifying molecular structure, but also our means of accessing chemistry in environments that cannot be reached physically, from planetary surfaces to the vicinity of black holes.

CEQPAS then shifted from spectroscopy to collisions. David Field (Aarhus University, Denmark) presented low-energy electron collisions in condensed molecular films and introduced *spontelectrics*: spontaneously polarised thin films where internal electric fields alter electron scattering.[15] Bobby Antony (Indian Institute of Technology Dhanbad, India) presented an overview of modern electron–molecule scattering theory,[16] outlining how current methods address a wide range of energies while still facing challenges for complex polyatomic and spin–relativistic targets, and showing how recent advances are beginning to make these systems tractable. Pamir Nag (J. Heyrovský Institute of Physical Chemistry, Czech Republic) showed that dissociative electron attachment can require symmetry lowering for bond cleavage to occur, providing an example where allowed and forbidden pathways depend on transient geometry.[17] Nikola Cvetanović showed how Stark spectroscopy serves as a non-intrusive probe of strong electric fields in low-temperature plasmas, using line splitting and shifts of hydrogen and helium emissions to map sheath fields that develop near plasma boundaries.[18] Nikola Škoro showed how non-thermal atmospheric-pressure plasma jets act as reactors that generate and deliver reactive oxygen and nitrogen species into water, illustrating how such plasmas can be harnessed for plasma-based water treatment with relevance to environmental remediation, agriculture and medicine.[19] The first day concluded with a tour of the IPB facilities and public lectures by Nenad Vukmirović, on quantum aspects of electron transport in solar-cell materials, and Slobodan Bubnjević, on the early history of quantum mechanics through key figures of the Solvay conferences. Framed by these broader perspectives, the day's programme reinforced that collision processes, once central to the derivation of quantum mechanics, now underpin applications in plasma agriculture, plasma medicine and environmental technologies.

The second day opened with a session on physical chemistry. After briefly linking quantum mechanics and spectroscopy to the design of functional molecules, including therapeutics relevant to neglected tropical diseases,[20] Felipe Fantuzzi (University of Kent, UK) argued that many core chemical concepts, devised before quantum mechanics, must be reformulated in a quantum language, recasting the foundations of chemistry itself. He then demonstrated that chemical bonding is a manifestation of quantum interference.[21] Cauê Souza (University of Kent, UK) presented a new computational protocol to reproduce the laboratory vacuum-ultraviolet absorption spectra of cryogenic ices, providing phase-sensitive benchmarks relevant to planetary and interstellar environments.[22,23] Dušan Veljković introduced strategies to reduce sensitivity in energetic materials by tuning local electrostatic potential,[24] and the discussion highlighted opportunities for collaboration with forensic science and dual-use research areas. Astrochemistry returned in the contribution by Heidy M. Quitián-Lara (Max Planck Institute for Extraterrestrial Physics, Germany), who showed how high-resolution spectroscopy and radiation-induced fragmentation experiments, paired with quantum-chemical calculations, can map the stability, reactivity and formation pathways of interstellar molecules and interpret astronomical observations.[25,26] The session concluded with a quantum-chemical study of non-covalent sulphur interactions by Ivana Veljković,[27] extending the σ-hole concept to rationalise chalcogen bonding.

The programme then turned to the conceptual foundations of quantum mechanics and to the emerging role of artificial intelligence (AI) and machine learning (ML) in physical science. Nenad Simonović discussed quantum diffraction and interference in atomic processes and showed that time-resolved superpositions of electron wave packets generate dynamic and exchange interference, enabling phase retrieval and the clear discrimination of competing scattering channels.[28] Igor Salom revisited the Wigner's friend paradox, challenging assumptions about the boundary between quantum and classical descriptions of observers. Saša Dujko re-examined the Franck–Hertz experiment with modern diagnostics, showing that energy exchange and electron spatial relaxation in gases are richer than the classic picture suggests.[29] Ivan Belča showed that an AI system can autonomously generate a complete spectroscopy workflow, raising the question of whether AI-generated datasets may eventually complement or replace new experiments. Vladimir Srećković demonstrated how small molecules shape astrophysical spectra through collisions and radiation, emphasising the need for accurate cross sections, robust databases and non-local thermodynamic equilibrium models, and noted that AI can help interpolate sparse data and guide future measurements.[30] Dimitrije Maletić reviewed how AI and ML support modern high-energy and nuclear-physics experiments, from event selection and pattern recognition to real-time decision systems. Lastly, Vladimir M. Petrović examined the capacities and limits of current AI, arguing that understanding it requires moving beyond black-box use toward transparent mechanisms tested across both physical and virtual environments.

The conference closed with remarks by Jelena Maljković, who emphasised that CEQPAS had showcased substantial progress, yet also revealed how much remains to be done. Across spectroscopy, collision science, physical chemistry, astrochemistry and AI, a recurring message emerged: quantum mechanics is not a finished theory, and spectroscopy remains the discipline that reveals where its limits and opportunities lie. Many speakers highlighted the need for coordinated infrastructures, openly accessible data and sustained training to ensure that experimental and computational knowledge does not dissipate as facilities evolve and generations change. CEQPAS demonstrated that quantum science has become a collective, international endeavour that links fundamental questions to applications with societal impact, from plasma medicine to environmental remediation and space missions.

Immediately after CEQPAS, the MOLecular Excited State spectroscopy (MOLESs)[31] initiative was launched at ICTM's historic building, where the Serbian Chemical Society was founded in 1897. MOLESs seeks to create a modern atlas of molecular excited states, taking inspiration from Melvin Robin's Higher Excited States of Polyatomic Molecules book series.[32–34] The consortium will assemble experimental and theoretical excited-state spectra across molecular families, phases and spectral regions, accompanied by reproducible protocols, benchmark datasets and fully accessible digital resources. If CEQPAS revisited the century that spectroscopy shaped, MOLESs prepares the century that spectroscopy will define; where CEQPAS celebrated the discovery of quantisation, MOLESs commits to charting the landscape of electronic structure. CEQPAS looked back to 1925; MOLESs looks forward.

In 1925, spectroscopy forced scientists to abandon classical pictures and create quantum mechanics. In 2025, spectroscopy again calls for collective action, not to reinvent quantum mechanics, but to organise and share the data required to use it. Belgrade, for one week in November, became a focal point where the legacy of quantum theory met its future applications in chemistry and molecular sciences, linking spectroscopy to planetary science, plasma medicine and data-driven discovery. The arc from Heisenberg in Helgoland to CEQPAS and MOLESs is continuous: spectroscopy reveals structure, quantum mechanics explains it, and the next century of discovery will depend on the ability to preserve, organise and interpret the spectra that have always been quantum mechanics' most important teacher.

Acknowledgements: The authors acknowledge the framework of the International Year of Quantum Science and Technology (IYQ2025), proclaimed by the United Nations and coordinated with the support of UNESCO, under which CEQPAS and MOLESs were organised. This work was supported by the Science Fund of the Republic of Serbia (grant no. 6821). F.F. gratefully acknowledges funding from the Royal Society ISPF International Collaboration Awards 2024 (grant no. ICAO\R1\241112) for the NUBIAN project. M.Z. thanks to the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (451-03-136/2025-03/200026).

И З В О Д

СТОГОДИШЊИЦА КВАНТНЕ ТЕОРИЈЕ У БЕОГРАДУ: CEQPAS И MOLESs ИНИЦИЈАТИВА

FELIPE FANTUZZI[1], JELENA B. MALJKOVIĆ[2], MATIJA ZLATAR[3], CAUÊ P. SOUZA[1], HEIDY M. QUITIÁN-LARA[4], PAMIR NAG[5], BOBBY ANTONY[6], BRATISLAV P. MARINKOVIĆ[2] AND NIGEL J. MASON[7]

[1]*School of Natural Sciences, University of Kent, Park Wood Rd, Canterbury CT2 7NH, UK,* [2]*Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade, Serbia,* [3]*Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000, Belgrade, Serbia,* [4]*Max Planck Institute for Extraterrestrial Physics, Gießenbachstraße 1, Garching 85748, Germany,* [5]*J. Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague, Czech Republic,* [6]*Department of Physics, Indian Institute of Technology (ISM), Dhanbad, 826004, Jharkhand, India,* [7]*School of Engineering, Mathematics and Physics, University of Kent, Park Wood Rd, Canterbury CT2 7NH, UK.*

Прва недеља новембра 2025. године у Београду била је обележена одржавањем два догађаја посвећена стогодишњици квантне механике и њеном утицају на хемију и молекулске науке. Конференција *Centennial of Quantum Theory: Progress in Atomic and Molecular Structure* (CEQPAS) окупила је истраживаче из Европе и света како би дискутовали о научном наслеђу квантне теорије и представили актуелна достигнућа у атомској и молекулској спектроскопији, сударним процесима релевантним за физику плазме, анализи хемијске везе и дизајну функционалних молекула, астрохемији, примени вештачке интелигенције и машинског учења у анализи и генерисању атомских и молекулских података, као и у ширим применама квантне науке. Одмах по завршетку CEQPAS-а покренута је нова међународна иницијатива: *MOLecular Excited State spectroscopy* (MOLESs), чији је примарни циљ развој атласа електронске структуре и спектроскопије ексцитованих стања молекула који ће ригорозно интегрисати експеримент и теорију. Заједно, CEQPAS и MOLESs повезују историјску перспективу са будућим могућностима, позиционирајући Београд као регионални центар молекулских наука заснованих на квантној механици.

(Примљено 18. новембра; ревидирано 18. новембра; прихваћено 25. новембра 2025.)

REFERENCES

1. M. Durrani, *Phys. World* **38** (2025) 35 (https://dx.doi.org/10.1088/2058-7058/38/08/28)
2. W. Heisenberg, *Zeitschrift Für Phys.* **33** (1925) 879 (https://dx.doi.org/10.1007/BF01328377)
3. M. Born, P. Jordan, *Zeitschrift Für Phys.* **34** (1925) 858 (https://dx.doi.org/10.1007/BF01328531)

4. W. Pauli, *Zeitschrift Für Phys.* **31** (1925) 765 (https://dx.doi.org/10.1007/BF02980631)
5. G. E. Uhlenbeck, S. Goudsmit, *Naturwissenschaften* **13** (1925) 953 (https://dx.doi.org/10.1007/BF01558878)
6. E. Schrödinger, *Phys. Rev.* **28** (1926) 1049 (https://dx.doi.org/10.1103/PhysRev.28.1049)
7. M. Born, *Zeitschrift Für Phys.* **38** (1926) 803 (https://dx.doi.org/10.1007/BF01397184)
8. J. B. Maljković, M. Zlatar, eds., *Centennial of Quantum Theory: Progress in Atomic and Molecular Structure - CEQPAS 2025, Book of Abstracts*, Belgrade, 2025 (https://dx.doi.org/10.5281/zenodo.17467615)
9. D. V. Mifsud, P. A. Hailey, A. Traspas Muiña, O. Auriacombe, N. J. Mason, S. Ioppolo, *Front. Astron. Sp. Sci.* **8** (2021) 757619 (https://dx.doi.org/10.3389/fspas.2021.757619)
10. X. Fu, Y. Liu, Q. Chen, Y. Fu, T. J. Cui, *Front. Phys.* **10** (2022) 869537 (https://dx.doi.org/10.3389/fphy.2022.869537)
11. A. B. Kovačević, *Appl. Spectrosc.* **79** (2025) 227 (https://dx.doi.org/10.1177/00037028241241308)
12. L. Lopes Cavalcante, E. C. Czaplinski, H. E. Maynard-Casely, M. L. Cable, N. Chaouche-Mechidal, R. Hodyss, C. Ennis, *Phys. Chem. Chem. Phys.* **26** (2024) 26842 (https://dx.doi.org/10.1039/D4CP03437F)
13. J. J. Jureta, A. R. Milosavljević, B. P. Marinković, *Int. J. Mass Spectrom.* **365–366** (2014) 114 (https://dx.doi.org/10.1016/j.ijms.2014.03.002)
14. J. Vukalović, B. P. Marinković, J. Rosado, F. Blanco, G. García, J. B. Maljković, *Phys. Chem. Chem. Phys.* **26** (2024) 985 (https://dx.doi.org/10.1039/D3CP05052A)
15. A. Cassidy, M. R. S. McCoustra, D. Field, *Acc. Chem. Res.* **56** (2023) 1909 (https://dx.doi.org/10.1021/acs.accounts.3c00094)
16. I. Chakraborty, N. Sinha, B. Antony, *Radiat. Phys. Chem.* **216** (2024) 111421 (https://dx.doi.org/10.1016/j.radphyschem.2023.111421)
17. P. Nag, M. Tarana, J. Fedor, *Phys. Rev. A* **103** (2021) 032830 (https://dx.doi.org/10.1103/PhysRevA.103.032830)
18. N. Cvetanović, M. M. Martinović, B. M. Obradović, M. M. Kuraica, *J. Phys. D. Appl. Phys.* **48** (2015) 205201 (https://dx.doi.org/10.1088/0022-3727/48/20/205201)
19. A. Kumar, N. Škoro, W. Gernjak, N. Puač, *Eur. Phys. J. D* **75** (2021) 283 (https://dx.doi.org/10.1140/epjd/s10053-021-00283-5)
20. E. R. S. Paz, C. P. Souza, J. C. De Oliveira, R. G. Almeida, C. Herrera-Acevedo, S. Lakoh, G. A. M. Jardim, E. N. da Silva Júnior, F. Fantuzzi, *ChemistryOpen* (2025) e202500465 (https://dx.doi.org/10.1002/open.202500465)
21. T. M. Cardozo, D. W. Oliveira De Sousa, F. Fantuzzi, M. A. C. Nascimento, *The Chemical Bond as a Manifestation of Quantum Mechanical Interference: Theory and Applications of the Interference Energy Analysis Using SCGVB Wave Functions*, in *Compr. Comput. Chem.*, Elsevier, 2024, pp. 552 (https://dx.doi.org/10.1016/B978-0-12-821978-2.00027-1)
22. J. Zhang, A. T. Muiña, D. V Mifsud, Z. Kaňuchová, K. Cielinska, P. Herczku, K. K. Rahul, S. T. S. Kovács, R. Rácz, J. C. Santos, A. T. Hopkinson, L. Craciunescu, N. C. Jones, S. V Hoffmann, S. Biri, I. Vajda, I. Rajta, A. Dawes, B. Sivaraman, Z. Juhász, B. Sulik, H. Linnartz, L. Hornekær, F. Fantuzzi, N. J. Mason, S. Ioppolo,

Mon. Not. R. Astron. Soc. **533** (2024) 826 (https://dx.doi.org/10.1093/mnras/stae1860)
23. M. D. Dickers, D. V. Mifsud, N. J. Mason, F. Fantuzzi, *Space Sci. Rev.* **221** (2025) 106 (https://dx.doi.org/10.1007/s11214-025-01228-9)
24. D. S. Kretić, I. S. Veljković, D. Ž. Veljković, *Chemistry* **5** (2023) 1843 (https://dx.doi.org/10.3390/chemistry5030126)
25. J. Londoño-Restrepo, S. Gómez, H. M. Quitián-Lara, F. Fantuzzi, A. Restrepo, *Chem. Sci.* **16** (2025) 3051 (https://dx.doi.org/10.1039/D4SC07986H)
26. H. M. Quitián-Lara, J. Londoño-Restrepo, S. Gómez, K. V García-González, A. Restrepo, N. J. Mason, P. Caselli, H. M. Boechat-Roberty, F. Fantuzzi, *Mon. Not. R. Astron. Soc.* **539** (2025) 3778 (https://dx.doi.org/10.1093/mnras/staf595)
27. D. S. Kretić, V. B. Medaković, I. S. Veljković, *Comput. Theor. Chem.* **1230** (2023) 114381 (https://dx.doi.org/10.1016/j.comptc.2023.114381)
28. N. S. Simonović, D. B. Popović, A. Bunjac, *Atoms* **11** (2023) 20 (https://dx.doi.org/10.3390/atoms11020020)
29. S. Dujko, J. Atić, D. Bošnjaković, R. D. White, P. Stokes, K. R. Hamilton, O. Zatsarinny, K. Bartschat, M. S. Rabasović, D. Šević, B. P. Marinković, D. V Fursa, I. Bray, R. P. McEachran, F. Blanco, G. García, D. B. Jones, L. Campbell, M. J. Brunger, *Plasma Sources Sci. Technol.* **30** (2021) 115019 (https://dx.doi.org/10.1088/1361-6595/ac3343)
30. V. Vujčić, B. P. Marinković, V. A. Srećković, S. Tošić, D. Jevremović, L. M. Ignjatović, M. S. Rabasović, D. Šević, N. Simonović, N. J. Mason, *Phys. Chem. Chem. Phys.* **25** (2023) 26972 (https://dx.doi.org/10.1039/D3CP03752E)
31. MOLecular Excited State spectroscopy - MOLESs https://www.moless-spectroscopy.org/ (accessed 19/11/2025)
32. M. B. Robin, *Higher Excited States of Polyatomic Molecules, Volume I*, Elsevier, New York, 1974 (https://dx.doi.org/10.1016/B978-0-12-589901-7.X5001-0)
33. M. B. Robin, *Higher Excited States of Polyatomic Molecules, Volume II*, Elsevier, New York, 1975 (https://dx.doi.org/10.1016/B978-0-12-589902-4.X5001-1)
34. M. B. Robin, *Higher Excited States of Polyatomic Molecules, Volume III*, Elsevier, Orlando, 1985 (https://dx.doi.org/10.1016/B978-0-12-589903-1.X5001-2).

JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. **00(0)**S1-S1 (2024) *Supplementary material*