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Research Article

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THEORETICAL STUDY OF ELECTRONIC AND STRUCTURAL PROPERTIES OF N-(2-OXO-2H-CHROMEN-3-CARBONYL)CYTISINE

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Abstract. *New compounds based on cytisine and coumarin are of interest to the pharmaceutical industry due to their promising biological activity. This activity, in turn, is closely related to the structure of the compound, which is manifested in its specific electronic properties. This paper presents the results of a theoretical study of the electronic and structural properties of recently synthesized N-(2-oxo-2H-chromen-3-carbonyl)cytisine. The molecular structure of the ground and first excited states is established. Their structural features are considered, taking into account their conformational diversity. The probabilities of vertical electronic transitions, which determine the intensities of bands in the emission spectrum, are calculated. The obtained theoretical results are compared with the measured luminescence spectrum of ethanol solution.*

Keywords: cytisine, coumarin, complex, density functional theory, Ultraviolet–visible spectroscopy, luminescence spectroscopy.

1. Introduction

Coumarin derivatives possess unique electronic properties, primarily manifested in their pronounced, intense luminescence, which allows them to serve as luminescent markers including luminescent probes [1], bioimaging marker [2], specific sensor [3, 4]. Another important feature is the biological activity exhibited by coumarin derivatives. Among other potential applications, the antidiabetic [5], antimicrobial [6,7] anti-inflammatory [8] and activity of a number of coumarin derivatives can be highlighted. The use of molecular hybridization with other biologically active substances opens up prospects for the creation of new compounds, thereby expanding the applications of coumarin derivatives. Of particular interest are compounds containing cytisine, a natural alkaloid with a pronounced affinity for binding to neuronal nicotinic acetylcholine receptors (nAChRs) [9]. This substance is considered an important factor playing a significant role in the study of central nervous system functioning [9]. As has been shown previously (see, for example, [10]), the biological activity of such complexes is closely linked to their molecular structure. Therefore, an important issue is the consideration of the complex's properties, taking into account its possible conformational diversity [9, 11, 12]. The object of study in this work is the recently obtained N-(2-oxo-2H-chromene-3-carbonyl) complex [13]. In previous works [13, 14], its structure and optical properties were investigated both in the crystalline state (vibrational properties, absorption in the UV-visible range) and in

ethanol solution (NMR spectra and absorption in the UV-visible range). At present, the luminescent properties of this compound remain unexplored.

The important reason for choosing luminescence spectra as research objects for the compounds containing a coumarin moiety is the presence of coumarin strong luminescence that is sensitive to its state [15]. This makes these compounds sensitive luminescent markers and probes [16]. This is especially important in drug research, as it allows us to understand, for example, where they accumulate, whether they undergo any reactions, or how they interact with proteins and enzymes. In this case, structure-sensitive luminescence will serve to understand the state of the molecule, i.e., as a state indicator.

In this regard, the present work aims to theoretically study using quantum chemical approach the structure of the molecule in its first excited state, the emission spectrum to the ground state, and compare it with the experimental luminescence spectrum. The results obtained will represent a continuation of the research on this substance, begun in the articles [13, 14], demonstrating novelty in the relevant aspects of the electronic structure of the first excited state of this recently synthesized substance.

2. Materials and methods

2.1. Experimental technique

For the measurements, ethanol solutions of N-(2-oxo-2H-chromene-3-carbonyl) cytisine with a concentration of 10^{-3} M were prepared. The starting material was synthesized according to the work [13]. Emission and luminescence excitation spectra were obtained on a Lumina fluorescence spectrometer (Thermo Fisher Scientific) in reflection geometry. Excitation spectra were recorded in the range of 290-420 nm, and luminescence spectra were recorded in the range of 380-700 nm.

2.2. Theoretical approach

Quantum chemical calculations were performed within the framework of the density functional theory with a hybrid exchange-correlation functional and a long-range dispersion correction wb97XD [17]. A doubly split-valence Pople-type basis set e 6-31G(d,p) [18,19] and the Gaussian G09W Rev. C program [20] were used. The calculation was performed for a single molecule in an ethanol medium. The influence of the medium was taken into account within the framework of the polarizable continuum model [21]. Optimization of the considered molecules was carried out for the ground (S_0) and first excited states (S_1) until the standard criteria were met for the maximum and root mean squared residual forces on atoms and atomic displacements.

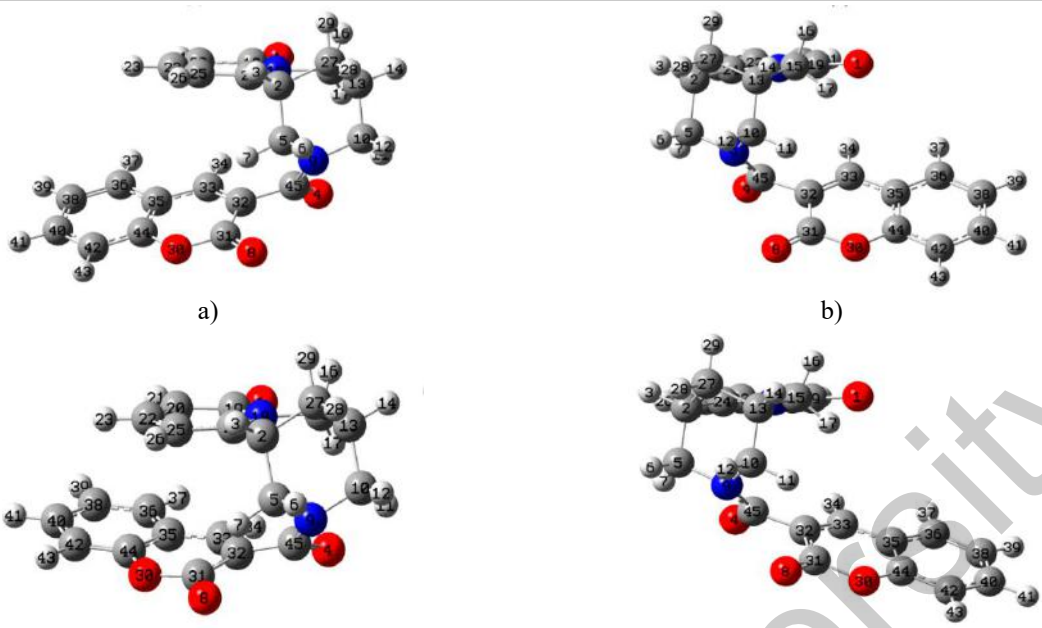
3. Results and discussion

3.1 Structural peculiarities

The molecule of the complex under study consists of three main moieties: the cytisine moiety, the intermediate moiety, and the coumarin moiety. A previous experimental and theoretical study [14] of the conformational states of the complex in solution revealed the presence of four conformer states that can transform into each other via internal rotations. Specifically, it was shown that the two lowest-energy conformers are formed by rotating the cytisine moiety relative to the coumarin and intermediate moieties. The other two conformers can be obtained from these conformers by rotating the coumarin moiety relative to the cytisine and intermediate moieties. The potential energy of the latter two conformers is higher, making them less populated at thermal equilibrium. Therefore, only the two lowest-energy states are considered in this study. Their geometries in the ground (S_0) and 1st excited state (S_1), determined by the method described in section (2.2), are shown in Figure 1.

To designate the two conformational states under consideration, the notations 1 were additionally introduced for the conformer observed in the crystalline state [13] and 2 for another conformer with a similar energy. The total energies of the S_1-1 and S_1-2 states are -1221.057229 and -1221.041763 Hartree, respectively. Thus, the energy of S_1-1 is lower by approximately 9.7 kcal/mol. Moreover, a comparison of the geometries of the ground (S_0-1) and first excited states (S_1-1) revealed a number of differences. Structural parameters that differ significantly in different conformer states are listed in Table 1.

The most significantly difference are as follows. In the S_1-1 state, the cytisine ring bordering the transition region is significantly distorted. This is manifested by longer C2C5 and C13C10 bonds and a shorter C5N9 bond and correlates with shorter O4H11 and O8H7 contacts. Much more significant changes occur in the intermediate moiety and the α-pyrone ring of the coumarin moiety.



a) b)

c) d)

Fig.1. Optimized geometries of S_0-1 (a), S_0-2 (b), S_1-1 (c), and S_1-2 (d) using the wb97XD/6-31G(d,p) method for the case of a single molecule in an ethanol medium, which is taken into account within the framework of the polarizable continuum model.

Table 1. Selected structural parameters for conformers 1 and 2 in ground (S_0) and excited (S_1) states.

Parameter*	Conformer and state			
	S_0-1	S_1-1	S_0-2	S_1-2
C2C5	1.545	1.559	1.546	1.547
C13C10	1.536	1.543	1.536	1.536
C5N9	1.456	1.447	1.456	1.457
C10N9	1.460	1.461	1.458	1.459
N9C45	1.360	1.394	1.358	1.359
C45O4	1.228	1.237	1.227	1.238
C45C32	1.505	1.474	1.507	1.480
C32C31	1.462	1.418	1.462	1.425
C31O8	1.211	1.229	1.211	1.219
C32C33	1.350	1.429	1.349	1.429
C31O30	1.368	1.398	1.367	1.414
O30C44	1.365	1.370	1.366	1.345
C33C35	1.436	1.400	1.438	1.391
O4H11 (O4H7)**	2.292	2.198	2.299	2.286
O8H7 (O8H11)**	2.262	2.031	2.960	2.505
C10N9C45	119.06	116.04	124.71	123.93
C9N45O4	123.04	118.44	123.39	122.55
C45C32C31	120.48	126.44	117.93	121.28
C32C31O8	125.59	128.97	125.19	128.45
C10N9C45O4	5.92	19.14	-168.70	-161.21
N9C45C32C31	-62.26	-44.93	74.58	55.24
C45C32C31O30	-178.93	172.54	175.01	173.40
C32C31O30C44	-1.03	-2.61	1.65	3.86
C33C32C31O30	-2.78	-9.96	-0.25	4.01
C44C35C33C32	-2.68	-6.09	1.99	6.61

* for two atoms, the bond length is given in Å, for three atoms, the planar angle is given in degrees (°), for four atoms, the dihedral angle is given in degrees (°).

** in some cases, similar structural parameters for S0-2 and S1-2 are given in brackets.

A rotation of the coumarin moiety's ring plane relative to the cytisine moiety's ring plane takes place due to the flexible intermediate moiety. In the S_1-1 state, a more negative charge is observed on the N9 and O4 atoms, which correlates with the longer C45N9 and C45O4 bonds and with an increase in the C10N9C45O4 dihedral angle. At the same time, a rotation of the coumarin moiety leads to a decrease in the O8H7 contact length. This is manifested by the larger absolute value of the dihedral angle N9C45C32C31. For the S_1-1 state, a greater deviation of the α-pyrone ring from planar geometry is observed. This is manifested by a greater deviation of the dihedral angles C45C32C31O30, C32C31O30C44, C33C32C31O30, and C44C35C33C32 from 180° or 0° in S_1-1. This ring contains longer oxygen-carbon bonds (C44-O30, O30-C31, and C31=O8).

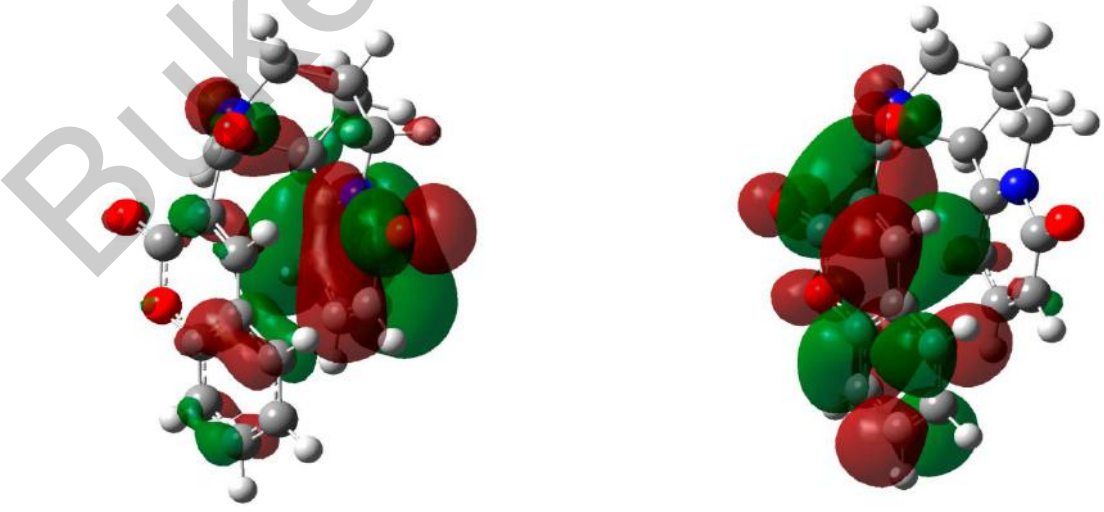
When comparing the optimized geometries of S_0-2 and S_1-2, a number of the following features can be noted. In the cytisine moiety, similar structural parameters are observed between S_0-2 and S_1-2, in contrast to S_0-1 and S_1-1. The C45C32 and C45O4 bonds are shorter in S_1-2 compared to S_0-2 while the C45N9 bonds are approximately the same. Just as in S_1-1, S_1-2 has a longer C32C33 bond and a shorter C32C31 bond compared to similar bond lengths in the ground state. In addition, S_1-2 also exhibits a greater deviation from the planar character of the α-pyrone ring in the coumarin moiety. A significant difference of S_1-2 is the longer hydrogen contacts O4H7 and O8H11, which is also manifested in a smaller value of the dihedral angle N9C45C32C31.

3.2 Electronic properties

For the optimized S_1-1 and S_1-2 states, the vertical transition energies and corresponding oscillator strengths were calculated. The longest-wavelength transition is to the ground state, i.e., S_1-1 → S_0-1 and S_1-2 → S_0-2, which is of practical interest in studying luminescence properties.

For the molecule the investigation of molecular orbitals plays the important role in understanding the electronic processes [22]. For S_1-1, the shortest-wavelength transition is the singlet-singlet transition between the 95 → 96 molecular orbitals (the orbital contribution is 98%, see Figure 2a). Its energy difference is 2.9109 eV, which corresponds to a wavelength of 425.93 nm, the oscillator strength is moderate, 0.0769.

For S_1-2, the shortest-wavelength transition is between the 94 → 96 orbitals (the orbital contribution is 96%). Its energy difference is significantly higher, 3.5964 eV, which corresponds to a wavelength of 344.74 nm, and the oscillator strength is 0.509. It should be noted that for S_1-1, a similar higher-energy transition between the same orbitals is also observed (94 → 96, the orbital contribution is 92%). However, its energy difference is significantly higher than 3.7607 eV, corresponding to a wavelength of 329.68 nm, and the oscillator strength is less than 0.3347. As part of this study, an experimental investigation of the luminescence properties of the complex was also conducted. Figure 3 shows the luminescence emission spectrum, which has a maximum at 453 nm (2.7373 eV). The luminescence excitation spectrum for this band was then obtained. The maximum in this spectrum is at 372 nm.



a) b)

Fig.2. View of the 95(HOMO) and 96(LUMO) molecular orbitals for S_1-1.

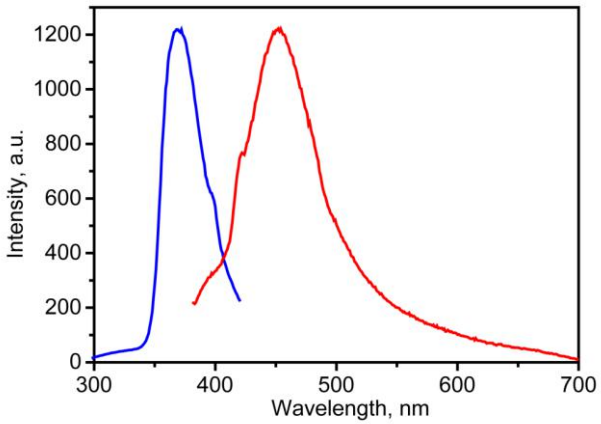


Fig.3. Luminescence emission spectrum at 453 nm (red) and luminescence excitation spectrum at 372 nm (blue).

The obtained theoretical estimates of the wavelength of the singlet-singlet transition from S_1-1 for conformational state 1 show a calculated value (426 nm) quite close to the experimentally observed luminescence maximum (453 nm). Based on this theoretically calculated transition, the radiative (luminescence) rate constant $\mathbf{k_r}$ was estimated according to the Strickler–Berg formula (1), [23]:

$$k_{r,i}(S_i \rightarrow S_0) = 2^{-i/2} f(S_i \rightarrow S_0) E^2(S_i \rightarrow S_0), \quad (1)$$

where i is the excited state number, $f(S_i\text{->}S_0)$ is the transition oscillator strength, $E(S_i \rightarrow S_0)$ is the electron transition energy (in cm^{-1}). For the case under consideration (i=1) the corresponding value $k_r=3\cdot10^7$.

The considered case of molecules corresponds to the case of addition of the intermediate part at atom 3 according to the IUPAC numbering of carbon atoms in the molecule of unsubstituted coumarin [24]. As an example of synthesized compounds with addition through the 3rd atom in the coumarin part, one can cite [25-27]. In these studies, it was noticed the presence of the strong luminescence in the experimental spectrum in the close region 460-480 nm. Nevertheless, it should be noted that the actual emission wavelength is quite sensitive to the structural peculiarities of the molecule as well as pH value or metal cation presence.

4. Conclusion

In this work, density functional theory methods were used to search for and optimize the geometry of the first excited state for two conformations of the N-(2-oxo-2H-chromen-3-carbonyl) cytisine molecule in an ethanol solution. Their energies were calculated. It was found that the first excited state of the conformer corresponding to the crystal structure is the most stable. A structural difference between the ground and first excited states was revealed. The wavelength of the transition from the first excited state to the ground state was calculated. The theoretical estimate of the luminescence maximum in the spectrum of the most stable conformer was 426 nm versus the value of 453 nm established experimentally. In addition, the radiation rate constant $k_r = 3\cdot10^7$ was estimated. An interpretation of this electronic transition is proposed based on an analysis of the molecular orbitals involved.

Conflict of interest statement

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

CRediT author statement

Turdybekov D.M.: Validation, Formal Analysis, Visualization, Supervision, Writing – Review & Editing; **Ibrayev N.Kh.:** Conceptualization, Investigation, Resources, Data Curation; **Kopbalina K.B.:** Conceptualization, Methodology, Software, Formal Analysis, Data Curation, Writing – Original Draft; **Kishkentayeva A.S.:** Validation, Investigation, Writing – Original Draft, Writing – Review & Editing;

Pankin D.V.: Conceptualization, Methodology, Software, Formal Analysis, Data Curation, Writing – Original Draft; **Smirnov M.B.:** Methodology, Software, Writing – Review & Editing.
The final manuscript was read and approved by all authors.

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References

1. Tian G., Zhang Z., Li H., Li D., Wang X., Qin C. (2020) Design, Synthesis and Application in Analytical Chemistry of Photo-Sensitive Probes Based on Coumarin. *Critical Reviews in Analytical Chemistry*, 51, 565–581. https://doi.org/10.1080/10408347.2020.1753163
2. Wang L., Li W., Zhi W., Ye D., Wang Y., Ni L., Bao X. (2017) A Rapid-Responsive Fluorescent Probe Based on Coumarin for Selective Sensing of Sulfite in Aqueous Solution and Its Bioimaging by Turn-on Fluorescence Signal. *Dyes and Pigments*, 147, 357–363. https://doi.org/10.1016/j.dyepig.2017.07.021
3. Li J., Zhang C.-F., Yang S.-H., Yang W.-C., Yang G.-F. (2014) A Coumarin-Based Fluorescent Probe for Selective and Sensitive Detection of Thiophenols and Its Application. *Analytical Chemistry*, 86, 3037–3042. https://doi.org/10.1021/ac403885n
4. Ray D., Bharadwaj P.K. (2008) A Coumarin-Derived Fluorescence Probe Selective for Magnesium. *Inorganic Chemistry*, 47, 2252–2254. https://doi.org/10.1021/ic702388z
5. Kenchappa R., Bodke Y.D., Chandrashekar A., Aruna Sindhe M., Peethambar S.K. (2017) Synthesis of Coumarin Derivatives Containing Pyrazole and Indenone Rings as Potent Antioxidant and Antihyperglycemic Agents. *Arabian Journal of Chemistry*, 10, S3895–S3906. https://doi.org/10.1016/j.arabjc.2014.05.029
6. Annunziata F., Pinna C., Dallavalle S., Tamborini L., Pinto A. (2020) An Overview of Coumarin as a Versatile and Readily Accessible Scaffold with Broad-Ranging Biological Activities. *International Journal of Molecular Sciences*, 21, 4618. https://doi.org/10.3390/ijms21134618
7. Alam M., Alam M.J., Azaz S., Parveen M., Park S., Ahmad S. (2018) DFT/TD-DFT Calculations, Spectroscopic Characterizations (FTIR, NMR, UV–Vis), Molecular Docking and Enzyme Inhibition Study of 7-Benzoyloxycoumarin. *Computational Biology and Chemistry*, 73, 65–78. https://doi.org/10.1016/j.compbiolchem.2018.01.007
8. Srikrishna D., Godugu C., Dubey P.K. (2018) A Review on Pharmacological Properties of Coumarins. *Mini-Reviews in Medicinal Chemistry*, 18, 113–141. https://doi.org/10.2174/1389557516666160801094919
9. Przybył A.K., Maj E., Wietrzyk J., Kubicki M. (2019) Spectroscopic, Structural and Anticancer Activity Studies of (−)-Cytisine Halogenated N-Benzyl Derivatives. *Journal of Molecular Structure*, 1176, 871–880. https://doi.org/10.1016/j.molstruc.2018.09.029
10. Pankin D. (2021) Laser-Induced Twisting of Phosphorus Functionalized Thiazolotriazole as a Way of Cholinesterase Activity Change. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 246, 118979. https://doi.org/10.1016/j.saa.2020.118979
11. Kopbalina K.B., Makhmutova A.S., Turdybekov D.M., Turdybekov K.M., Tolenova G.K. (2025) Quantum-Chemical Study of the Structure and Properties of Molecule of the Lupinine Alkaloid Derivative. *Bulletin of the Karaganda University. Physics Series*, 105(1), 14–22. https://doi.org/10.31489/2023No4/33-38
12. He L., Xu Q., Liu Y., Wei H., Tang Y., Lin W. (2015) Coumarin-Based Turn-On Fluorescence Probe for Specific Detection of Glutathione over Cysteine and Homocysteine. *ACS Applied Materials & Interfaces*, 7, 12809–12813. https://doi.org/10.1021/acsami.5b01934
13. Kishkentayeva A., Kopbalina K., Shaimerdenova Z., Shults E., Gatilov Y., Pankin D., Smirnov M., Povolotckaia A., Turdybekov D., Mazhenov N. (2025) Investigation of N-(2-oxo-2H-chromen-3-carbonyl)cytisine's Crystal Structure and Optical Properties. *Materials*, 18, 3153. https://doi.org/10.3390/ma18133153
14. Kopbalina K., Adekenova A., Shaimerdenova Zh., Kairatova Zh., Shakarimova K., Pankin D., Smirnov M., Kishkentayeva A., Artykbayeva M., Jalmakhanbetova R. (2025) Investigation of N-(2-oxo-2H-chromen-3-carbonyl)cytisine's Molecular Structure in Solution. *Molecules*, 30(20), 4139. https://doi.org/10.3390/molecules30204139

15. Gawad S.A.A., Sakr M.A.S. (2022) Spectroscopic Investigation, DFT and TD-DFT Calculations of 7-(Diethylamino) Coumarin (C466) *J. Mol. Struct.* 1248, 131413. https://doi.org/10.1016/j.molstruc.2021.131413

16. Tian G., Zhang Z., Li H., Li D., Wang X., Qin C. (2020) Design, Synthesis and Application in Analytical Chemistry of Photo-Sensitive Probes Based on Coumarin. *Crit. Rev. Anal. Chem.* 51, 565–581. https://doi.org/10.1080/10408347.2020.1753163

17. Chai J., Head-Gordon M. (2008) Long-Range Corrected Hybrid Density Functionals with Damped Atom–Atom Dispersion Corrections. *Physical Chemistry Chemical Physics*, 10, 6615–6620. https://doi.org/10.1039/b810189b

18. Ditchfield R., Hehre W.J., Pople J.A. (1971) Self-Consistent Molecular Orbital Methods. 9. Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules. *Journal of Chemical Physics*, 54, 724. https://doi.org/10.1063/1.1674902

19. Hehre W.J., Ditchfield R., Pople J.A. (1972) Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular-Orbital Studies of Organic Molecules. *Journal of Chemical Physics*, 56, 2257. https://doi.org//10.1063/1.1677527

20. Frisch M.J., Trucks G.W., Schlegel H.B., Scuseria G.E., Robb M.A., Cheeseman J.R., Scalmani G., Barone V., Mennucci B., Petersson G.A., et al. (2013) *Gaussian 09, Revision D.01*. Gaussian, Inc., Wallingford CT. Available at: https://www.scirp.org/reference/referencespapers?referenceid=2418053

21. Tomasi J., Mennucci B., Cammi R. (2005) Quantum Mechanical Continuum Solvation Models. *Chemical Reviews*, 105, 2999–3093. https://doi.org/10.1021/cr9904009

22. Kopbalina K.B., Makhmutova A.S., Turdybekov D.M., Turdybekov K.M., Tolenova G.K. (2024) Quantum-Chemical Study of the Structure and Properties of Molecule of the Lupinine Alkaloid Derivative. *Eurasian Physical Technical Journal,* 4(46), 33-38. https://doi.org/10.31489/2023No4/33-38

23. Ibrayev N.Kh., Valiev R.R., Seliverstova E.V., Menshova E.P., Nasibullin R.T., Sundholm D. (2024) Molecular phosphorescence enhancement by the plasmon field of metal nanoparticles. *Physical Chemistry Chemical Physics*, 26, 14624-1436. https://doi.org/10.1039/d4cp01281j

24. Sun X.Y., Liu T., Sun J., Wang X.J. (2020). Synthesis and application of coumarin fluorescence probes. *RSC advances*, 10(18), 10826-10847. https://doi.org/10.1039/C9RA10290F

25. Xu Y., Jiang Z., Xiao Y., Bi F.Z., Miao J.Y., Zhao B.X. (2014). A new fluorescent pH probe for extremely acidic conditions. *Analytica chimica acta*, 820, 146-151. https://doi.org/10.1016/j.aca.2014.02.029

26. Chen Y., Clouthier C.M., Tsao K., Strmiskova M., Lachance H., Keillor J.W. (2014). Coumarin-Based Fluorogenic Probes for No-Wash Protein Labeling, *Angew. Chem. Int. Ed.*, 53, 13785–13788. https://doi.org/10.1002/anie.201408015

27. You Q.H., Lee A.W.M., Chan W.H., Zhu X.M., Leung K.C.F. (2014). A coumarin-based fluorescent probe for recognition of Cu 2+ and fast detection of histidine in hard-to-transfect cells by a sensing ensemble approach. *Chemical Communications*, 50(47), 6207-6210. https://doi.org/10.1039/C4CC00521J

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