QUANTUM–CHEMICAL STUDY OF SOME TRIS(PYRROLO)BENZENES AND TRIS(PYRROLO)-1,3,5-TRIAZINES

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Russian Supercomputing Days 2023

Development of high-energy components of rocket fuels in FRC PCP MC RAS

- FRC PCP MC RAS in collaboration with other RAS institutes for more than 60 years has been developing high-energy substances.
- In recent years more attention is paid to quantum calculations of physical and chemical properties (Gaussian).
- Computer design of substances not yet synthesized.

High-energy density materials (HEDM)

military affairs

mineral exploration

rocket and space technology

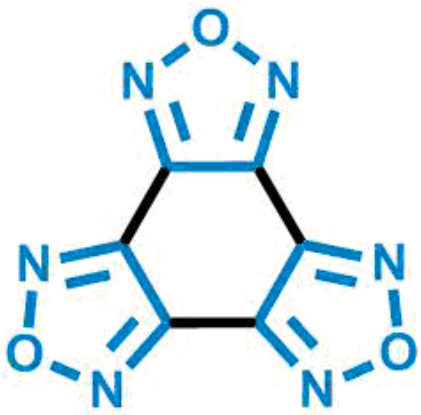
construction

metallurgy

mining

Enthalpy of formation

$$\Delta_f H^0_{298}$$



Quantum-chemical ab initio calculations

Stationary Schrödinger Equation

$$\hat{H}(\vec{r},\vec{R})\psi(\vec{r},\vec{R}) = E\psi(\vec{r},\vec{R})$$

Hamiltonian of a polyatomic molecule

$$\hat{H} = \sum_i \hat{T}_i + \sum_\alpha \hat{T}_\alpha + \sum_{i>k} V_{ik} + \sum_{i,\alpha} V_{i\alpha} + \sum_{\alpha>\beta} V_{\alpha\beta} + V_{so}$$

Electronic and nuclear kinetic energies

Electronic and nuclear Coulomb interaction energies

Spin-orbital interaction

Approximations of ab initio calculations

- Adiabatic approximation - the kinetic energy of nuclei is neglected
- Self-consistent field - the electron moves in the effective field of the remaining electrons
- Rectification of the electron correlation

Quantum-chemical calculation methods

GAUSSIAN 09

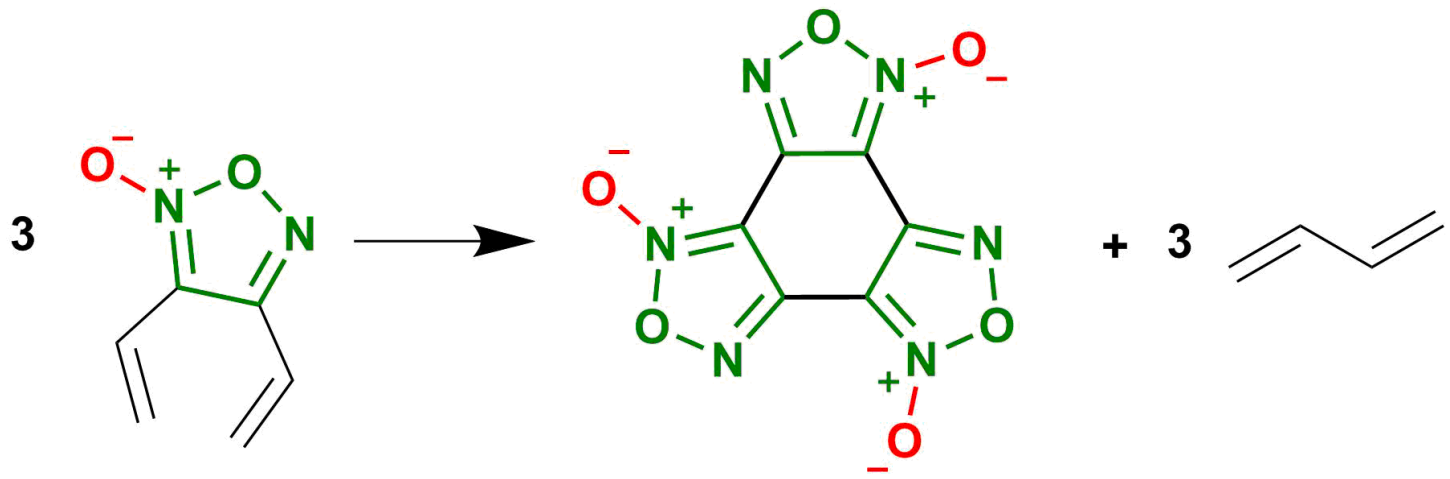
- DFT/B3LYP with the 6-311G+(2d,p) basis
- G4(MP2)
- G4

Calculating the enthalpy of formation

The atomization reaction

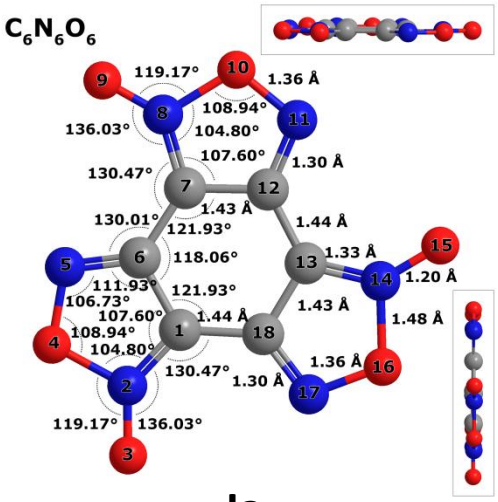
$$\Delta H_f: wC(g) + xH(g) + yN(g) + zO(g) = C_wH_xN_yO_z(g)$$

The reaction scheme

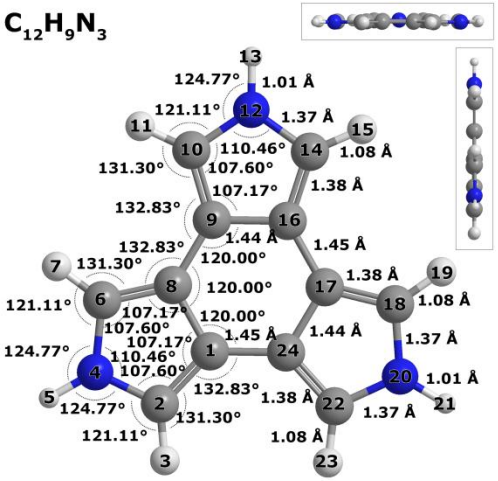


Optimized geometry

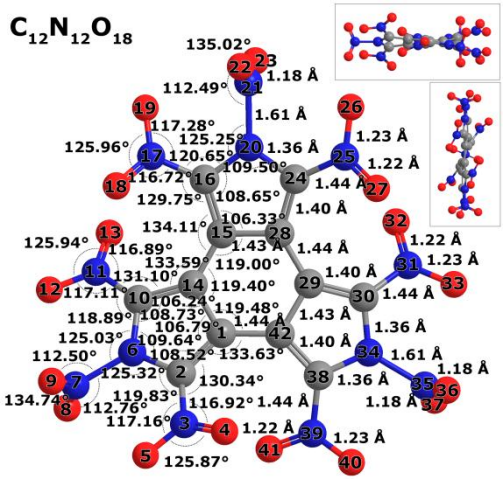
Calculation level: **B3LYP/6-311+G(2d,p)**



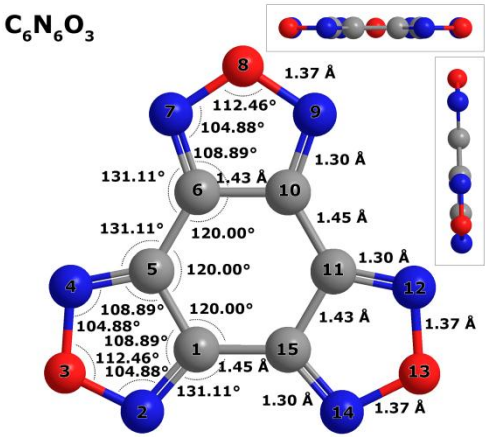
Ia



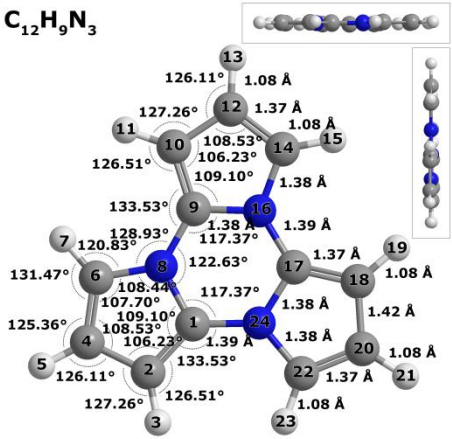
IIa



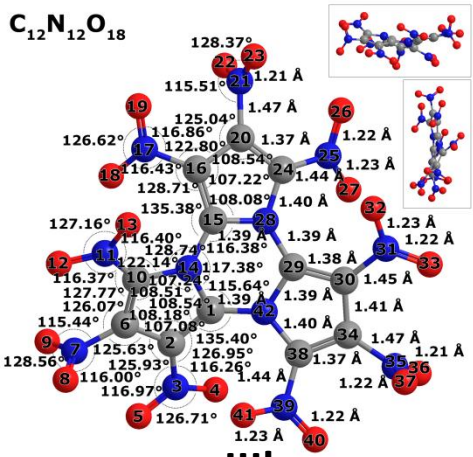
IIIa



Ib

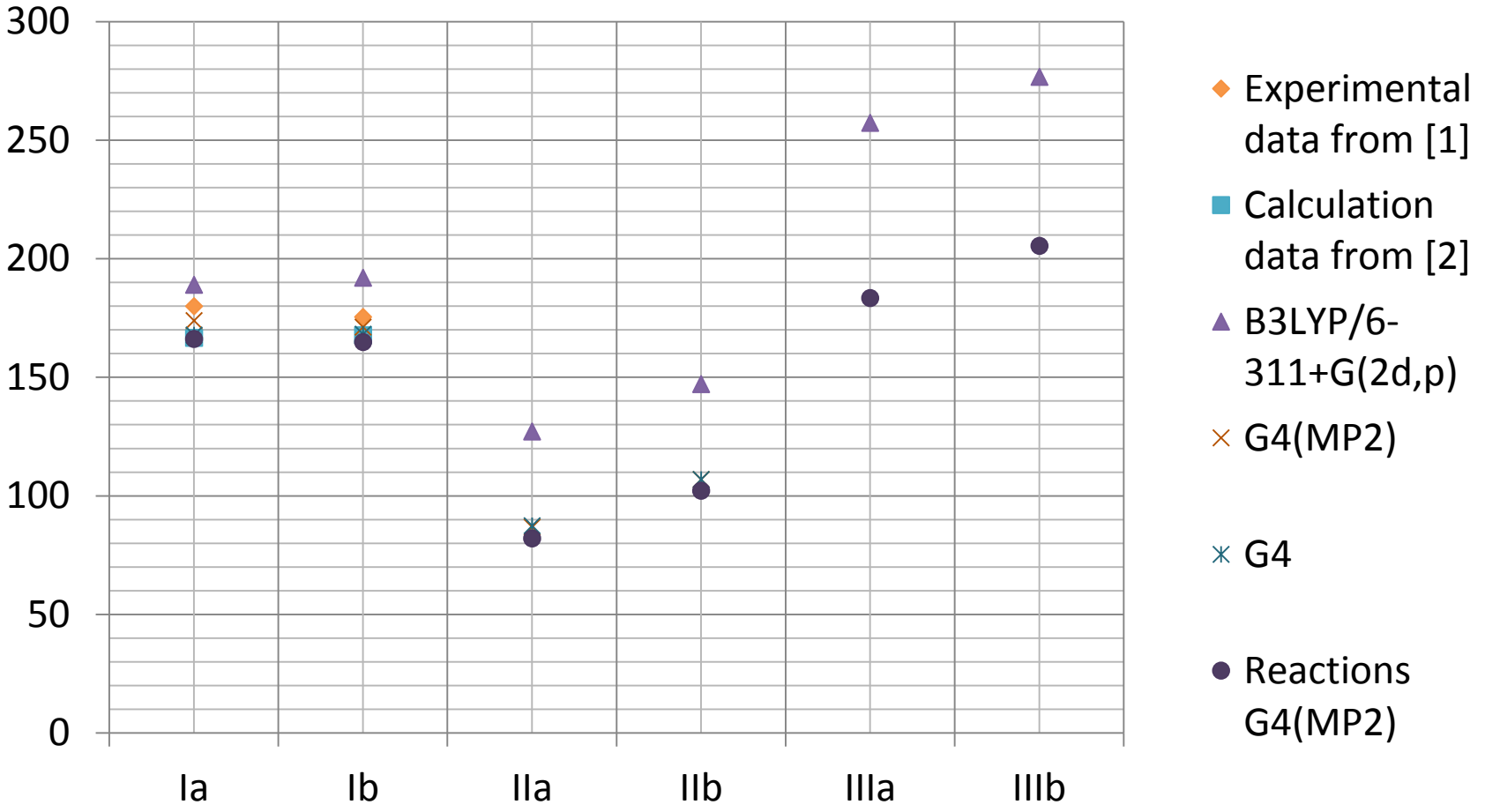


IIb



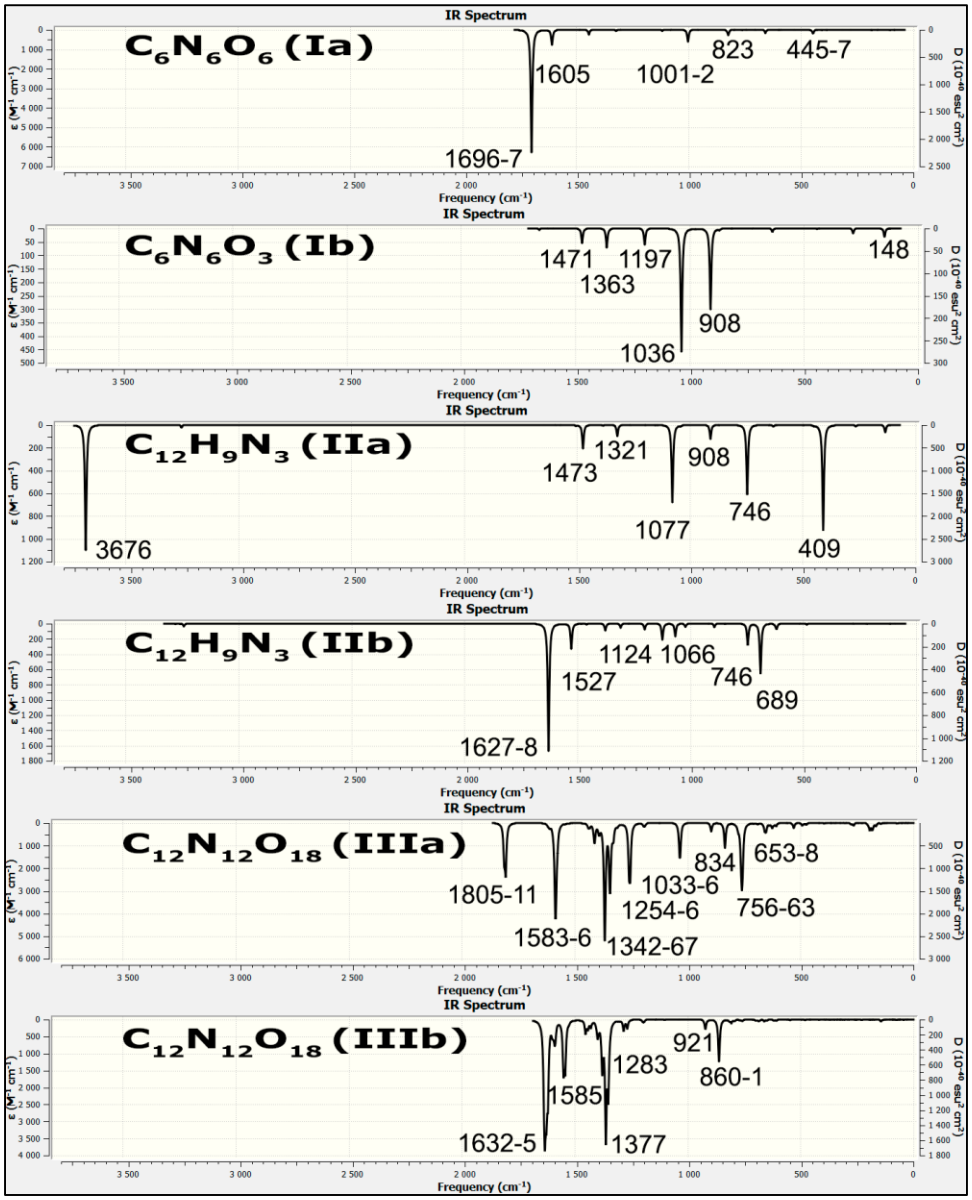
IIIb

Enthalpy of formation

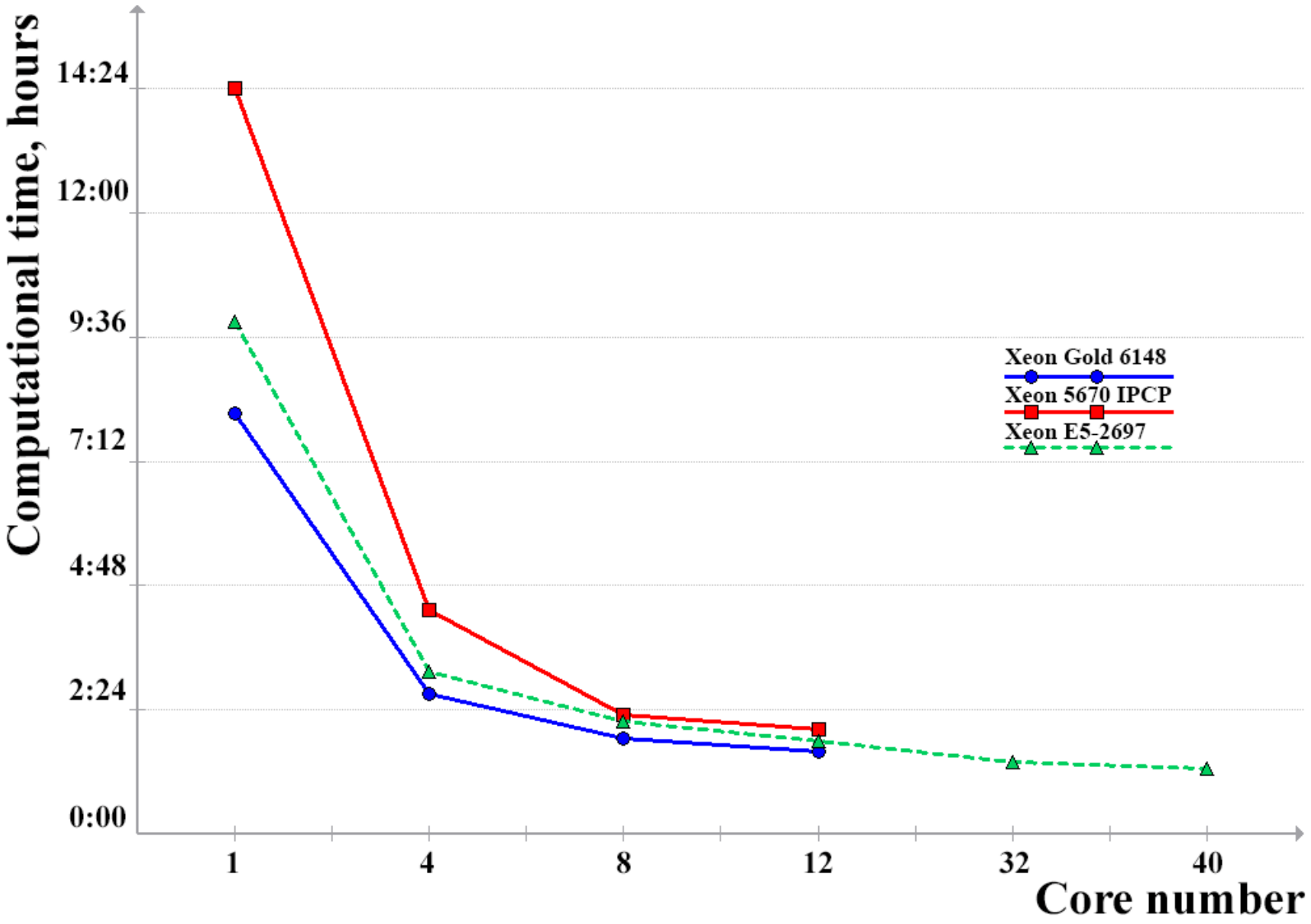


[1] Matyushin, Yu.N., Lebedev, V.P., Chironov, V.V., Pepekin, V.I.: Energy of the NO bond in benzofuroxanes. Khimicheskaya zika, 21, pp. 58{61 (2002) (in Russian).
[2] Suntsova, M.A.: Forecasting the enthalpies of formation new nitrogen-containing high-energy compounds based on quantum-chemical calculations. Candidate's Dissertation in Chemistry, Moscow (2016) (in Russian).

The IR absorption spectra



Computational details



Calculation time (CPU*hours)

	B3LYP	G4(MP2)	G4	Reaction
Ia	11	109	658	23*
Ib	6	42	170	17*
IIa	10	68	136*	22*
IIb	13	71	152	25*
IIIa	506			637*
IIIb	547			674*

Conclusions

- Geometric and thermochemical parameters of a number of tetracyclic compounds have been obtained by ab initio quantum-chemical methods (Gaussian 09).
- For known substances, the results of our calculations showed a slight deviation (within 4%) from the literature data, and for new, not yet synthesized pyrrole-annelated tetracycles, the data were obtained for the first time.
- The dependence of the enthalpy of formation on the structure of the compounds has been established.
- This work is the first stage of a systematic study of the energy potential of a wide series of tetracycles.

The work was performed using the equipment of the Center for Collective Use of Super High-Performance Computing Resources of the Lomonosov Moscow State University.

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THANK YOU FOR THE ATTENTION!