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	α-Napthalene sulfonamide, β-Napthalene sulfonamide, 1,5-Napthalene disulfonylchloride, b-Naphthalene sulphonylchloride, a-Naphthalene sulphonylchloride IR spectrum *N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, V. N. Petrova* *Manuscript in progress*
$C_{28}H_{28}N_4Ni$ $NiN_4C_{28}H_{28}$	**Nickel octamethylporphirin** Structure by GED/MS and QC *Alexander E. Pogonin , Arseniy A. Otlyotov, Yury Minenkov, Alexander S. Semeikin, Yuriy A. Zhabanov, Sergey A. Shlykov, Georgiy V. Girichev,* https://doi.org/10.3390/ijms23010320
$C_{32}H_{36}N_4Ni$ $NiN_4C_{32}H_{36}$	**Nickel-etioporphyrin-II** Structure by GED/MS and QC *G.V. Girichev, A.E. Pogonin, N.V. Tverdova, N.I.Giricheva* *Manuscript in preparation*
$C_{14}H_{10}$ $C_{14}H_{10}$	**Anthracene** Structure by GED/MS and QC *N. W. Mitzel, Yu. Vishnevskiy, N.V. Tverdova, A.A. Otlyotov, N.I. Giricheva, G. V. Girichev* *Manuscript in preparation*
$C_{14}H_{14}O_2$	**1,2-Diphenoxyethane** Structure by GED/MS and QC

Ph-OCH_2CH_2O-Ph	*J.-H. Weddeling, T. Glodde, I. Yu. Kurochkin, A.A. Otlyotov, N.W. Mitzel, G.V. Girichev* *Manuscript in preparation*
$C_{14}H_9F_5O_2$ Ph-OCH_2CH_2O-Ph_f	**1-Phenoxy-2-pentafluorophenoxy-ethane** Structure by GED/MS and QC *J.-H. Weddeling, T. Glodde, I. Yu. Kurochkin, A.A. Otlyotov, N.W. Mitzel, G.V. Girichev* *Manuscript in preparation*
$C_{10}H_{18}Si_2$ $(CH_3)_3Si$-C-C≡C-C-$Si(CH_3)_3$	**1,4-Bis(trimethylsilyl)-1,3-butadiyne** Structure by GED/MS and QC *A.A. Otlyotov, Yu.V. Vishnevskiy, J.-H. Lamm, H.-G. Stammler, N.W. Mitzel, G.V. Girichev* *Manuscript in preparation*
$C_{12}H_{10}$ $C_{12}H_{10}$	**Acenaphthene** Structure by GED/MS and QC *A.A. Otlyotov, Yu.V. Vishnevskiy, J.-H. Lamm, H.-G. Stammler, N.W. Mitzel, G.V. Girichev* *Manuscript in preparation*
$C_{30}H_{54}Co_4O_{13}$ $Co_4O(OOCCMe_3)_6$	**Cobalt oxopivalate** Structure by GED/MS and QC calculations *A.S.Alikhanyan, G.V. Girichev, N.I. Giricheva, E.A. Morozova, V.V. Sliznev* *Manuscript in preparation*
$C_4H_{14}OSi_3$ $C_3Si_3(OCH)_3H_{11}$	**1-Methoxy-1,3,5-trisilacyclohexane** Structure by GED/MS and QC *S.A. Shlykov, I. Arnason, L.E. Kuzmina* *Refinement in progress*
$C_4H_{14}Si_3$ $C_3Si_3(CH)_3H_{11}$	**1-methyl-1,3,5-trisilacyclohexane** Structure by GED/MS and QC *S.A. Shlykov, I. Arnason, L.E. Kuzmina* *Refinement in progress*
F_5Mo MoF_5	**Molibdenum pentafluoride** Structure by GED/MS QC calculations *V.V.Sliznev, O.A.Pimenov, G.V.Girichev* *J. Mol. Struct., 1199, 2020, p.126884*
	5,10,15,20-Tetraphenyl-21-thia-porphyrin **5,10,15,20-tetraphenyl-21,23-dithia-porphyrin** Electronic absorption spectra and QC calculation *S.G. Pukhovskaya, I.A. Kuzmin, S.A. Shlykov, O.A. Pimenov* *Manuscript in preparation*
	5,10,15,20-Tetraphenyl-21-oxa-porphyrin, **5,10,15,20-tetraphenyl-21-thia-porphyrin,** **5,10,15,20-tetraphenyl-21,23-dithia-porphyrin** Thermodynamic and enthalpy of sublimation by MS *I.A. Kuzmin, S.A. Shlykov, A.V.Krasnov* *Refinement in progress*
$C_{44}N_3H_{29}S$ SPh_4porphyrin	**5,10,15,20-Tetraphenyl-21-thia-porphyrin** Structure by GED/MS and QC calculations *I.A. Kuzmin, S.A. Shlykov* *Refinement in progress*
$C_{44}N_4H_{26}Cl_4$ $4C_6H_4Cl$ - H_2P	**5,10,15,20-Tetrakis(4'chlorinophenyl)porphyrin** Structure by GED/MS and QC calculations, Enthalpy of sublimation by MS *Pogonin A.E., Kurochkin I.Yu., Otlyotov A.A., Kiselev A.N., Shlykov S.A., Girichev G.V.*

	Manuscript in preparation
$C_{44}N_4H_{26}Br_4$ $4C_6H_4Br - H_2P$	**5,10,15,20-Tetrakis(4'-brominophenyl)porphyrin** Structure by GED/MS and QC calculations, Enthalpy of sublimation by MS *Pogonin A.E., Kurochkin I.Yu., Otlyotov A.A., Kiselev A.N., Shlykov S.A., Girichev G.V.* *Manuscript in preparation*
	Ca(II), Ni(II) and Zn(II) with hemi- and dicarbahemiporphyrazine Structure and electronic absorption spectra by QC calculations *Alexey V. Eroshin, Arseniy A. Otlyotov, Yuriy A. Zhabanov, Vladimir V. Veretennikov, Mikhail K. Islyaikin* *Macroheterocycles, 2021 14(2) 119-129*
$C_7H_{15}NO_3Si$ $C_7H_{15}NO_3Si$	**1-Methylsilatrane** Structure by GED and QC calculations *E.F. Belogolova, S.A. Shlykov, A.V. Eroshin, E. P. Doronina, V. F. Sidorkin* *Phys. Chem. Chem. Phys., 2021,23, 2762-2774* *https://doi.org/10.1039/D0CP05872F*
$C_6H_{12}NO_3SiCl$ $C_6H_{12}NO_3SiCl$	**1-Chlorosilatrane** Structure by QC calculations *S.A. Shlykov, A.V. Eroshin* *Manuscript in progress*
$C_{11}H_{13}NO$ $O{=}C_5H_8NC_6H_5$	**1-Phenyl-piperidin-4-one** Structure by GED and QC calculations *A.V. Eroshin, S.A. Shlykov* *GED experiment performed, refinement in progress*
$C_{15}H_{21}O_6Sc$ $ScC_{15}H_{21}O_6$	**Tris-acetylacetonate scandium** Structure by GED/MS and QC calculations *N.I.Giricheva, N.V.Tverdova, S.A.Shlykov, G.V.Girichev* *Manuscript is ready*
$C_{10}H_{14}O_4Sc$ $ScC_{10}H_{14}O_4$	**bis-acetylacetonate scandium** Structure by GED/MS and QC calculations *N.I.Giricheva, N.V.Tverdova, S.A.Shlykov, G.V.Girichev* *Manuscript is ready*
	4- (4-tritylphenoxy) phthalonitrile Structure by QC calculations *N.V.Tverdova, N.I.Giricheva, V.E.Maizlish, N.E.Galanin, G.V.Girichev* *journal Macroheterocycles (accepted)*
$C_{44}H_{28}N_4Pt$ $C_{44}H_{28}N_4Pt(II)$	**5,10,15,20-Tetraphenylporphyrinato platinum(II)** Structure by GED/MS and QC calculations *I.Yu.Kurochkin, N.V.Tverdova, N.I.Giricheva, V.A.Olshevskaya, A.V. Zaitsev, N.W.Mitzel, G.V.Girichev* *Manuscript in preparation*
$C_{44}H_8N_4F_{20}Pt$ $C_{44}H_8N_4F_{20}Pt(II)$	**5,10,15,20-Perfluoroteraphenylporphyrinato platinum(II)** Structure by GED/MS and QC calculations *I.Yu.Kurochkin, N.V.Tverdova, N.I.Giricheva, V.A.Olshevskaya, A.V. Zaitsev, N.W.Mitzel, G.V.Girichev* *Manuscript in preparation*
	5,10,15,20-Tetraphenylporphyrinato platinum(II), **5,10,15,20-perfluoroteraphenylporphyrinato platinum(II),** **5,10,15,20-teraphenylporphyrin** IR spectrum *Ivan Yu. Kurochkin, Valentina A. Olshevskaya, Andrei V. Zaitsev, Nina I. Giricheva, Georgy G. Girichev* *journal Macroheterocycles (accepted)*

	4-*n* -Propyloxycinnamic, 4-n-propyloxybenzoic, 4-n-propylbenzoic carboxylic acids Structural and dynamic non-rigidity of hydrogen-bonded complexes of A···A and A···B···A types and odd–even effect *N.I. Giricheva, K.E. Bubnova, Yu.A. Zhabanov, M.S. Fedorov, G.V. Girichev* *Journal of Molecular Liquids 350 (2022) 118521*
	Ultrafast electron microscopy - instrument of XXI century *S.A.Aseev, B.N.Mironov, E.A.Ryabov, A.S.Avilov. G.V.Girichev. A.A.Ischenko* *Crystallography (Rus.) 2021, V. 66, N4, P. 509–527*
LaI_3 LaI_3	**Lanthanun triiodide** Structure by GED/MS and QC *Valery V. Sliznev, Sergey V. Smorodin, Nina I. Giricheva, Georgiy V. Girichev* *Journal of Molecular Structure 1251 (2022) 132048*
	Structural aspects of trans-cis isomerisation of azobenzene, 4-4'-azopyridine and azoxybenzene *N.I.Giricheva, I.S.Lebedev, M.F.Fedorov, K.E. Bubnova. G.V.Girichev* *J.Struct. Chem. 2021, 62(12) p. 2096-2107*
	New supramolecular hydrogen-bonded liquid crystals based on 4-alkylbenzenesulfonic acids and 4-pyridyl 4′-alkyloxybenzoates: quantum chemical modeling and mesomorphic properties *Fedorov M.S., Giricheva N.I., Syrbu S.A., Belova E.A., Filippov I.A., Kiselev M.R.* *Journal of Molecular Structure. 2021. V. 1244. 130890.* *DOI 10.1016/j.molstruc.2021.130890*
	Influence of structural features of azo-, azoxy-, azodioxy pyridins on mesomorphic properties of system on their base *N.I.Giricheva, I.S. Lebedev, M.F.Fedorov* *Liquid Crystals and their Application. 2021. Vol. 21, № 4. P. 19–28*
	The study of interaction of sodium dodecylsulphate with L-triptophan by densitometry of QC modeling *M.S.Kurbatova, G.N.Tarasova, E.Yu.Tynina, N.I.Giricheva* *Rus. J. Phys. Chem., 2021, Vol. 95, No. 8, pp. 1216–1224* *DOI: 10.1134/S0036024421080161*
	Derivatives of phthalocyaini and porphyrine of A3B-type: Qc modeling of dimeres *A.I.Smirnova, N.I.Giricheva, K.M.Soldatova, A.D.Ezhov, E.G.Glikhovskiy, N.V.Usoltseva* *Liq. Cryst. and their Appl., 2021, 21 (1), 71–81* *DOI: 10.18083/LCAppl.2021.1.71*
	Quantum-chemical modeling of interaction of balenine with dodecylsulpfate sodium dimer as a fragment of anionic micella. *V.P.Barannikov, M.S.Kurbatova, N.I.Giricheva* *Journal of Structural Chemistry, 2021, T. 62, №2, C. 209-218*
	4-Methyl-pyridine-N-oxide, 4-nitro-pyridine-N-oxide 4-metoxy-pyridine-N-oxide, 2-methyl-4-nitro-pyridine-N-oxide 3-methyl-4-nitro-pyridine-N-oxide Enthalpy of sublimation by MS

	N.V. Belova, N.I. Giricheva, Y.A. Zhabanov, V.P.Andreev, G.V. Girichev *Russian Journal of General Chemistry, V.91, N10, 2021, p.1932-1937*
	Amine-N-oxide, Phosphin-P-oxide, Tricloro-amine-N-oxide, Tricloro-phosphin-P-oxide, Trifluoro-amine-N-oxide, Trifluoro-phosphin-P-oxide, Pyridine, Phosphorine, Pyridine-N-oxide, Phosphorin 1-oxide, 4-Methylpyridine-N-oxide, 4-Methyl-phosphorin-1-oxide, 4-Nitropyridine-N-oxide, 4-Nitrophosphorin 1-oxide, 3-Methylpyridine-N-oxide, 2-Methylpyridine-N-oxide, 3-Nitropyridine-N-oxide, 2-Nitropyridine-N-oxide, 4-Methoxypyridine- N-oxide, Pyridine-N-oxide-bortrifluorid, 3-Methyl-4-nitropyridine-N-Oxide, 2-Methyl-4-nitropyridine-N-Oxide, 2,6-Dimethyl-4-nitro-pyridine-N-Oxide, 4-Chloropyridine-N-Oxide Structure and electron density distribution analysis by QC calculations *N.V.Belova, V.V.Sliznev, H.Oberhammer* *Journal of Molecular Structure 1255 (2022) 132409,* *https://doi.org/10.1016/j.molstruc.2022.132409*
	Copper trithiadodecaazahexaphyrin **Nickel trithiadodecaazahexaphyrin** Structure and electron density analysis by QC calculations *Dmitry I. Nazarov, Mikhail K. Islyaikin, Evgenii N. Ivanov, Oskar I. Koifman, Mikhail S. Batov, Leokadiya V. Zorina, Salavat S. Khasanov, Alexander F. Shestakov, Evgeniya I. Yudanova, Yuriy A. Zhabanov, Dmitriy A. Vyalkin, Akihiro Otsuka, Hideki Yamochi, Hiroshi Kitagawa, Tomas Torres, and Dmitri V. Konarev* *Inorg. Chem. https://doi.org/10.1021/acs.inorgchem.1c01132*
	Tetra-3-(4-cyclohexylphenoxy)phthalocyanines zinc tetra-4-(4-cyclohexylphenoxy)phthalocyanines aluminum Structure and electron density analysis by QC calculations *Yuriy A. Zhabanov, Dmitriy A. Vyalkin, Tatiyana V. Tikhomirova, Kristina K. Kazaryan* *Manuscript in preparation*
	Tetrabenzoporphyrin and its metal complexes with Zn, Cd, Al, Ga, In Structure and electron density analysis by DFT calculations *Alexey V. Eroshin, Arseniy A. Otlyotov, Ilya A. Kuzmin, Pavel A. Stuzhin and Yuriy A. Zhabanov* *Manuscript in preparation*
	Tetra(1,2,5-thiadiazolo)porphyrazines yttrium(III) and lutetium(III) Structure and electronic absorption spectra by QC calculations *Ekaterina A. Tarakanova, Mahmoud Hamdoush, Alexey V. Eroshin, Igor V. Ryzhov, Yuriy A. Zhabanov, Pavel A Stuzhin* *Polyhedron - 2021, 193(1), 114877*
	Y, La and Lu complexes with porphyrazine and tetrakis(1,2,5-thiadiazole)porphyrazine Structure and electronic absorption spectra by QC calculations *Yuriy A. Zhabanov, Igor V. Ryzhov, Ilya A. Kuzmin, Alexey V. Eroshin and Pavel A. Stuzhin* *Molecules 2021, 26(1)* *113 https://doi.org/10.3390/molecules26010113*
	Metal-free and nickel complex of tetrakis(1,2,5-thiadiazolo)porphyrazine MS, structure and spectral characteristics by QC calculations *Zhabanov, Y.A.; Eroshin, A.V.; Ryzhov, I.V.; Kuzmin, I.A.; Finogenov, D.N.; Stuzhin, P.A.*

	Molecules 2021, 26, 2945 *https://doi.org/10.3390/molecules26102945*
	Al, Ga, In and metal-free complexes with octachloropyrazinoporphirazines structure and spectral characteristics by QC calculations *Y. A. Zhabanov, A. V. Eroshin, I. V. Ryzhov, A. A. Otlyotov* *Manuscript in preparation*