ISSN 0022-4766, *Journal of Structural Chemistry, 2024, Vol. 65, No. 7, pp. 1412-1419. © Pleiades Publishing, Ltd., 2024.*
Russian Text © The Author(s), 2024, published in Zhurnal Strukturnoi Khimii, 2024, Vol. 65, No. 7, 129642.

MIXED-LIGAND CHLORIDE COMPLEX OF Co(II) WITH *E*-2-(((4-IODOPHENYL)IMINO)METHYL) PHENOL: CRYSTAL STRUCTURE AND FEATURES OF HALOGEN BONDING IN A SOLID

S. A. Adonin[1,2]*, P. A. Abramov[1], A. S. Zaguzin[1],
and A. S. Novikov[3]

Neutral complex [L_2CoCl_2] is obtained by the reaction of cobalt(II) chloride with *E*-(((4-iodophenyl)imino)methyl)phenol (L), and its structure is studied by single crystal X-ray diffraction. The structure contains I···Cl halogen bonds whose energies are estimated by quantum chemical calculations.

DOI: 10.1134/S0022476624070126

Keywords: cobalt, halide complexes, halogen bond, crystal structure.

INTRODUCTION

A halogen bond (XB) is a special type of non-covalent interactions in which halogen atoms (usually iodine) play an unusual role of an electrophile [1-3]. This phenomenon as well as the other “atypical” bonding modes (for example, chalcogen bonding [4-10]) has been actively studied for at least the previous decade [11-17]. This is due to both purely fundamental interest in the development of supramolecular chemistry in general and possible applications of this effect in materials science.

One of general tasks in the research area has been repeatedly noted–the search for new building blocks capable of forming XBs. Perfluorinated iodo- and bromoarenes [18-23], di- and polyhalides [24-28], hypervalent iodine compounds [29-34], etc. can be noted among the most frequently occurring objects. However, although Schiff bases represent a vast class of compounds widely used in coordination chemistry as ligands [35-44] and provide a variety of synthetic routes to introduce halogen atoms available for the XB formation, they are rarely considered from this point of view.

It is well known that in [$L_2M^{II}X_2$]-type complexes, where X = halide, L = halogenated pyridine, the formation of strong XBs is the rule rather than the exception [45-51]. It is logical to assume that the complexes with Schiff bases containing a sterically available iodarene substituent can exhibit similar behavior. To test this hypothesis, we synthesized *E*-(((4-iodophenyl)imino)methyl)phenol (L) that was reacted with cobalt dichloride to give neutral complex [L_2CoCl_2] (**1**), and its structure was studied by single crystal X-ray diffraction (XRD). In the structure of **1** there are indeed I···Cl XBs the energies of which were estimated by quantum chemical calculations.

---

[1]Nikolaev Institute of Inorganic Chemistry, Siberian Branch, Russian Academy of Sciences, Novosibirsk, Russia; *adonin@niic.nsc.ru. [2]Favorsky Irkutsk Institute of Chemistry, Siberian Branch, Russian Academy of Sciences, Irkutsk, Russia. [3]St. Petersburg State University, Institute of Chemistry, St. Petersburg, Russia. Original article submitted January 31, 2024; revised March 25, 2024; accepted March 27, 2024.

TABLE 1. Crystallographic Characteristics and Details of the Diffraction Experiment for the Crystal of **1**

Parameter	**1**
Chemical formula	$C_{26}H_{20}Cl_2CoI_2N_2O_2$
M	776.07
Crystal system	Triclinic
Space group	$P\overline{1}$
a, b, c, Å	7.9849(2), 12.6574(4), 13.3733(3)
α, β, γ, deg	97.138(2), 95.681(2), 93.246(2)
V, Å^3	1331.30(6)
Z	2
μ, mm^{-1}	3.19
Reflection index ranges	$h = -10\rightarrow 9$, $k = -16\rightarrow 14$, $l = -17\rightarrow 14$
Reflections: measured / independent / with $I > 2\sigma(I)$	10148 / 5809 / 4673
$R(F^2 > 2\sigma(F^2))$, $wR(F^2)$, S	0.033, 0.065, 1.03
$\Delta\rho_{min}$ / $\Delta\rho_{max}$, e/Å^3	0.70 / –0.82

EXPERIMENTAL

The chemically pure grade reagents (or their analogues) were purchased from commercial sources and used without further purification. L was obtained from salicylic aldehyde and 4-iodoaniline by the procedure [52].

Synthesis of 1. L (50 mg, 0.155 mmol) and $CoCl_2{\cdot}6H_2O$ (18 mg, 0.078 mmol) were dissolved in 7 mL of acetonitrile with stirring. Gradual evaporation of the solvent results in the formation of blue-green crystals of **1**. Yield: 79%.

Single crystal XRD. The structure of complex **1** was determined following the standard procedure on an Agilent Xcalibur diffractometer with an area AtlasS2 detector (graphite monochromator, $\lambda(MoK_\alpha) = 0.71073$ Å, ω-scanning). Integration was performed, absorption corrections were applied, and unit cell parameters were determined using the CrysAlisPro software. The structure was solved using SHELXT [53] and refined by the full-matrix least squares method (LSM) in the anisotropic approximation for non-hydrogen atoms by the SHELXL 2017\1 algorithm [54] in the ShelXle program [55]. The details are given in Table 1. Atomic coordinates and other parameters of single crystal XRD experiments have been deposited with the Cambridge Structural Database under No. 2329207; deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk/data_request/cif).

RESULTS AND DISCUSSION

Although L (Fig. 1) can act as a N,O-donor chelate ligand, in the case of **1** there is monodentate coordination through oxygen atoms of hydroxyl groups which remain protonated. Co(II) has a tetrahedral coordination environment (Fig. 2). The Co–O and Co–Cl distances are 1.942-1.945 Å and 2.236-2.287 Å respectively.

As already mentioned, a distinctive feature of the structure of **1** is a pronounced XB between chloride ligands and iodine atoms in L. The respective distances are 3.337 Å, which is significantly less than the sum of the corresponding Bondi Van der Waals radii (3.73 Å). Due to the interactions of this type, neutral $[L_2CoCl_2]$ moieties are organized into infinite 1D supramolecular chains (Fig. 3).

In order to understand the nature and estimate the energy of non-covalent I···Cl interactions in the crystal of **1** (these short contacts can be classified as typical XBs [3]), we performed quantum chemical calculations within density functional theory (ωB97XD/DZP-DKH) [56, 57] using the Gaussian09 software and the topological analysis of the electron density distribution by the QTAIM method [58] using the Multiwfn program [59] (version 3.7). A supramolecular dimeric cluster

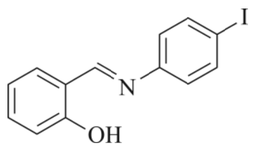

Fig. 1. L ligand structure.

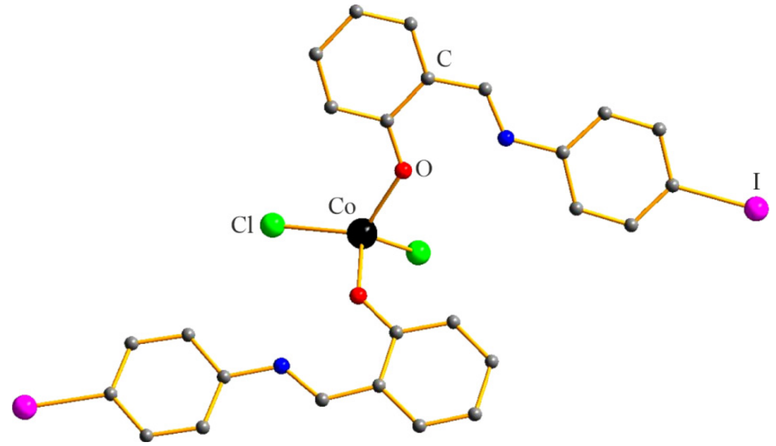

Fig. 2. Structure of **1**. Hereinafter, Co is black, C is gray, Cl is green, O is red, I is purple; H atoms are omitted.

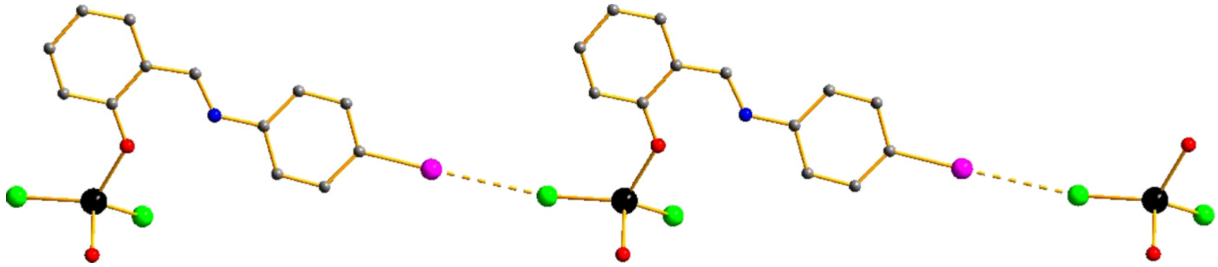

Fig. 3. I···Cl XB in **1**.

(idealized isolated model system for which the quantum chemistry calculations were performed) was analyzed without the geometry optimization. The results are shown in Table 2. I···Cl XBs in the crystal of **1** were visualized within the formalism of the non-covalent interaction analysis in the model supramolecular associate (NCI analysis [60]) (Fig. 4). Electron densities, the Laplacian of the electron density, the total energy density, the potential energy density, and the Lagrangian of the kinetic energy in the (3, –1) bond critical point corresponding to non-covalent I···Cl interactions in the crystal of **1**, are

TABLE 2. Electron Density $\rho(\mathbf{r})$, Laplacian of the Electron Density $\nabla^2\rho(\mathbf{r})$, Total Energy Density H_b, Potential Energy Density $V(\mathbf{r})$, and Lagrangian of the Kinetic Energy $G(\mathbf{r})$ (a.u.) in the (3, –1) Bond Critical Point Corresponding to Non-Covalent I···Cl Interactions in the Crystal of **1**, the Lengths of these Contacts l (Å) and their Energies E (kcal/mol)

Contact	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	H_b	$V(\mathbf{r})$	$G(\mathbf{r})$	l[#1]	E[#2]
I···Cl	0.015	0.049	0.001	–0.010	0.011	3.337	4.6

[#1] The smallest Van der Waals radii (by Bondi) for chlorine and iodine atoms are 1.75 Å and 1.98 Å respectively [61].

[#2] $E = 0.67G(\mathbf{r})$ (the correlation was developed specifically to estimate the energy of non-covalent interactions involving iodine atoms) [62].

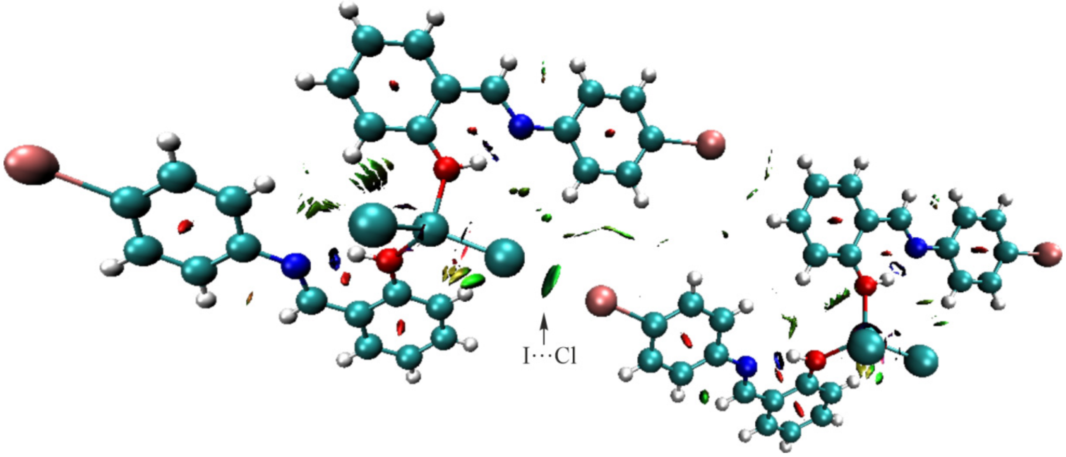

Fig. 4. Visualization of I···Cl XBs in the crystal of **1** within the formalism of the non-covalent interaction analysis in the model supramolecular associate (NCI analysis [60]).

quite typical of such supramolecular contacts involving halogen atoms. The ratio of the potential energy density and the Lagrangian of the kinetic energy (3, –1) in the bond critical point corresponding to non-covalent I···Cl interactions in **1** indicates that the fraction of the covalent component is not significant in these supramolecular contacts.

FUNDING

This work was supported by the Ministry of Science and Higher Education of the Russian Federation (structural characterization of the samples, 121031700313-8).

CONFLICT OF INTERESTS

The authors of this work declare that they have no conflicts of interest.

REFERENCES

1. G. R. Desiraju, P. S. Ho, L. Kloo, A. C. Legon, R. Marquardt, P. Metrangolo, P. Politzer, G. Resnati, and K. Risanen. Definition of the halogen bond (IUPAC recommendations 2013). *Pure Appl. Chem.*, **2013**, *85*(8), 1711-1713. https://doi.org/10.1351/pac-rec-12-05-10
2. G. Cavallo, P. Metrangolo, T. Pilati, G. Resnati, M. Sansotera, and G. Terraneo. Halogen bonding: a general route in anion recognition and coordination. *Chem. Soc. Rev.*, **2010**, *39*(10), 3772. https://doi.org/10.1039/b926232f
3. G. Cavallo, P. Metrangolo, R. Milani, T. Pilati, A. Priimagi, G. Resnati, and G. Terraneo. The halogen bond. *Chem. Rev.*, **2016**, *116*(4), 2478-2601. https://doi.org/10.1021/acs.chemrev.5b00484
4. E. A. Suturina, N. A. Semenov, A. V. Lonchakov, I. Y. Bagryanskaya, Y. V. Gatilov, I. G. Irtegova, N. V. Vasilieva, E. Lork, R. Mews, N. P. Gritsan, and A. V. Zibarev. Interaction of 1,2,5-chalcogenadiazole derivatives with thiophenolate: Hypercoordination with formation of interchalcogen bond versus reduction to radical anion. *J. Phys. Chem. A*, **2011**, *115*(18), 4851-4860. https://doi.org/10.1021/jp2019523
5. E. A. Radiush, E. A. Pritchina, E. A. Chulanova, A. A. Dmitriev, I. Y. Bagryanskaya, A. M. Z. Slawin, J. D. Woollins, N. P. Gritsan, A. V. Zibarev, and N. A. Semenov. Chalcogen-bonded donor–acceptor complexes of 5,6-dicyano[1,2,5]selenadiazolo[3,4-*b*]pyrazine with halide ions. *New J. Chem.*, **2022**, *46*(30), 14490-14501. https://doi.org/10.1039/d2nj02345h

6. E. A. Katlenok, M. L. Kuznetsov, N. A. Semenov, N. A. Bokach, and V. Y. Kukushkin. A new look at the chalcogen bond: π-hole-based chalcogen (Se, Te) bonding which does not include a σ-hole interaction. *Inorg. Chem. Front.*, **2023**, *10*(10), 3065-3081. https://doi.org/10.1039/d3qi00087g
7. E. A. Radiush, H. Wang, E. A. Chulanova, Y. A. Ponomareva, B. Li, Q. Y. Wei, G. E. Salnikov, S. Y. Petrakova, N. A. Semenov, and A. V. Zibarev. Halide complexes of 5,6-dicyano-2,1,3-benzoselenadiazole with 1:4 stoichiometry: Cooperativity between chalcogen and hydrogen bonding. *ChemPlusChem*, **2023**, *88*(11). https://doi.org/10.1002/cplu.202300523
8. A. N. Isaev. Effect of halogen at the divalent sulfur atom on the properties of complexes with a chalcogen and hydrogen bond. *Russ. J. Phys. Chem. A*, **2023**, *97*(5), 955-964. https://doi.org/10.1134/s0036024423050114
9. A. A. Artemjev, A. S. Kubasov, V. P. Zaytsev, A. V. Borisov, A. S. Kritchenkov, V. G. Nenajdenko, R. M. Gomila, A. Frontera, and A. G. Tskhovrebov. Novel chalcogen bond donors derived from [3+2] cycloaddition reaction between 2-pyridylselenyl reagents and isocyanates: Synthesis, structures and theoretical studies. *Cryst. Growth Des.*, **2023**, *23*(4), 2018-2023. https://doi.org/10.1021/acs.cgd.3c00101
10. A. A. Sapronov, A. S. Kubasov, V. N. Khrustalev, A. A. Artemjev, G. M. Burkin, E. A. Dukhnovsky, A. O. Chizhov, A. S. Kritchenkov, R. M. Gomila, A. Frontera, and A. G. Tskhovrebov. Se···π chalcogen bonding in 1,2,4-selenodiazolium tetraphenylborate complexes. *Symmetry*, **2023**, *15*(1), 212. https://doi.org/10.3390/sym15010212
11. A. B. Đunović and D. Ž. Veljković. Halogen bonds as a tool in the design of high energetic materials: Evidence from crystal structures and quantum chemical calculations. *CrystEngComm*, **2021**, *23*(39), 6915-6922. https://doi.org/10.1039/d1ce00854d
12. A. Lazić, N. Trišović, L. Radovanović, J. Rogan, D. Poleti, Ž. Vitnik, V. Vitnik, and G. Ušćumlić. Towards understanding intermolecular interactions in hydantoin derivatives: The case of cycloalkane-5-spirohydantoins tethered with a halogenated benzyl moiety. *CrystEngComm*, **2017**, *19*(3), 469-483. https://doi.org/10.1039/c6ce02210c
13. M. Moradkhani, A. Naghipour, and Y. Abbasi Tyula. Competition and interplay between hydrogen, tetrel, and halogen bonds from interactions of $COCl_2$ and HX ($X = F$, Cl, Br, and I). *Comput. Theor. Chem.*, **2023**, *1223*, 114099. https://doi.org/10.1016/j.comptc.2023.114099
14. K. Mandal, S. Sarkar, P. Ghosh, V. R. Hathwar, and D. Chopra. Quantitative insights into noncovalent interactions involving halogen and tetrel bonds in 2,4,6-trimethylpyrylium tetrafluoroborate. *Acta Crystallogr.*, *Sect. C: Struct. Chem.*, **2022**, *78*(11), 597-605. https://doi.org/10.1107/s2053229622009469
15. A. Hasija, S. Som, and D. Chopra. Investigation of crystal structures, energetics and isostructurality in halogen-substituted phosphoramidates. *Acta Crystallogr.*, *Sect. B: Struct. Sci. Cryst. Eng. Mater.*, **2022**, *78*(2), 179-194. https://doi.org/10.1107/s2052520622000889
16. K. M. Bairagi, K. S. Ingle, R. Bhowal, S. A. Mohurle, A. Hasija, O. I. Alwassil, K. N. Venugopala, D. Chopra, and S. K. Nayak. Interplay of halogen and hydrogen bonding through co-crystallization in pharmacologically active dihydropyrimidines: Insights from crystal structure and energy framework. *ChemPlusChem*, **2021**, *86*(8), 1167-1176. https://doi.org/10.1002/cplu.202100259
17. R. Shukla and D. Chopra. Chalcogen and pnictogen bonds: Insights and relevance. *Curr. Sci.*, **2021**, *120*(12), 1848. https://doi.org/10.18520/cs/v120/i12/1848-1853
18. E. A. Katlenok, M. Haukka, O. V. Levin, A. Frontera, and V. Y. Kukushkin. Supramolecular assembly of metal complexes by (aryl)I···d_{z^2}[Pt^{II}] halogen bonds. *Chem. - Eur. J.*, **2020**, *26*(34), 7692-7701. https://doi.org/10.1002/chem.202001196
19. A. V. Rozhkov, A. S. Novikov, D. M. Ivanov, D. S. Bolotin, N. A. Bokach, and V. Y. Kukushkin. Structure-directing weak interactions with 1,4-diiodotetrafluorobenzene convert one-dimensional arrays of $[M^{II}(acac)_2]$ species into three-dimensional networks. *Cryst. Growth Des.*, **2018**, *18*(6), 3626-3636. https://doi.org/10.1021/acs.cgd.8b00408

20. M. A. Kryukova, A. V. Sapegin, A. S. Novikov, M. Krasavin, and D. M. Ivanov. New crystal forms for biologically active compounds. Part 2: Anastrozole as N-substituted 1,2,4-triazole in halogen bonding and lp-π interactions with 1,4-diiodotetrafluorobenzene. *Crystals*, **2020**, *10*(5), 371. https://doi.org/10.3390/cryst10050371

21. A. A. Eliseeva, D. M. Ivanov, A. S. Novikov, and V. Y. Kukushkin. Recognition of the π-hole donor ability of iodopentafluorobenzene - a conventional σ-hole donor for crystal engineering involving halogen bonding. *CrystEngComm*, **2019**, *21*(4), 616-628. https://doi.org/10.1039/c8ce01851k

22. V. V. Suslonov, A. A. Eliseeva, A. S. Novikov, D. M. Ivanov, A. Y. Dubovtsev, N. A. Bokach, and V. Y. Kukushkin. Tetrachloroplatinate(II) anion as a square-planar tecton for crystal engineering involving halogen bonding. *CrystEngComm*, **2020**, *22*(24), 4180-4189. https://doi.org/10.1039/d0ce00576b

23. A. A. Eliseeva, D. M. Ivanov, A. V. Rozhkov, I. V. Ananyev, A. Frontera, and V. Y. Kukushkin. Bifurcated halogen bonding involving two rhodium(I) centers as an integrated σ-hole acceptor. *JACS Au*, **2021**, *1*(3), 354-361. https://doi.org/10.1021/jacsau.1c00012

24. Y. V. Torubaev, I. V. Skabitskiy, A. V. Pavlova, and A. A. Pasynskii. First structural evidence of a Se-Br–Br halogen-bonded molecular complex. *New J. Chem.*, **2017**, *41*(9), 3606-3611. https://doi.org/10.1039/c6nj04096a

25. T. A. Shestimerova, N. A. Yelavik, A. V. Mironov, A. N. Kuznetsov, M. A. Bykov, A. V. Grigorieva, V. V. Utochnikova, L. S. Lepnev, and A. V. Shevelkov. From isolated anions to polymer structures through linking with I_2: Synthesis, structure, and properties of two complex bismuth(III) iodine iodides. *Inorg. Chem.*, **2018**, *57*(7), 4077-4087. https://doi.org/10.1021/acs.inorgchem.8b00265

26. A. Eich, R. Köppe, P. W. Roesky, and C. Feldmann. The bromine-rich bromido metallates $[BMIm]_2[SnBr_6]\cdot(Br_2)$ and $[MnBr(18\text{-crown-}6)]_4[SnBr_6]_2\cdot(Br_2)_{4.5}$. *Eur. J. Inorg. Chem.*, **2019**, *2019*(9), 1292-1298. https://doi.org/10.1002/ejic.201900018

27. A. V. Bykov, T. A. Shestimerova, M. A. Bykov, L. A. Osminkina, A. N. Kuznetsov, V. E. Gontcharenko, and A. V. Shevelkov. Synthesis, crystal, and electronic structure of $(HpipeH_2)_2[Sb_2I_{10}](I_2)$, with I_2 molecules linking Sb_2X_{10} dimers into a polymeric anion: A strategy for optimizing a hybrid compound′s band gap. *Int. J. Mol. Sci.*, **2023**, *24*(3), 2201. https://doi.org/10.3390/ijms24032201

28. T. A. Shestimerova, N. A. Golubev, N. A. Yelavik, M. A. Bykov, A. V. Grigorieva, Z. Wei, E. V. Dikarev, and A. V. Shevelkov. Role of I_2 molecules and weak interactions in supramolecular assembling of pseudo-three-dimensional hybrid bismuth polyiodides: Synthesis, structure, and optical properties of phenylenediammonium polyiodobismuthate(III). *Cryst. Growth Des.*, **2018**, *18*(4), 2572-2578. https://doi.org/10.1021/acs.cgd.8b00179

29. V. V. Suslonov, N. S. Soldatova, D. M. Ivanov, B. Galmés, A. Frontera, G. Resnati, P. S. Postnikov, V. Y. Kukushkin, and N. A. Bokach. Diaryliodonium tetrachloroplatinates(II): Recognition of a trifurcated metal-involving μ_3-I···(Cl,Cl,Pt) halogen bond. *Cryst. Growth Des.*, **2021**, *21*(9), 5360-5372. https://doi.org/10.1021/acs.cgd.1c00654

30. N. S. Soldatova, V. V. Suslonov, T. Y. Kissler, D. M. Ivanov, A. S. Novikov, M. S. Yusubov, P. S. Postnikov, and V. Y. Kukushkin. Halogen bonding provides heterooctameric supramolecular aggregation of diaryliodonium thiocyanate. *Crystals*, **2020**, *10*(3), 230. https://doi.org/10.3390/cryst10030230

31. I. S. Aliyarova, D. M. Ivanov, N. S. Soldatova, A. S. Novikov, P. S. Postnikov, M. S. Yusubov, and V. Y. Kukushkin. Bifurcated halogen bonding involving diaryliodonium cations as iodine(III)-based double-σ-hole donors. *Cryst. Growth Des.*, **2021**, *21*(2), 1136-1147. https://doi.org/10.1021/acs.cgd.0c01463

32. N. S. Soldatova, P. S. Postnikov, V. V. Suslonov, T. Y. Kissler, D. M. Ivanov, M. S. Yusubov, B. Galmés, A. Frontera, and V. Y. Kukushkin. Diaryliodonium as a double σ-hole donor: The dichotomy of thiocyanate halogen bonding provides divergent solid state arylation by diaryliodonium cations. *Org. Chem. Front.*, **2020**, *7*(16), 2230-2242. https://doi.org/10.1039/d0qo00678e

33. A. D. Radzhabov, A. I. Ledneva, N. S. Soldatova, I. I. Fedorova, D. M. Ivanov, A. A. Ivanov, M. S. Yusubov, V. Y. Kukushkin, and P. S. Postnikov. Halogen bond-involving self-assembly of iodonium carboxylates: Adding a dimension to supramolecular architecture. *Int. J. Mol. Sci.*, **2023**, *24*(19), 14642. https://doi.org/10.3390/ijms241914642

34. A. V. Semenov, S. V. Baykov, N. S. Soldatova, K. K. Geyl, D. M. Ivanov, A. Frontera, V. P. Boyarskiy, P. S. Postnikov, and V. Y. Kukushkin. Noncovalent chelation by halogen bonding in the design of metal-containing arrays: Assembly of double σ-hole donating halolium with Cu^I-containing O,O-donors. *Inorg. Chem.*, **2023**, *62*(15), 6128-6137. https://doi.org/10.1021/acs.inorgchem.3c00229
35. I. V. Smolyaninov, D. A. Burmistrova, N. P. Pomortseva, M. A. Polovinkina, O. P. Demidov, N. R. Al′myasheva, A. I. Poddel′skii, and N. T. Berberova. Triphenylphosphine thiolate gold(I) complexes with redox-active schiff bases: Synthesis, electrochemical properties, and biological activity. *Russ. J. Coord. Chem.*, **2023**, *49*(9), 577-592. https://doi.org/10.1134/s1070328423600420
36. M. S. Denisov and Y. A. Beloglazova. Nitro-substituted pyridinimine complexes of Pd(II): Synthesis and inhibition of MAO-B ex vivo. *Russ. J. Coord. Chem.*, **2023**, *49*(9), 565-576. https://doi.org/10.1134/s1070328423600626
37. S. V. Baryshnikova, M. V. Arsen′ev, R. V. Rumyantsev, I. A. Yakushev, and A. I. Poddel′skii. Copper(II) *o*-iminophenolate complexes based on catecholaldimines. *Russ. J. Coord. Chem.*, **2023**, *49*(7), 429-436. https://doi.org/10.1134/s107032842360016x
38. I. V. Smolyaninov, D. A. Burmistrova, N. P. Pomortseva, Y. K. Voronina, A. I. Poddel′sky, N. T. Berberova, and I. L. Eremenko. Complexes $R_2Sn(IV)L$ with O,N,O′-donor Schiff bases: Synthesis, structures, and redox properties. *Russ. J. Coord. Chem.*, **2023**, *49*(3), 124-141. https://doi.org/10.1134/s1070328423700446
39. B. Dag, Y. Tenekecioğlu, T. Aral, H. Kızılkaya, R. Erenler, and N. Genc. Synthesis, characterization, and antioxidant activity of a novel Schiff base, an amine and amine–metal complexes. *Russ. J. Bioorg. Chem.*, **2023**, *49*(4), 861-866. https://doi.org/10.1134/s1068162023040106
40. M. A. Latif, T. Ahmed, M. S. Hossain, B. M. Chaki, A. Abdou, and M. Kudrat-E-Zahan. Synthesis, spectroscopic characterization, DFT calculations, antibacterial activity, and molecular docking analysis of Ni(II), Zn(II), Sb(III), and U(VI) metal complexes derived from a nitrogen-sulfur Schiff base. *Russ. J. Gen. Chem.*, **2023**, *93*(2), 389-397. https://doi.org/10.1134/s1070363223020214
41. S. A. Nikolaevskii, M. A. Kiskin, Y. V. Koshchienko, A. S. Burlov, A. G. Starikov, and I. L. Eremenko. Structure of 4-methyl-N-{2-[2-alkylamino-5-nitrophenyliminomethyl]phenyl}benzenesulfonamides. *Crystallogr. Rep.*, **2013**, *58*(3), 437-441. https://doi.org/10.1134/s1063774513030164
42. A. S. Burlov, S. A. Nikolaevskii, A. S. Bogomyakov, I. S. Vasil′chenko, Y. V. Koshchienko, V. G. Vlasenko, A. I. Uraev, D. A. Garnovskii, E. V. Sennikova, G. S. Borodkin, A. D. Garnovskii, and V. I. Minkin. New magnetically active metal complexes of tridentate Schiff bases of phenylazosalicylaldehyde. *Russ. J. Coord. Chem.*, **2009**, *35*(7), 486-491. https://doi.org/10.1134/s1070328409070045
43. A. S. Burlov, A. I. Uraev, V. N. Ikorskii, S. A. Nikolaevskii, Y. V. Koshchienko, I. S. Vasil′chenko, D. A. Garnovskii, V. G. Vlasenko, Y. V. Zubavichus, L. N. Divaeva, G. S. Borodkin, and A. D. Garnovskii. Molecular design of new magnetically active copper complexes with heteroaromatic schiff bases and azo compounds. *Russ. J. Gen. Chem.*, **2008**, *78*(6), 1230-1235. https://doi.org/10.1134/s1070363208060224
44. A. S. Burlov, Y. V. Koshchienko, V. N. Ikorskii, V. G. Vlasenko, I. A. Zarubin, A. I. Uraev, I. S. Vasil′chenko, D. A. Garnovskii, G. S. Borodkin, S. A. Nikolaevskii, and A. D. Garnovskii. New magnetoactive copper complexes with Schiff's bases. *Russ. J. Inorg. Chem.*, **2006**, *51*(7), 1065-1070. https://doi.org/10.1134/s0036023606070096
45. F. Zordan and L. Brammer. M–X···X′–C halogen-bonded network formation in MX_2(4-halopyridine)$_2$ complexes (M = Pd, Pt; X = Cl, I; X′ = Cl, Br, I). *Cryst. Growth Des.*, **2006**, *6*(6), 1374-1379. https://doi.org/10.1021/cg050670m
46. R. Wang, T. S. Dols, C. W. Lehmann, and U. Englert. The halogen bond made visible: Experimental charge density of a very short intermolecular Cl···Cl donor–acceptor contact. *Chem. Commun.*, **2012**, *48*(54), 6830. https://doi.org/10.1039/c2cc32647g
47. F. F. Awwadi, R. D. Willett, S. F. Haddad, and B. Twamley. The electrostatic nature of aryl–bromine–halide synthons: The role of aryl–bromine–halide synthons in the crystal structures of the *trans*-bis(2-bromopyridine)dihalocopper(II)

and *trans*-bis(3-bromopyridine)dihalocopper(II) complexes. *Cryst. Growth Des.*, **2006**, *6*(8), 1833-1838. https://doi.org/10.1021/cg060154b

48. F. Awwadi, S. F. Haddad, R. D. Willett, and B. Twamley. The analogy of C–Br···Br–C, C–Br···Br–Fe, and Fe–Br···Br–Fe contacts: Crystal structures of (26DAPH)$FeBr_4$ and $(26DA35DBPH)_2FeBr_4 \cdot Br$. *Cryst. Growth Des.*, **2010**, *10*(1), 158-164. https://doi.org/10.1021/cg900762s
49. C. A. Krasinski, B. L. Solomon, F. F. Awwadi, C. P. Landee, M. M. Turnbull, and J. L. Wikaira. Copper(II) halide salts and complexes of 4-amino-2-fluoropyridine: Synthesis, structure and magnetic properties. *J. Coord. Chem.*, **2017**, *70*(5), 914-935. https://doi.org/10.1080/00958972.2016.1278213
50. F. F. Awwadi, R. D. Willett, B. Twamley, M. M. Turnbull, and C. P. Landee. Dual behavior of bromine atoms in supramolecular chemistry: The crystal structure and magnetic properties of two copper(II) coordination polymers. *Cryst. Growth Des.*, **2015**, *15*(8), 3746-3754. https://doi.org/10.1021/acs.cgd.5b00393
51. F. F. Awwadi, M. M. Turnbull, M. I. Alwahsh, and S. F. Haddad. May halogen bonding interactions compete with Cu···Cl semi-coordinate bonds? Structural, magnetic and theoretical studies of two polymorphs of *trans*-bis(5-bromo-2-chloro pyridine)dichlorocopper(II) and *trans*-bis(2,5-dichloropyridine)dichlorocopper(II). *New J. Chem.*, **2018**, *42*(13), 10642-10650. https://doi.org/10.1039/c8nj00422f
52. G. C. Percy and D. A. Thornton. N-aryl salicylaldimine complexes: Infrared and PMR spectra of the ligands and vibrational frequencies of their metal(II) chelates. *J. Inorg. Nucl. Chem.*, **1972**, *34*(11), 3357-3367. https://doi.org/10.1016/0022-1902(72)80230-6
53. G. M. Sheldrick. SHELXT - Integrated space-group and crystal-structure determination. *Acta Crystallogr.*, *Sect. A: Found. Adv.*, **2015**, *71*(1), 3-8. https://doi.org/10.1107/s2053273314026370
54. G. M. Sheldrick. Crystal structure refinement with SHELXL. *Acta Crystallogr.*, *Sect. C: Struct. Chem.*, **2015**, *71*(1), 3-8. https://doi.org/10.1107/s2053229614024218
55. C. B. Hübschle, G. M. Sheldrick, and B. Dittrich. ShelXle: a Qt graphical user interface for SHELXL. *J. Appl. Crystallogr.*, **2011**, *44*(6), 1281-1284. https://doi.org/10.1107/s0021889811043202
56. J.-D. Chai and M. Head-Gordon. Long-range corrected hybrid density functionals with damped atom–atom dispersion corrections. *Phys. Chem. Chem. Phys.*, **2008**, *10*(44), 6615. https://doi.org/10.1039/b810189b
57. C. L. Barros, P. J. P. de Oliveira, F. E. Jorge, A. Canal Neto, and M. Campos. Gaussian basis set of double zeta quality for atoms Rb through Xe: application in non-relativistic and relativistic calculations of atomic and molecular properties. *Mol. Phys.*, **2010**, *108*(15), 1965-1972. https://doi.org/10.1080/00268976.2010.499377
58. R. F. W. Bader. A quantum theory of molecular structure and its applications. *Chem. Rev.*, **1991**, *91*(5), 893-928. https://doi.org/10.1021/cr00005a013
59. T. Lu and F. Chen. Multiwfn: A multifunctional wavefunction analyzer. *J. Comput. Chem.*, **2012**, *33*(5), 580-592. https://doi.org/10.1002/jcc.22885
60. E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, and W. Yang. Revealing noncovalent interactions. *J. Am. Chem. Soc.*, **2010**, *132*(18), 6498-6506. https://doi.org/10.1021/ja100936w
61. A. Bondi. Van der Waals volumes and radii of metals in covalent compounds. *J. Phys. Chem.*, **1966**, *70*(9), 3006-3007. https://doi.org/10.1021/j100881a503
62. E. V. Bartashevich and V. G. Tsirelson. Interplay between non-covalent interactions in complexes and crystals with halogen bonds. *Russ. Chem. Rev.*, **2014**, *83*(12), 1181-1203. https://doi.org/10.1070/rcr4440