



SUPPLEMENTARY MATERIAL TO
**Synthesis and structural characterization of Cd(II) complexes
with 2-acetylpyridine-aminoguanidine – A novel
coordination mode**

MIRJANA M. RADANOVIĆ^{1*}, SLAĐANA B. NOVAKOVIĆ², MARKO V. RODIĆ¹,
LJILJANA S. VOJINOVIĆ-JEŠIĆ¹, CHRISTOPH JANIYAK³
and VUKADIN M. LEOVAC¹

¹University of Novi Sad Faculty of Sciences, Trg D. Obradovića 3, 21000 Novi Sad, Serbia,
²“Vinča” Institute of Nuclear Sciences, National Institute of the Republic of Serbia, Univer-
sity of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia and ³Heinrich-Heine-Universität
Düsseldorf, Institute for Inorganic Chemistry and Structural Chemistry, Universitätsstraße 1,
Düsseldorf, D-40225, Germany

J. Serb. Chem. Soc. 87 (11) (2022) 1259–1272

TABLE S-I. Complexes with a monodentate aminoguanidine-derived Schiff base ligand

REFCODE	Reference
GAKSIW	O. T. Ujam, S. M. Devoy, W. Henderson, B. K. Nicholson, T. S. A. Hor, <i>Inorg. Chim. Acta</i> 363 (2010) 3558 (https://doi.org/10.1016/j.ica.2010.07.011)

TABLE S-II. Complexes with a tridentate aminoguanidine-derived Schiff base ligand

REFCODES	References
GOTGEE	B. W. Skelton, V. N. Kokozay, O. Yu. Vassilyeva, E. A. Buvaylo (2019) <i>CSD Communication (Private Communication)</i> (https://doi.org/10.5517/ccdc.csd.cc23rl6p)
BUWNUE	M. G. Jelic, N. Boukos, M. M. Lalovic, N. Z. Romcevic, V. M. Leovac, B. B. Hadzic, S. S. Balos, L. S. Jovanovic, M. P. Slankamenac, M. B. Zivanov, L. S. Vojinovic-Jesic, <i>Opt. Mater.</i> 35 (2013) 2728 (https://doi.org/10.1016/j.optmat.2013.08.023)
BUWQOB	M. M. Radanovic, M. V. Rodic, S. A. Armakovic, S. J. Armakovic, L. S. Vojinovic-Jesic, V. M. Leovac, <i>J. Coord. Chem.</i> 70 (2017) 2870 (https://doi.org/10.1080/00958972.2017.1367388)
CEKNIS	M. M. Lalovic, L. S. Jovanovic, L. S. Vojinovic-Jesic, V. M. Leovac, V. I. Cesljevic, M. V. Rodic, V. Divjakovic, <i>J. Coord. Chem.</i> 65 (2012) 4217 (https://doi.org/10.1080/00958972.2012.737916)
CELHIM	E. A. Buvaylo, V. N. Kokozay, O. Yu. Vassilyeva, B. W. Skelton, O. V. Nesterova, A. J. L. Pombeiro, <i>Inorg. Chem. Commun.</i> 78 (2017) 5 (https://doi.org/10.1016/j.inoche.2017.03.008)
CELHOS	
GANQEU	
GEMJOY	Yu. M. Chumakov, V. I. Tsapkov, G. Bocelli, B. Ya. Antosyak, S. G. Shova, A. P. Gulya, <i>Crystallogr. Rep.</i> 51 (2006) 66 (https://doi.org/10.5517/cc8w217)

*Corresponding author. E-mail: mirjana.lalovic@dh.uns.ac.rs

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IPOFAN	E. A. Buvaylo, K. A. Kasyanova, O. Y. Vassilyeva, B. W. Skelton, <i>Acta Crystallogr., Sect. E: Cryst. Commun.</i> 72 (2016) 907 (https://doi.org/10.1107/S2056989016008690)
IQEDOZ	
IQEDOZ01	L. S. Vojinovic-Jesic, M. M. Radanovic, M. V. Rodic, V. Zivkovic-Radovanovic, L.
IQEFAN	S. Jovanovic, V. M. Leovac, <i>Polyhedron</i> 117 (2016) 526
IQEFER	(https://doi.org/10.1016/j.poly.2016.06.032)
IQEFIV	
MECJOV	M. M. Lalovic, L. S. Vojinovic-Jesic, L. S. Jovanovic, V. M. Leovac, V. I. Cesljevic, V. Divjakovic, <i>Inorg. Chim. Acta</i> 388 (2012) 157 (https://doi.org/10.1016/j.ica.2012.03.026)
MEXGED	E. A. Buvaylo, V. N. Kokozay, O. Yu. Vassilyeva, B. W. Skelton, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> 69 (2013) m165 (https://doi.org/10.1107/S1600536813004534)
MOHHIC	L. S. Vojinovic-Jesic, M. M. Radanovic, M. V. Rodic, L. S. Jovanovic, V. I.
MOHHOI	Cesljevic, M. D. Joksovic, <i>Polyhedron</i> 80 (2014) 90
MOHHUO	(https://doi.org/10.1016/j.poly.2014.02.003)
QEHSUT	V. Jevtovic, D. Vidovic, S. Ivkovic, <i>Cont. Mat.</i> 2 (2011) 55 (https://doi.org/10.5767/anurs.cmat.110201.en.055J)
QEHSUT01	M. M. Radanovic, M. V. Rodic, S. A. Armakovic, S. J. Armakovic, L. S. Vojinovic-Jesic, V. M. Leovac, <i>J. Coord. Chem.</i> 70 (2017) 2870 (https://doi.org/10.1080/00958972.2017.1367388)
QELKIE	M. M. Radanovic, M. V. Rodic, L. S. Vojinovic-Jesic, S. Armakovic, S. J.
QELKUQ	Armakovic, V. M. Leovac, <i>Inorg. Chim. Acta</i> 473 (2018) 160 (https://doi.org/10.1016/j.ica.2017.12.038)
QOHDEY	M.M.Lalovic, V.M.Leovac, L.S.Vojinovic-Jesic, M.V.Rodic, L.S.Jovanovic,
QOHDUO	V.I.Cesljevic, <i>J. Serb. Chem. Soc.</i> 78 (2013) 1161 (https://doi.org/10.2298/JSC130326038L)
RIYMIV	K. D. Onuska, N. J. Taylor, J. Carsky, <i>J. Chem. Cryst.</i> 26 (1996) 841
RIYMIV01	(https://doi.org/10.1007/BF01670317)
WIDTIN	V. M. Leovac, M. D. Joksovic, V. Divjakovic, L. S. Jovanovic, Z. Saranovic, A. Pevec, <i>J. Inorg. Biochem.</i> 101 (2007) 1094 (https://doi.org/10.1016/j.jinorgbio.2007.04.004)
XEDDEE	M. M. Radanovic, S. B. Novakovic, L. S. Vojinovic-Jesic, M. V. Rodic, V. M. Leovac, <i>J. Serb. Chem. Soc.</i> 83 (2018) 157 (https://doi.org/10.2298/JSC170922116R)
XIXTOO	C. I. Turta, L. F. Chapurina, I. G. Donica, V. Voronkova, E. R. Healey, V. Ch.
XIXVAC	Kravtsov, <i>Inorg. Chim. Acta</i> 361 (2008) 309 (https://doi.org/10.1016/j.ica.2007.07.017)
YEDJOM	E. B. Shamuratov, Kh. T. Sharipov, A. S. Batsanov, Yu. T. Struchkov, A. B. Khudoyarov, F. F. Mirdzhalalov, <i>Koord. Khim. (Russ.)(Coord. Chem.)</i> 19 (1993) 155
YUCMOZ	V. M. Leovac, L. S. Vojinovic-Jesic, V. I. Cesljevic, S.B.Novakovic, G.A.Bogdanovic, <i>Acta Crystallogr. Sect. C: Cryst. Struct. Commun.</i> 65 (2009) m337 (https://doi.org/10.1107/S0108270109029023)
YUJGIV	G. R. Andrade, J. Kunsminkas, L. Pizzuti, A. dos Anjos, S. D. Inglez, B. Tirloni, P.
YUJGIV01	H. Suegama, <i>Inorg. Chem. Commun.</i> 61 (2015) 210
YUJGIV02	(https://doi.org/10.1016/j.inoche.2015.09.022)
HUDHAE	A. Mondal, C. Das, M. Corbella, A. Bauza, A. Frontera, M. Saha, S. Mondal, K. D. Saha, S. K. Chattopadhyay, <i>New J. Chem.</i> 44 (2020) 7319 (https://doi.org/10.1039/C9NJ05712A)

TABLE S-III. Complexes with a tetradentate aminoguanidine-derived Schiff base ligands

REFCODES	References
GOQMAD	O. Yu. Vassilyeva, E. A. Buvaylo, V. N. Kokozay, S. L. Studzinsky, B. W. Skelton, G. S. Vasyliiev, <i>Acta Crystallogr., Sect. E: Cryst. Commun.</i> 78 (2022) 173 (https://doi.org/10.1107/S2056989022000317)
GOTFIH	B. W. Skelton, V. N. Kokozay, O. Yu. Vassilyeva, <i>CSD Communication (Private Communication)</i> (2019) (https://doi.org/10.5517/ccdc.csd.cc23rkxc)
TUFDAZ	Z. A. Starikova, A. I. Yanovsky, Yu. T. Struchkov, S. V. Zubkov, I. I. Seifullina, <i>Izv. Akad. Nauk SSSR, Ser. Khim. (Russ.) (Russ. Chem. Bull.)</i> (1996) 2157
YUJGIV	G. R. Andrade, B. Tirloni, (2015) <i>CSD Communication (Private Communication)</i> (https://doi.org/10.5517/cc1j9wxm)
YUJGIV01	G. R. Andrade, J. Kunsminskas, L. Pizzuti, A. dos Anjos, S. D. Inglez, B. Tirloni, P. H. Suegama, <i>Inorg. Chem. Commun.</i> 61 (2015) 210. (https://doi.org/10.1016/j.inoche.2015.09.022)
YUJGIV02	G. R. Andrade, B. Tirloni, (2015) <i>CSD Communication (Private Communication)</i> (https://doi.org/10.5517/cc1j9wvk)

TABLE S-IV. Complexes in which a Schiff base of aminoguanidine has a role of a counter-ion

REFCODE	Reference
QIBPIA	J. Valdes-Martinez, J. H. Alstrum-Acevedo, R. A. Toscano, G. Espinosa-Perez, B. A. Helfrich, D. X. West, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> 57 (2001) m137 (https://doi.org/10.1107/S1600536801003725)
QELLAX	M. M. Radanovic, M. V. Rodic, L. S. Vojinovic-Jesic, S. Armakovic, S. J. Armakovic, V. M. Leovac, <i>Inorg. Chim. Acta</i> 473 (2018) 160 (https://doi.org/10.1016/j.ica.2017.12.038)
QELKOK	M. M. Radanovic, M. G. Jelic, N. Z. Romcevic, N. Boukos, L. S. Vojinovic-Jesic, V. M. Leovac, B. B. Hadzic, B. M. Bajac, L. F. Nad, C. Chandrinou, S. S. Balos, <i>Mater. Res. Bull.</i> 70 (2015) 951 (https://doi.org/10.1016/j.materresbull.2015.06.034)
MINQIJ	J. Valdes-Martinez, J. H. Alstrum-Acevedo, R. A. Toscano, S. Hernandez-Ortega,
MINQOP	G. Espinosa-Perez, D. X. West, B. Helfrich, <i>Polyhedron</i> 21 (2002) 409
MINQUV	(https://doi.org/10.1016/S0277-5387(01)01006-3)
FOWLEJ	Rui-jun Xu, <i>Acta Crystallogr., Sect. E: Struct. Rep. Online</i> , 65 (2009) m951 (https://doi.org/10.1107/S1600536809027196)
YUMZUD	M. M. Radanovic, M. G. Jelic, N. Z. Romcevic, N. Boukos, L. S. Vojinovic-Jesic, V. M. Leovac, B. B. Hadzic, B. M. Bajac, L. F. Nad, C. Chandrinou, S. S. Balos, <i>Mater. Res. Bull.</i> 70 (2015) 951 (https://doi.org/10.1016/j.materresbull.2015.06.034)
GEMJIS	Yu. M. Chumakov, V. I. Tsapkov, G. Bocelli, B. Ya. Antosyak, S. G. Shova, A. P. Gulya, <i>Kristallografiya (Russ.) (Crystallogr. Rep.)</i> 51 (2006) 66 (https://doi.org/10.5517/cc8w206)
YEDJUM	E. B. Shamuratov, Kh. T. Sharipov, A. S. Batsanov, Yu. T. Struchkov, A. B. Khudoyarov, F. F. Mirdzhalalov, <i>Koord. Khim. (Russ.) (Coord. Chem.)</i> 19 (1993) 155
KABLEH	Xiaoni Gao, Ting An, Jizhen Li, Fengqi Zhao, Xuezhong Fan, Xinyan Li, Guofang Zhang, Ziwei Gao, <i>Z. Anorg. Allg. Chem.</i> 642 (2016) 155 (https://doi.org/10.1002/zaac.201500690).

TABLE S-V. Coordination bond distances and angles in $[\text{Cd}_2\text{Cl}_6(\text{HL})_2]$.

Bond	Bond distance, Å	Bonds	Bond angle, °
Cd1–Cl1	2.5632(3)	Cl1–Cd1–Cl3	112.948(9)
Cd1–Cl2	2.5638(3)	Cl2–Cd1–Cl3	96.734(9)
Cd1–Cl3	2.5272(3)	N3–Cd1–Cl3	85.334(18)
Cd1–Cl1 ⁱ	2.7148(3)	N5–Cd1–Cl2	96.50(2)
Cd1–N3	2.7483(8)	Cl1–Cd1–N3	161.69(3)
Cd1–N5	2.2992(8)	Cl2–Cd1–Cl1 ⁱ	174.132(7)

Symmetry code: (i) 1–x, 1–y, 2–z.

TABLE S-VI. Coordination bond distances and angles in $[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{XY}]\cdot\text{H}_2\text{O}$

Bond	Bond distance, Å	Bonds	Bond angle, °
Cd1–N7	2.285(2)	N7–Cd1–N5a	88.46(8)
Cd1–N8	2.348(2)	N7–Cd1–N3a	78.18(8)
Cd1–Cl1/Br1	2.580(14)/2.636(3)	N7–Cd1–N8	166.11(9)
Cd1–S1/Br2	2.663(3)/2.72(2)	N8–Cd1–N3a	88.24(8)
Cd1–N3	2.605(2)	N5a–Cd1–N8	88.66(8)
Cd1–N5	2.348(2)	N5a–Cd1–Cl1	99.6(3)
		N5a–Cd1–Br1	97.73(8)
		N3a–Cd1–S1	98.99(8)
		N3a–Cd1–Br2	99.3(6)

TABLE S-VII. Potential interactions in $[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{XY}]\cdot\text{H}_2\text{O}$ involving substitutionally disordered ligands

D–H···A	$d(\text{D–H}) / \text{Å}$	$d(\text{H···A}) / \text{Å}$	$\angle(\text{D–H···A}) / ^\circ$	Symmetry codes:
N2a–H2a···N6 _c	0.86	2.057	159.31	–x+1, –y+1, –z+2
N4a–H4a···N6 _c	0.86	2.451	143.07	x+1, –y+1, –z+2
C7a–H7a···Br1 _a	0.93	3.103	125.78	
N2a–H2a···Br1 _a	0.86	2.601	143.44	–x+1, –y+1, –z+1
N2a–H2a···Cl1 _b	0.86	2.464	142.65	–x+1, –y+1, –z+1
N4a–H2a···Br1 _a	0.86	2.854	139.63	–x+1, –y+1, –z+1
N4a–H2a···Cl1 _b	0.86	2.636	140.57	–x+1, –y+1, –z+1
O1–H1a···S1 _c	0.92	2.511	164.41	x–1, y, z

TABLE S-VIII. Global packing features of idealized structures derived from complex **2**.

Idealized structure	Crystal packing coefficient	Anion volume defined by Hirshfeld surface, Å ³	Anion mole ratio in 2
$[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{Br}(\text{SCN})]\cdot\text{H}_2\text{O}$	0.675	468.9	0.61
$[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{Cl}(\text{SCN})]\cdot\text{H}_2\text{O}$	0.669	466.8	0.35
$[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{Br}_2]\cdot\text{H}_2\text{O}$	0.653	466.8	0.03
$[\text{HL}][\text{Cd}(\text{HL})(\text{NCS})_2\text{BrCl}]\cdot\text{H}_2\text{O}$	0.647	464.8	0.01