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Zinc Coordination Polymers Containing Isomeric Forms of p-(Thiazolyl)benzoic Acid: Blue-Emitting Materials with a Solvatochromic Response to Water

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Abstract

© 2017 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim Two coordination polymers of assorted dimensionality (1D, 2D) have been prepared, namely [Zn 3 (L 2Th) 4 (OH) 2 ·2(HL 2Th)] ∞ (1) and [Zn(L 5Th)(OAc)] ∞ (2), starting from Zn II salts and the isomeric forms of the organic linker p-(thiazolyl)benzoic acid: p-(2-thiazolyl)benzoic acid (HL 2Th) and p-(5-thiazolyl)benzoic acid (HL 5Th). The isomers have been prepared ad hoc, following straightforward Pd-catalyzed C–C coupling reaction protocols. In 1, the deprotonated ligand is coordinated through its carboxylate group only, with dangling thiazole groups. The –COO – units are bridging adjacent metal centers, thus creating a 1D chain. The Zn 3 cluster is made of one six-coordinate (O h) and two four-coordinate (T d) Zn II ions; triple-bridging μ 3 -OH groups are balancing the overall positive charge. The structure of 2 is instead made of Zn 2 (carboxylate) 4 “paddle-wheel” dimers as the constituting inorganic node. The octahedral metal coordination sphere includes two μ-(κ-COO) benzoate spacers, two μ-(κ-COO) acetate ions, the thiazole N atoms coming from adjacent building blocks, and a weak Zn···Zn axial interaction. The resulting final assembly is two-dimensional (2D), where p-(5-thiazolyl)benzoate adopts a genuine μ-[κ(COO):κ(N)] bridging coordination mode. The luminescent properties of both polymers have been analyzed in the solid state; they feature ligand-centered emissions at λ = 434 nm (1) and λ = 427 nm (2). These electronic transitions fall in the visible region, giving the samples a characteristic blue color under an ordinary UV lamp (excitation at λ = 254 nm). The theoretical analysis of the electronic features of the ligands and related molecular orbitals reveals that the observed transitions are mainly of π→π* nature, involving π orbitals delocalized on both aromatic cycles. A significant (reversible) blueshift of the emission maximum of ca. 60 nm, from the visible to the UV region, has been observed for 1 when suspended in water.

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Keywords

Coordination polymers, Luminescence, Solvatochromism, Thiazole, Zinc

References

[1] For recent general reviews/articles on the MOF topic, see: a) Metal–Organic Frameworks and Hybrid Materials (themed issue), CrystEngComm 2015, 17;

[2] Metal–Organic Frameworks (themed issue), Chem. Soc. Rev. 2014, 43
[3] J.-R. Li, J. Sculley and H.-C. Zhou, Chem. Rev., 2012, 112, 869–932;
[4] J.-R. Li, R. J. Kuppler and H.-C. Zhou, Chem. Soc. Rev., 2009, 38, 1477–1504.
[5] A. Dhakshinamoorthy and E. Garcia, Chem. Soc. Rev., 2012, 41, 5262–5284;
[6] M. Yoon, R. Srirambalaji and K. Kim, Chem. Rev., 2012, 112, 1196–1231;
[7] K. P. Lillerud, U. Olsbye and M. Tilset, Top. Catal., 2010, 53, 859–868.
[8] C. M. Doherty, D. Buso, A. J. Hill, S. Furukawa, S. Kitagawa and P. Falcaro, Acc. Chem. Res., 2014, 47, 396–405;
[9] R. Ricco, L. Malfatti, M. Takahashi, A. J. Hill and P. Falcaro, J. Mater. Chem. A, 2013, 1, 13033–13045;
[10] E. Coronado and G. M. Espallargas, Chem. Soc. Rev., 2013, 42, 1525–1539.
[11] H. Li, M. Eddaoudi, M. O'Keeffe and O. M. Yaghi, Nature, 1999, 402, 276–279.
[12] D. T. Vodak, M. E. Braun, J. Kim, M. Eddaoudi and O. M. Yaghi, Chem. Commun., 2001, 2534–2535.
[13] M. E. Chapman, P. Ayyappan, B. M. Foxman, G. T. Yee and W. Lin, Cryst. Growth Des., 2001, 1, 159–163.
[14] Y.-C. He, J. Yang, G.-C. Yang, W.-Q. Kann and J.-F. Ma, Chem. Commun., 2012, 48, 7859–7861.
[15] F. Yi, D. Chen, M. Wu, L. Han and H. Jiang, ChemPlusChem, 2016, 81, 675–690;
[16] J. Heine and K. Müller-Buschbaum, Chem. Soc. Rev., 2013, 42, 9232–9242;
[17] L. E. Kreno, K. Leong, O. K. Farha, M. Allendorf, R. P. Van Duyne and J. T. Hupp, Chem. Rev., 2012, 112, 1105–1125;
[18] Y. Cui, Y. Yue, G. Qian and B. Chen, Chem. Rev., 2012, 112, 1126–1162.
[19] Some examples are: a) D. Chen, N.-N. Zhang, C.-S. Liu and M. Du, J. Mater. Chem. C, 2017, 5, 2311–2317;
[20] W. Yan, C. Zhang, S. Chen, L. Han and H. Zheng, ACS Appl. Mater. Interfaces, 2017, 9, 1629–1634;
[21] G. Zeng, S. Xing, X. Wang, Y. Yang, D. Ma, H. Liang, L. Gao, J. Hua, G. Li, Z. Shi and S. Feng, Inorg. Chem., 2016, 55, 1089–1095;
[22] X.-M. Lin, J.-L. Niu, P.-X. Wen, Y. Pang, L. Hu and Y.-P. Cai, Cryst. Growth Des., 2016, 16, 4705–4710;
[23] X.-Z. Song, S.-Y. Song, S.-N. Zhao, Z.-M. Hao, M. Zhu, X. Meng, L.-L. Wu and H.-J. Zhang, Adv. Funct. Mater., 2014, 24, 4034–4041;
[24] Z. Hao, X. Song, M. Zhu, X. Meng, S. Zhao, S. Su, W. Yang and S. Song, J. Mater. Chem. A, 2013, 1, 11043–11050.
[25] A. Douvali, A. C. Tsipis, S. V. Eliseeva, S. Petoud, G. S. Papaefstathiou, C. D. Malliakas, I. Papadas, G. S. Armatas, I. Margiolaki, M. G. Kanatzidis, T. Lazarides and M. J. Manos, Angew. Chem. Int. Ed., 2015, 54, 1651–1656;
[26] Angew. Chem., 2015, 127, 1671.
[27] F. Drache, V. Bon, I. Senkovska, M. Adam, A. Eychmüller and S. Kaskel, Eur. J. Inorg. Chem., 2016, 4483–4489.
[28] S. L. Jackson, A. Rananaware, C. Rix, S. V. Bhosale and K. Latham, Cryst. Growth Des., 2016, 16, 3067–3071;
[29] F. Wang, W. Liu, S. J. Teat, F. Xu, H. Wang, X. Wang, L. An and J. Li, Chem. Commun., 2016, 52, 10249–10252;
[30] X.-L. Hu, C. Qin, L. Zhao, F.-H. Liu, K.-Z. Shao and Z.-M. Su, RSC Adv., 2015, 5, 49606–49613;
[31] J. Yang, L. Zhang, X. Wang, R. Wang, F. Dai and D. Sun, RSC Adv., 2015, 5, 62982–62988;
[32] J. Cui, Y. Li, Z. Guo and H. Zheng, Chem. Commun., 2013, 49, 555–557;
[33] J. Cui, Z. Lu, Y. Li, Z. Guo and H. Zheng, Chem. Commun., 2012, 48, 7967–7969;
[34] R. Grünker, V. Bon, A. Heerwig, N. Klein, P. Müller, U. Stoeck, I. A. Baburin, U. Mueller, I. Senkovska and S. Kaskel, Chem. Eur. J., 2012, 18, 13299–13303.
[35] Y. Yu, J.-P. Ma, C.-W. Zhao, J. Yang, X.-M. Zhang, Q.-K. Liu and Y.-B. Dong, Inorg. Chem., 2015, 54, 11590–11592;
[36] J.-H. Wang, M. Li and D. Li, Chem. Sci., 2013, 4, 1793–1801.
[37] H.-R. Tian, C.-Y. Gao, Y. Yang, J. Ai, C. Liu, Z.-G. Xu and Z.-M. Sun, New J. Chem., 2017, 41, 1137–1141;
[38] F.-Y. Yi, Y. Wang, J.-P. Li, D. Wu, Y.-Q. Lan and Z.-M. Sun, Mater. Horiz., 2015, 2, 245–251.
[39] C. I. C. Esteves, A. M. F. Silva, M. M. M. Raposo and S. P. G. Costa, Tetrahedron, 2009, 65, 9373–9377;
[40] R. M. F. Batista, S. P. G. Costa and M. M. M. Raposo, Tetrahedron Lett., 2004, 45, 2825–2828.
[41] S.-H. Lee, A. Otomo, T. Nakahama, T. Yamada, T. Kamikado, S. Yokoyama and S. Mashiko, J. Mater. Chem., 2002, 12, 2187–2188;
[42] E. M. Breitung, C.-F. Shu and R. J. McMahon, J. Am. Chem. Soc., 2000, 122, 1154–1160.
[43] A. Dessì, M. Calamante, A. Mordini, M. Peruzzini, A. Sinicropi, R. Basosi, F. Fabrizi de Biani, M. Taddei, D. Colonna, A. di Carlo, G. Reginato and L. Zani, RSC Adv., 2015, 5, 32657–32668;
[44] A. Dessì, M. Calamante, A. Mordini, M. Peruzzini, A. Sinicropi, R. Basosi, F. Fabrizi de Biani, M. Taddei, D. Colonna, A. di Carlo, G. Reginato and L. Zani, Chem. Commun., 2014, 50, 13952–13955;

[45] A. Dessì, M. Calamante, A. Mordini, L. Zani, M. Taddei and G. Reginato, RSC Adv., 2014, 4, 1322–1328.

[46] A. Rossin and G. Giambastiani, CrystEngComm, 2015, 17, 218–228;

[47] A. Rossin, G. Tuci, G. Giambastiani and M. Peruzzini, ChemPlusChem, 2014, 79, 406–412;

[48] G. Tuci, G. Giambastiani, S. Kwon, P. C. Stair, R. Q. Snurr and A. Rossin, ACS Catal., 2014, 4, 1032–1039;

[49] A. Rossin, B. Di Credico, G. Giambastiani, M. Peruzzini, G.-Pescitelli, G. Reginato, E. Borfecchia, D. Gianolio, C. Lamberti and S. Bordiga, J. Mater. Chem., 2012, 22, 10335–10344;

[50] A. Rossin, B. Di Credico, G. Giambastiani, L. Gonsalvi, M. Peruzzini and G. Reginato, Eur. J. Inorg. Chem., 2011, 539–548.

[51] S. Staderini, G. Tuci, M. D'Angelantonio, F. Manoli, I. Manet, G. Giambastiani, M. Peruzzini and A. Rossin, ChemistrySelect, 2016, 1, 1123–1131.

[52] The ligand is insoluble in water at pH ≤ 6. Consequently, no reaction occurs in the absence of an auxiliary base.

[53] Some (selected) examples are: a) Y. Fu, G. Li, F. Liao, M. Xiong and J. Lin, J. Mol. Struct., 2011, 1004, 252–256;

[54] K.-Z. Shao, Y.-H. Zhao, Y.-Q. Lan, X.-L. Wang, Z.-M. Su and R.-S. Wang, CrystEngComm, 2011, 13, 889–896;

[55] S. Hazra, B. Sarkar, S. Naiya, M. G. B. Drew and A. Ghosh, Polyhedron, 2012, 46, 8–15;

[56] E.-C. Yang, H.-K. Zhao, B. Ding, X.-G. Wang and X.-J. Zhao, Cryst. Growth Des., 2007, 7, 2009–2015;

[57] N. L. Rosi, J. Kim, M. Eddaoudi, B. Chen, M. O'Keeffe and O. M. Yaghi, J. Am. Chem. Soc., 2005, 127, 1504–1518;

[58] T. Loiseau, H. Muguerra, G. Ferey, M. Haouas and F. Taulelle, J. Solid State Chem., 2005, 178, 621–628;

[59] X.-L. Wang, C. Qin, E.-B. Wang, Z.-M. Su, L. Xu and S. R. Batten, Chem. Commun., 2005, 4789–4791.

[60] V. A. Blatov, A. P. Shevchenko, D. M. Proserpio, Cryst. Growth Des. 2014, 14, 3576-3586. http://topospro.com/.

[61] Some (selected) examples are: a) F.-K. Wang, S.-Y. Yang, R.-B. Huang, L.-S. Zheng and S. R. Batten, CrystEngComm, 2008, 10, 1211–1215;

[62] H. Kwak, S. H. Lee, S. H. Kim, Y. M. Lee, B. K. Park, E. Y. Lee, Y. J. Lee, C. Kim, S.-Y. Kim and Y. Kim, Polyhedron, 2008, 27, 3484–3492;

[63] Y.-G. Lee, H. R. Moon, Y. E. Cheon and M. P. Suh, Angew. Chem. Int. Ed., 2008, 47, 7741–7745;

[64] Angew. Chem., 2008, 120, 7855;

[65] B.-Q. Ma, K. L. Mulfort and J. T. Hupp, Inorg. Chem., 2005, 44, 4912–4914;

[66] R. N. Devi, M. Edgar, J. Gonzalez, A. M. Z. Slawin, D. P. Tunstall, P. Grewal, P. A. Cox and P. A. Wright, J. Phys. Chem. B, 2004, 108, 535–543;

[67] B. Moulton, H. Abourahma, M. W. Bradner, J. Lu, G. J. McManus and M. J. Zaworotko, Chem. Commun., 2003, 1342–1343.

[68] Similar Zn–N(thiazole) distances can be found in: a) L. You, S. R. Long, V. M. Lynch and E. V. Anslyn, Chem. Eur. J., 2011, 17, 11017–11023;

[69] S. W. Suh, C.-H. Kim and I. H. Kim, Acta Crystallogr., Sect. E: Struct. Rep. Online, 2011, 67, m135–m136;

[70] L.-Y. Zhang, X.-C. Shen, Y. Yang and H. Liang, Acta Crystallogr., Sect. E: Struct. Rep. Online, 2009, 65, m1517;

[71] L.-Y. Wang, C.-X. Zhang, D.-Z. Liao, Z.-H. Jiang and S.-P. Yan, J. Mol. Struct., 2003, 657, 1–6.

[72] S. C. Abrahams and J. L. Bernstein, Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem., 1969, 25, 1233–1236.

[73] The difference between the calculated and experimental values is due to the underestimation of the HOMO–LUMO gap that normally occurs with DFT methods. See: G. Zhang and C. B. Musgrave, J. Phys. Chem. A, 2007, 111, 1554–1561.

[74] R. Ye, L. Ling and Y. Yao, Inorg. Chim. Acta, 2016, 453, 8–15;

[75] R. Ye, X. Zhang, J. Zhai, Y. Qin, L. Zhang, Y. Yao and J. Zhang, CrystEngComm, 2015, 17, 9155–9166;

[76] L. Yang, L. Zeng, W. Gu, J. Tian, S. Liao, M. Zhang, X. Wei, L. Xin and X. Liu, Inorg. Chem. Commun., 2013, 29, 76–81.

[77] R. Siebert, Y. Tian, R. Camacho, A. Winter, A. Wild, A. Krieg, U. S. Schubert, J. Popp, I. G. Scheblykin and B. Dietzek, J. Mater. Chem., 2012, 22, 16041–16050.

[78] L. Chen, J.-W. Ye, H.-P. Wang, M. Pan, S.-Y. Yin, Z.-W. Wei, L.-Y. Zhang, K. Wu, Y.-N. Fan and C.-Y. Su, Nat. Commun., 2017, 8, 15985;

[79] L. Chen, S.-Y. Yin, M. Pan, K. Wu, H.-P. Wang, Y.-N. Fana and C.-Y. Su, J. Mater. Chem. C, 2016, 4, 6962–6966.

[80] A. Dondoni, M. Fogagnolo, A. Medici and E. Negrini, Synthesis, 1987, 2, 185–186;

[81] A. Dondoni, A. R. Mastellari, A. Medici, E. Negrini and P. Pedrini, Synthesis, 1986, 9, 757–760.

[82] CrysAlis CCD 1.171.31.2 (release 07–07– 2006), CrysAlis171.NET, Oxford Diffraction Ltd.

[83] CrysAlis RED 1.171.31.2 (release 07–07– 2006), CrysAlis171.NET, Oxford Diffraction Ltd.

[84] A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, J. Appl. Crystallogr., 1999, 32, 115–119.

[85] G. M. Sheldrick, SHELXL, 1997, University of Göttingen, Göttingen, Germany.

[86] M. Nardelli, Comput. Chem., 1983, 7, 95–98.

[87] L. J. Farrugia, J. Appl. Crystallogr., 1997, 30, 565.

[88] A. Pérez-Perarnau, S. Preciado, C. M. Palmeri, C. Moncunill-Massaguer, D. Iglesias-Serret, D. M. Gonzales-Gironès, M. Miguel, S. Karasawa, S. Sakamoto, A. M. Cosialls, C. Rubio-Patiño, J. Saura-Esteller, R. Ramón, L. Caja, I. Fabregat, G. Pons, H. Handa, F. Albericio, J. Gil and R. Lavilla, Angew. Chem. Int. Ed., 2014, 53, 10150–10154;

[89] Angew. Chem., 2014, 126, 10314.

[90] J. Albaneze-Walker, R. Raju, J. A. Vance, A. J. Goodman, M. R. Reeder, J. Liao, M. T. Maust, P. A. Irish, P. Espino and D. R. Andrews, Org. Lett., 2009, 11, 1463–1466.

[91] The C{H} NMR assignments for tertiary C atoms have been made through 2D H–C HETCOR experiments (see also Figure S5), while for quaternary C atoms, the assignment has been made through a comparison with the (known) starting materials.

[92] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT.

[93] Y. Zhao and D. G. Truhlar, Theor. Chem. Acc., 2008, 120, 215–241.