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Smart Polymorphism of Thiacalix[4]arene with Long-Chain Amide Containing Substituents

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Abstract

© 2017 American Chemical Society. A problem of controlled (smart) formation of polymorphs was solved for a set of tert-butylthiacalix[4]arene derivatives with four N-(--acetoxyethyl)carbamoylmethoxy substituents at the lower rim with 1,3-alternate, cone, and partial cone conformations. For this, an effective polymorph screening with a reproducible influence of preparation history was achieved using guest vapor inclusion and a standard state of host glass powder. By this procedure with consequent guest release and heating, the ability of the studied calixarenes for polymorphism was investigated and compared as a function of their macrocycle conformation. The data of simultaneous thermogravimetry and differential scanning calorimetry with mass spectrometry of evolved vapors were determined together with the data of powder X-ray diffraction for the initial host samples, intermediate clathrates, and final polymorphs. In addition, single crystal X-ray diffraction data were obtained for four crystalline forms of the studied calixarenes. The results yielded a structure-property relationship, where 1,3-alternate calixarene without an extended H-bonded supramolecular network at least in one crystalline form has a much higher ability for polymorphism than the other two conformations. Thus, 10 polymorphs with essentially different crystal packing were found for this calixarene including a unique tetramorphism with four consecutive melting points of guest-free polymorph and corresponding three crystallization ranges. This ability of 1,3-alternate calixarene is linked with its other smart property: selective crystallization of its compact glass in vapors of binary liquid mixtures, which can be used for visual detection of very small benzene impurities (0.5% (v/v)) in cyclohexane.

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References

[1] Hilfiker, R.; Blatter, F.; von Raumer, M. Relevance of Solid-state Properties for Pharmaceutical Products. In Polymorphism in the Pharmaceutical Industry; Hilfiker, R., Eds.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, 2006; pp 1-19.

[2] Zhang, G. G. Z.; Zhou, D. Crystalline and Amorphous Solids. In Developing Solid Oral Dosage Forms, 1 st ed.; Qiu, Y., Chen, Y., Zhang, G. G. Z., Liu, L., Porter, W., Eds.; Academic Press: New York, 2009; pp 25-60.

[3] Lee, E. H. Asian J. Pharm. Sci. 2014, 9, 163-175 10.1016/j.ajps.2014.05.002

[4] Bernstein, J. Polymorphism in Molecular Crystals, 1 st ed.; Oxford University Press: New York, 2002.

[5] Fraxedas, J. Molecular Organic Materials From Molecules to Crystalline Solids, 1 st ed.; Cambridge University Press: Cambridge, 2006.

[6] Price, S. L. Chem. Soc. Rev. 2014, 43, 2098-2111 10.1039/C3CS60279F

[7] Bucar, D.-K.; Lancaster, R. W.; Bernstein, J. Angew. Chem., Int. Ed. 2015, 54, 6972-6993 10.1002/anie.201410356

[8] Aitipamula, S.; Chow, P. S.; Tan, R. B. H. CrystEngComm 2014, 16, 3451-3465 10.1039/c3ce42008f

[9] Park, Y.; Lee, J.; Lee, S. H.; Choi, H. G.; Mao, C.; Kang, S. K.; Choi, S.-E.; Lee, E. H. Cryst. Growth Des. 2013, 13, 5450-5458 10.1021/cg401405g

[10] Yu, L.; Reutzel-Edens, S. M.; Mitchell, C. A. Org. Process Res. Dev. 2000, 4, 396-402 10.1021/op000028v

[11] Thirunahari, S.; Aitipamula, S.; Chow, P. S.; Tan, R. B. H. J. Pharm. Sci. 2010, 99, 2975-2990 10.1002/jps.22061

[12] Grzesiak, A. L.; Lang, M.; Kim, K.; Matzger, A. J. J. Pharm. Sci. 2003, 92, 2260-2271 10.1002/jps.10455

[13] Nangia, A. Acc. Chem. Res. 2008, 41, 595-604 10.1021/ar700203k

[14] Llinàs, A.; Goodman, J. M. Drug Discovery Today 2008, 13, 198-210 10.1016/j.drudis.2007.11.006

[15] Kelly, R. C.; Rodríguez-Hornedo, N. Org. Process Res. Dev. 2009, 13, 1291-1300 10.1021/op900133z

[16] Gu, C.-H.; Young, V., Jr.; Grant, D. J. W. J. Pharm. Sci. 2001, 90, 1878-1890 10.1002/jps.1137.abs

[17] Lee, J.; Boerrigter, S. X. M.; Jung, Y. W.; Byun, Y.; Yuk, S. H.; Byrn, S. R.; Lee, E. H. Eur. J. Pharm. Sci. 2013, 50, 253-262 10.1016/j.ejps.2013.07.004

[18] Lang, P.; Kiss, V.; Ambrus, R.; Farkas, G.; Szabo-Revesz, P.; Aigner, Z.; Varkonyi, E. J. Pharm. Biomed. Anal. 2013, 84, 177-183 10.1016/j.jpba.2013.06.002

[19] Thallapally, P. K.; McGrail, B. P.; Atwood, J. L.; Gaeta, C.; Tedesco, C.; Neri, P. Chem. Mater. 2007, 19, 3355-3357 10.1021/cm0709121

[20] Tian, J.; Thallapally, P. K.; McGrail, B. P. CrystEngComm 2012, 14, 1909-1919 10.1039/c2ce06457j

[21] Thallapally, P. K.; McGrail, B. P.; Dalgarno, S. J.; Schaef, H. T.; Tian, J.; Atwood, J. L. Nat. Mater. 2008, 7, 146-150 10.1038/nmat2097

[22] Herbert, S. A.; Janiak, A.; Thallapally, P. K.; Atwood, J. L.; Barbour, L. J. Chem. Commun. 2014, 50, 15509-15512 10.1039/C4CC07366E

[23] Tian, J.; Thallapally, P. K.; Dalgarno, S. J.; Atwood, J. L. J. Am. Chem. Soc. 2009, 131, 13216-13217 10.1021/ja904658p

[24] Aaltonen, J.; Alleso, M.; Mirza, S.; Koradia, V.; Gordon, K. C.; Rantanen Eur. J. Pharm. Biopharm. 2009, 71, 23-37 10.1016/j.ejpb.2008.07.014

[25] Bolla, G.; Mittapalli, S.; Nangia, A. Cryst. Growth Des. 2014, 14, 5260-5274 10.1021/cg5010424

[26] Giron, D. J. Therm. Anal. Calorim. 2001, 64, 37-60 10.1023/A:1011572610005

[27] Näther, C.; Jess, I.; Seyfarth, L.; Bärwinkel, K.; Senker, J. Cryst. Growth Des. 2015, 15, 366-373 10.1021/cg501464m

[28] Huang, J.; Dali, M. J. Pharm. Biomed. Anal. 2013, 86, 92-99 10.1016/j.jpba.2013.08.004

[29] Uzoh, O. G.; Cruz-Cabeza, A. J.; Price, S. L. Cryst. Growth Des. 2012, 12, 4230-4239 10.1021/cg3007348

[30] López-Mejías, V.; Matzger, A. J. Cryst. Growth Des. 2015, 15, 3955-3962 10.1021/acs.cgd.5b00570

[31] Zipp, C. F.; Dirr, H. W.; Fernandes, M. A.; Marques, H. M.; Michael, J. P. Cryst. Growth Des. 2013, 13, 3463-3474 10.1021/cg400356s

[32] Thakur, T. S.; Dubey, R.; Desiraju, G. R. Annu. Rev. Phys. Chem. 2015, 66, 21-42 10.1146/annurev-physche--040214-121452

[33] Desiraju, G. R. Angew. Chem., Int. Ed. Engl. 1995, 34, 2311-2327 10.1002/anie.199523111

[34] Shishkin, O. V.; Zubatyuk, R. I.; Shishkina, S. V.; Dyakonenko, V. V.; Medviediev, V. V. Phys. Chem. Chem. Phys. 2014, 16, 6773-6786 10.1039/c3cp55390f

[35] Dunitz, J. D. Chem. Commun. 2003, 545-548 10.1039/b211531j

[36] Cruz-Cabeza, A. J.; Reutzel-Edens, S. M.; Bernstein, J. Chem. Soc. Rev. 2015, 44, 8619-8635 10.1039/C5CS00227C

[37] Lhotak, P.; Himl, M.; Stibor, I.; Petrickova, H. Tetrahedron Lett. 2002, 43, 9621-9624 10.1016/S0040-4039(02)02391-2

[38] Galyaltdinov, S. F.; Ziganshin, M. A.; Drapailo, A. B.; Gorbatchuk, V. V. J. Phys. Chem. B 2012, 116, 11379-11385 10.1021/jp3065739

[39] Gataullina, K. V.; Ziganshin, M. A.; Stoikov, I. I.; Gubaidullin, A. T.; Gorbatchuk, V. V. Phys. Chem. Chem. Phys. 2015, 17, 15887-15895 10.1039/C5CP02042E

[40] Yakimov, A. V.; Ziganshin, M. A.; Gubaidullin, A. T.; Gorbatchuk, V. V. Org. Biomol. Chem. 2008, 6, 982-985 10.1039/b800187a

[41] Safina, G. D.; Gavrilova, O. M.; Ziganshin, M. A.; Stoikov, I. I.; Antipin, I. S.; Gorbatchuk, V. V. Mendeleev Commun. 2011, 21, 291-292 10.1016/j.mencom.2011.09.022

[42] Nomura, E.; Takagaki, M.; Nakaoka, C.; Taniguchi, H. J. Org. Chem. 2000, 65, 5932-5936 10.1021/jo000165q

[43] Dalgarno, S. J.; Tian, J.; Warren, J. E.; Clark, T. E.; Makha, M.; Raston, C. L.; Atwood, J. L. Chem. Commun. 2007, 4848-4850 10.1039/b712621b

[44] Atwood, J. L.; Barbour, L. J.; Jerga, A. Chem. Commun. 2002, 2952-2953 10.1039/b209718b

[45] Smith, V. J.; Marais, C. G.; Suwińska, K.; Lipkowski, J.; Szumna, A.; Esterhuysen, C.; Barbour, L. J. CrystEngComm 2015, 17, 5129-5133 10.1039/C5CE00362H

[46] Surov, O. V.; Voronova, M. I.; Smirnov, P. R.; Mamardashvili, N. Z.; Shaposhnikov, G. P. CrystEngComm 2012, 14, 533-536 10.1039/C1CE05469D

[47] Morohashi, N.; Ebata, K.; Nakayama, H.; Noji, S.; Hattori, T. Cryst. Growth Des. 2017, 17, 891-900 10.1021/acs.cgd.6b01765

[48] Morohashi, N.; Shibata, O.; Miyoshi, I.; Kitamoto, Y.; Ebata, K.; Nakayama, H.; Hattori, T. Cryst. Growth Des. 2016, 16, 4671-4678 10.1021/acs.cgd.6b00748

[49] Brouwer, E. B.; Enright, G. D.; Udachin, K. A.; Lang, S.; Ooms, K. J.; Halchuk, P. A.; Ripmeester, J. A. Chem. Commun. 2003, 1416-1417 10.1039/b301739g

[50] Atwood, J. L.; Barbour, L. J.; Lloyd, G. O.; Thallapally, P. K. Chem. Commun. 2004, 922-923 10.1039/b402452b

[51] Thallapally, P. K.; Lloyd, G. O.; Atwood, J. L.; Barbour, L. J. Angew. Chem., Int. Ed. 2005, 44, 3848-3851 10.1002/anie.200500749

[52] Newman, A. Am. Pharm. Rev. 2011, 14, 44-46

[53] Gorbatchuk, V. V.; Gatiatulin, A. K.; Ziganshin, M. A. Gas/Solid Complexation and Inclusion. In Reference Module in Chemistry, Molecular Sciences and Chemical Engineering; Elsevier, 2016.

[54] Yakimova, L. S.; Ziganshin, M. A.; Sidorov, V. A.; Kovalev, V. V.; Shokova, E. A.; Tafeenko, V. A.; Gorbatchuk, V. V. J. Phys. Chem. B 2008, 112, 15569-15575 10.1021/jp804277u

[55] Gorbatchuk, V. V.; Tsifarkin, A. G.; Antipin, I. S.; Solomonov, B. N.; Konovalov, A. I.; Seidel, J.; Baitalov, F. J. Chem. Soc., Perkin Trans.2 2000, 2, 2287-2294 10.1039/b003477k

[56] Gorbatchuk, V. V.; Tsifarkin, A. G.; Antipin, I. S.; Solomonov, B. N.; Konovalov, A. I.; Lhotak, P.; Stibor, I. J. Phys. Chem. B 2002, 106, 5845-5851 10.1021/jp014352j

[57] Ziganshin, M. A.; Yakimov, A. V.; Safina, G. D.; Solovieva, S. E.; Antipin, I. S.; Gorbatchuk, V. V. Org. Biomol. Chem. 2007, 5, 1472-1478 10.1039/B701082F

[58] Andronis, V.; Yoshioka, M.; Zografi, G. J. Pharm. Sci. 1997, 86, 346-351 10.1021/js9602711

[59] Nguyen Thi, Y.; Rademann, K.; Emmerling, F. CrystEngComm 2015, 17, 9029-9036 10.1039/C5CE01583A

[60] Green, D. P.; Jain, V.; Bailey, B.; Wagner, M.; Clark, M.; Valeri, D.; Lakso, S. Proc. SPIE 2013, 8679, 867912-867925 10.1117/12.2011805

[61] Kaestner, M.; Hofer, M.; Rangelow, I. W. Proc. SPIE 2013, 8680, 868019-868028 10.1117/12.2011535

[62] Nimse, S. B.; Kim, T. Chem. Soc. Rev. 2013, 42, 366-386 10.1039/C2CS35233H

[63] Hilfiker, R.; De Paul, S. M.; Szelagiewicz, M. Approaches to Polymorphism Screening. In Polymorphism in the Pharmaceutical Industry; Hilfiker, R., Eds.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, 2006; pp 287-308.

[64] Strydom, S.; Liebenberg, W.; Yu, L.; de Villiers, M. Int. J. Pharm. 2009, 379, 72-81 10.1016/j.ijpharm.2009.06.012

[65] Petit, S.; Coquerel, G. The Amorphous State. In Polymorphism in the Pharmaceutical Industry; Hilfiker, R., Eds.; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, 2006; pp 259-285.

[66] Gorbachuk, E. V.; Badeeva, E. K.; Zinnatullin, R. G.; Pavlov, P. O.; Dobrynin, A. B.; Gubaidullin, A. T.; Ziganshin, M. A.; Gerasimov, A. V.; Sinyashin, O. G.; Yakhvarov, D. G. J. Organomet. Chem. 2016, 805, 49-53 10.1016/j.jorganchem.2016.01.008

[67] Surana, R.; Pyne, A.; Suryanarayanan, R. Pharm. Res. 2004, 21, 1167-1176 10.1023/B:PHAM.0000033003.17251.c3

[68] Safina, G. D.; Validova, L. R.; Ziganshin, M. A.; Stoikov, I. I.; Antipin, I. S.; Gorbatchuk, V. V. Sens. Actuators, B 2010, 148, 264-268 10.1016/j.snb.2010.04.032

[69] Thallapally, P. K.; Dobrzańska, L.; Gingrich, T. R.; Wirsig, T. B.; Barbour, L. J.; Atwood, J. L. Angew. Chem. 2006, 118, 6656-6659 10.1002/ange.200601391

[70] Zhukov, A. Yu.; Fink, T. A.; Stoikov, I. I.; Antipin, I. S. Russ. Chem. Bull. 2009, 58, 1007-1014 10.1007/s11172-009-0129-9

[71] APEX2 (Version 2.1), SAINTPlus. Data Reduction and Correction Program (Version 7.31A, Bruker Advanced X-ray Solutions; BrukerAXS Inc.: Madison, Wisconsin, USA, 2006.

[72] Sheldrick, G. M. SADABS, Program for Empirical X-ray Absorption Correction; Bruker-Nonius, 2004.

[73] Sheldrick, G. M. SHELXTL v.6.12, Structure Determination Software Suite; Bruker AXS: Madison, WI, 2000.

[74] Farrugia, L. J. J. Appl. Crystallogr. 1999, 32, 837-838 10.1107/S0021889899006020

[75] Bruker, APEX3, SAINT and SADABS; Bruker AXS Inc.: Madison, Wisconsin, USA, 2015.

[76] Sheldrick, G. M. Acta Crystallogr., Sect. A: Found. Adv. 2015, 71, 3-8 10.1107/S2053273314026370

[77] Sheldrick, G. M. Acta Crystallogr. 2015, C71, 3-8

[78] Macrae, C. F.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Shields, G. P.; Taylor, R.; Towler, M.; van de Streek, J. J. Appl. Crystallogr. 2006, 39, 453-457 10.1107/S002188980600731X

[79] Spek, A. L. J. Appl. Crystallogr. 2003, 36, 7-13 10.1107/S0021889802022112

[80] Kawakami, K. J. Pharm. Sci. 2007, 96, 982-989 10.1002/jps.20748

[81] Bachler, J.; Fuentes-Landete, V.; Jahn, D. A.; Wong, J.; Giovambattista, N.; Loerting, T. Phys. Chem. Chem. Phys. 2016, 18, 11058-11068 10.1039/C5CP08069J

[82] Ostwald, W. Z. Phys. Chem. 1897, 22, 289-330

[83] Wang, F. C.; Feve, M.; Lam, T. M.; Pascault, J.-P. J. Polym. Sci., Part B: Polym. Phys. 1994, 32, 1305-1313 10.1002/polb.1994.090320801

[84] Amombo Noa, F. M.; Bourne, S. A.; Nassimbeni, L. R. Cryst. Growth Des. 2015, 15, 3271-3279 10.1021/acs.cgd.5b00402