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References and Notes

- [1] R. S. Shallenberger, *J. Food Sci.* **1963**, *28*, 584-589.
- [2] R. S. Shallenberger and T. E. Acree, *Nature* **1967**, *216*, 480-482; *J. Agric. Food Chem.* **1969**, *17*, 701-703.
- [3] L. B. Kier, *J. Pharm. Sci.* **1972**, *61*, 1394-1397.
- [4] For a pertinent review, see: C.-K. Lee, *Adv. Carbohydr. Chem. Biochem.* **1987**, *45*, 199-351.
- [5] A. Faurion and P. MacLeod, in: *Nutritive Sweeteners* (Eds.: G. G. Birch and K. J. Parker), Applied Science Publ., London / New Jersey, **1982**, pp. 247-273.
- [6] A. Faurion, *Progr. Sensory Physiology* **1987**, *8*, 129-201.
- [7] (a) A. Faurion, S. Saito, and P. MacLeod, *Chem. Senses* **1980**, *5*, 107-121. – (b) A. Faurion, *Progress in Sensory Physiology*, Springer-Verlag Berlin / Heidelberg, **1987**, pp. 129-201.
- [8] G. E. DuBois, D. E. Walters, S. S. Schiffmann, Z. S. Warwick, B. J. Booth, S. D. Pecore, K. Gibes, B. T. Carr, and L. M. Bran, in: *Sweeteners: Discovery, Molecular Design, and Chemoreception* (Eds.: D. E. Walter, F. T. Orthoefer, and G. E. DuBois), ACS Symposium Series #450, Am. Chem. Soc., Washington, D.C., **1991**, pp. 261-276.
- [9] A. Faurion and C. Vayssettes-Courchay, *Brain Res.* **1990**, *512*, 317-332.
- [10] G. G. Birch, *Food Technol.* **1991**, *45*, 114-120.
- [11] (a) D. Lancet and N. Ben-Arie, in: *Sweeteners: Discovery, Molecular Design, and Chemoreception* (Eds.: D. E. Walter, F. T. Orthoefer, and G. E. DuBois), ACS Symposium Series #450, Am. Chem. Soc., Washington, D.C., **1991**, pp. 226-236. – (b) S. A. Simon, *ibid.*, pp. 237-250.
- [12] G. E. DuBois, D. E. Walters, and M. S. Kellogg, in: *Sweet Taste Chemoreception* (Eds.: G. G. Birch, J. A. Kanters, and M. Mathlouthi), Elsevier Appl. Science, London / New York, **1993**, pp. 237-267.
- [13] I. Tvaroška and S. Pérez, *Carbohydr. Res.* **1986**, *149*, 389-410.
- [14] A. D. French and J. W. Brady, Eds., *Computer Modeling of Carbohydrate Molecules*, ACS Symposium Series #430, Am. Chem. Soc., Washington, D.C., **1990**.
- [15] B. Meyer, *Top. Curr. Chem.* **1990**, *154*, 141-208.
- [16] J. W. Brady, *Adv. Biophys. Chem.* **1990**, *1*, 155-202.
- [17] F. W. Lichtenthaler, S. Immel, and U. Kreis, *Starch / Stärke* **1991**, *43*, 121-132; and in: *Carbohydrates as Organic Raw Materials* (Ed.: F. W. Lichtenthaler), VCH Publ., Weinheim / New York, **1991**, pp. 1-32.
- [18] F. W. Lichtenthaler, *Zuckerindustrie (Berlin)* **1991**, *116*, 701-712.
- [19] F. W. Lichtenthaler and S. Immel, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London / New York, **1993**, pp. 21-53.
- [20] M. Mathlouthi and M. O. Portmann, *J. Mol. Struct.* **1990**, *237*, 327-338.
- [21] L. Hough and R. Khan, in: *Progress in Sweeteners* (Ed.: T. H. Grenby), Elsevier Appl. Science, London / New York, **1989**, pp. 97-120.
- [22] C. E. James, L. Hough, and R. Khan, *Progr. Chem. Org. Nat. Prod.* **1989**, *55*, 117-184.

- [23] (a) L. Hough, in: *Carbohydrates as Organic Raw Materials* (Ed.: F. W. Lichtenthaler), VCH Publ., Weinheim / New York, **1991**, pp. 33-55. – (b) L. Hough and R. Khan, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London / New York, **1993**, pp. 91-102 and 269-282.
- [24] R. S. Shallenberger, *Agric. Sci. Rev.* **1964**, *2*, 11-20; see also Ref. [4], p. 260.
- [25] G. M. Brown, and H. A. Levy, *Science* **1963**, *141*, 921-923; *Acta Crystallogr., Sect. B*, **1973**, *29*, 790-797.
- [26] J. C. Hanson, L. C. Sieker, and L. H. Jensen, *Acta Crystallogr., Sect. B*, **1973**, *29*, 797-808.
- [27] A. Allerhand, D. Doddrell, and R. Komoroski, *J. Chem. Phys.* **1971**, *55*, 189-198.
- [28] K. Bock, B. Meyer, and M. Vignon, *J. Mag. Reson.* **1980**, *38*, 545-551.
- [29] K. Bock and R. U. Lemieux, *Carbohydr. Res.* **1982**, *100*, 63-74.
- [30] J. C. Christofides and D. B. Davies, *J. Chem. Soc., Chem. Commun.* **1985**, 1533-1534.
- [31] D. C. McCain and J. L. Markley, *Carbohydr. Res.* **1986**, *152*, 73-80; *J. Am. Chem. Soc.* **1986**, *108*, 4259-4264; *J. Mag. Reson.* **1987**, *73*, 244-251.
- [32] D. B. Davies and J. C. Christofides, *Carbohydr. Res.* **1987**, *163*, 269-274.
- [33] H. Kovacs, S. Bagley, and J. Kowalewski, *J. Mag. Reson.* **1989**, *85*, 530-541.
- [34] L. Poppe and H. van Halbeek, *J. Am. Chem. Soc.* **1992**, *114*, 1092-1094.
- [35] B. Adams and L. Lerner, *J. Mag. Reson.* **1992**, *96*, 604-607.
- [36] B. Adams and L. Lerner, *J. Am. Chem. Soc.* **1992**, *114*, 4827-4829.
- [37] J. M. Duker and A. S. Serianni, *Carbohydr. Res.* **1993**, *249*, 281-303.
- [38] (a) V. H. Tran and J. W. Brady, *Biopolymers* **1990**, *29*, 961-976; 977-997. – (b) J. W. Brady, *Adv. Biophys. Chem.* **1990**, *1*, 155-202. – (c) V. H. Tran and J. W. Brady, in: *Computer Modeling of Carbohydrate Molecules* (Eds.: A. D. French and J. W. Brady), ACS Symposium Series #430, Am. Chem. Soc., Washington D. C., **1990**, pp. 213-226.
- [39] C. H. du Penhoat, A. Imberty, N. Roques, V. Michon, J. Mentech, G. Descotes, and S. Pérez, *J. Am. Chem. Soc.* **1991**, *113*, 3720-3727.
- [40] S. Pérez, C. Meyer, A. Imberty, and A. D. French, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London / New York, **1993**, pp. 55-73.
- [41] E. S. Stevens and C. A. Duda, *J. Am. Chem. Soc.* **1991**, *113*, 8622-8627.
- [42] A. D. French and L. Schäfer, S. Q. Newton, *Carbohydr. Res.* **1993**, *239*, 51-60.
- [43] A. D. French and M. K. Dowd, *J. Mol. Struct. (Theochem)* **1993**, *286*, 183-201.
- [44] R. R. W. Hooft, *Ph.D. Thesis*, University of Utrecht, **1993**.
- [45] (a) H. J. Lindner, *PIMM88 – Closed Shell PI-SCF-LCAO-MO-Molecular Mechanics Program*, Technische Hochschule Darmstadt, **1988**. – (b) H. J. Lindner, *Tetrahedron* **1974**, *30*, 1127-1132. – (c) A. E. Smith, *Ph.D. Thesis*, Technische Hochschule Darmstadt, **1989**. – (d) A. E. Smith and H. J. Lindner, *J. Comput.-Aided Mol. Des.* **1991**, *5*, 235-262.
- [46] (a) F. M. Richards, *Ann. Rev. Biophys. Bioeng.* **1977**, *6*, 151-176; *Carlsberg. Res. Commun.* **1979**, *44*, 47-63. – (b) M. L. Connolly, *J. Appl. Cryst.* **1983**, *16*, 548-558; *Science* **1983**, *221*, 709-713.
- [47] B. Lee and F. M. Richards, *J. Mol. Biol.* **1971**, *55*, 379-400.
- [48] (a) J. Brickmann, *MOLCAD – MOLEcular Computer Aided Design*, Technische Hochschule Darmstadt, **1992**. The major part of the MOLCAD program is included in the MOLCAD-module of the SYBYL package of TRIPOS Associates, St. Louis, USA. – (b) J. Brickmann and M. Waldherr-Teschner, *Labo (Hoppenstedt Verlag, Darmstadt)* **1989**, *10*, 7-14; *Informationstechnik (Oldenburg Verlag, München)* **1991**, *33*, 83-90. – (c) J. Brickmann, *J. Chim. Phys.* **1992**, *89*, 1709-1721. – (d) M. Waldherr-Teschner,

- T. Goetze, W. Heiden, M. Knoblauch, H. Vollhardt, and J. Brickmann, in: *Advances in Scientific Visualization* (Eds.: F. H. Post, A. J. S. Hin), Springer Verlag, Heidelberg, **1992**, pp. 58-67. – (e) J. Brickmann, T. Goetze, W. Heiden, G. Moeckel, S. Reiling, H. Vollhardt, and C.-D. Zachmann, *Interactive Visualization of Molecular Scenarios with MOLCAD/SYBYL*, in: *Insight and Innovation in Data Visualization* (Ed.: J. E. Bowie), Manning Publications Co., Greenwich, **1994**, in press.
- [49] (a) P. K. Weiner, R. Langridge, J. M. Blaney, R. Schaefer, and P. A. Kollman, *Proc. Natl. Acad. Sci. USA* **1982**, *79*, 3754-3758. – (b) C. E. Dykstra, *Chem. Rev.* **1993**, *93*, 2339-2353.
- [50] J. J. P. Stewart, *J. Comput.-Aided Mol. Des.* **1990**, *4*, 1-105; *MOPAC V5.0, Quantum Chem. Prog. Exch., Program No. 455*, **1983**.
- [51] M. J. S. Dewar, E. G. Zoebisch, E. F. Healy, and J. J. P. Stewart, *J. Am. Chem. Soc.* **1985**, *107*, 3902-3909.
- [52] (a) G. A. Jeffrey, *Carbohydr. Res.* **1973**, *28*, 233-241. – (b) G. A. Jeffrey, M. E. Gress, and S. Takagi, *J. Am. Chem. Soc.* **1977**, *99*, 609-611. – (c) Y.-C. Tse and M. D. Newton, *J. Am. Chem. Soc.* **1977**, *99*, 611-613. – (d) G. A. Jeffrey and L. Lewis, *Carbohydr. Res.* **1978**, *60*, 179-182. – (e) G. A. Jeffrey and S. Takagi, *Acc. Chem. Res.* **1978**, *11*, 264-270. – (f) G. A. Jeffrey and J. Mitra, *Acta Crystallogr., Sect. B*, **1983**, *39*, 469-480. – (g) G. A. Jeffrey, *Acta Crystallogr., Sect. B*, **1990**, *46*, 89-103.
- [53] G. A. Jeffrey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer Verlag, Berlin / New York, **1991**.
- [54] G. A. Jeffrey, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London / New York, **1993**, pp. 1-10.
- [55] C. H. Hamann, J. Schneider, P. Schmittinger, and R. Stephan, *Ger. Offen.* DE 3.346.131 (**1985**) [*Chem. Abstr.* **1985**, *103*, 61502g].
- [56] S. Nakajima, T. Masumizu, K. Arai, C. Shaw, K. Nozawa, and K. Kawai, *Stud. Org. Chem. (Recent Adv. Electroorg. Synth.)* **1987**, *30*, 265-268 [*Chem. Abstr.* **1988**, *108*, 94168j].
- [57] (a) P. Wolf, H. Polligkeit, and C. H. Hamann, *Dechema-Monographie 124*, VCH Verlagsgesellschaft, Weinheim / New York, **1991**, pp. 525-532. – (b) S. Fischer, H. Polligkeit, P. Wolf, and C. H. Hamann, *Dechema-Monographie 125*, VCH Verlagsgesellschaft, Weinheim / New York, **1992**, pp. 649-658. – (c) C. H. Hamann, S. Fischer, H. Polligkeit, and P. Wolf, *J. Carbohydr. Chem.* **1993**, *12*, 173-190.
- [58] W. Heiden, G. Moeckel, and J. Brickmann, *J. Comput.-Aided Mol. Des.* **1993**, *7*, 503-514.
- [59] M. Teschner, C. Henn, H. Vollhardt, S. Reiling, and J. Brickmann, *J. Mol. Graphics* **1994**, *12*, 98-105.
- [60] See Ref. [22], p. 166.
- [61] See Ref. [21], p. 108.
- [62] L. Hough, *Internat. Sugar J.* **1989**, *91*, 23-37.
- [63] M. G. Lindley, G. G. Birch, and R. Khan, *J. Sci. Food Agric.* **1976**, *27*, 140-144.
- [64] L. Hough and R. Khan, *Trends Biochem. Sci.* **1978**, *3*, 61-63.
- [65] L. Hough and E. O'Brien, *Carbohydr. Res.* **1980**, *84*, 95-102.
- [66] For pyranoses in general, the conformation of the endocyclic 6-CH₂OH hydroxymethyl groups is defined by the two torsion angles O₅-C₅-C₆-O₆ ($\equiv \omega$, $g = gauche$, $t = trans$) and C₄-C₅-C₆-O₆; accordingly, the three staggered rotamers are gg ($\omega = -60^\circ$), gt ($\omega = +60^\circ$), and tg ($\omega = \pm 180^\circ$); see also Fig. 6-1 on p. 149.
- [67] O. Hassel and B. Ottar, *Acta Chem. Scand.* **1947**, *1*, 929-942.
- [68] R. U. Lemieux and J. T. Brewer, *Adv. Chem. Ser.* **1973**, *117*, 121-146.
- [69] S. Pérez, J. St.-Pierre, and R. H. Marchessault, *Can. J. Chem.* **1978**, *56*, 2866-2871.

- [70] R. H. Marchessault and S. Pérez, *Biopolymers* **1979**, *18*, 2369-2374.
- [71] J. W. Brady, *J. Am. Chem. Soc.* **1986**, *108*, 8153-8160.
- [72] L. M. J. Kroon-Batenburg and J. Kroon, *Biopolymers* **1990**, *29*, 1243-1248.
- [73] K. Bock and J. Ø. Duus, *J. Carbohydr. Chem.* **1994**, *13*, 513-543.
- [74] L. Hough and S. P. Phadnis, *Nature* **1976**, *263*, 800.
- [75] L. Hough, *Chem. Soc. Rev.* **1985**, *14*, 357-374.
- [76] M. R. Jenner, in: *Developments in Food Carbohydrates* (Ed.: C. K. Lee), Elsevier Appl. Science, London / New York, Vol. 2, **1981**, pp. 91-143.
- [77] M. R. Jenner, in: *Progress in Sweeteners* (Ed.: T. H. Grenby), Elsevier Appl. Science, London / New York, **1989**, pp. 121-141.
- [78] M. R. Jenner, in: *Sweeteners: Discovery, Molecular Design, and Chemoreception* (Eds.: D. E. Walter, F. T. Orthofer, and G. E. DuBois), ACS Symposium Series #450, Am. Chem. Soc., Washington, D.C., **1991**, pp. 68-87.
- [79] C. K. Lee, *Carbohydr. Res.* **1987**, *162*, 53-63.
- [80] (a) L. Hough, S. P. Phadnis, R. A. Khan, and M. R. Jenner (Tate & Lyle), *Brit. Pat.* 1.543.167 (1977), *Ger. Offen.* 2.700.917 (1977) [*Chem. Abstr.* **1977**, *87*, 202019v]. – (b) L. Hough, S. P. Phadnis, R. A. Khan, and M. R. Jenner (Tate & Lyle), *Ger. Offen.* 2.700.036 (1977) [*Chem. Abstr.* **1977**, *87*, 202020p]. – (c) R. A. Khan, L. Hough, and S. P. Phadnis (Tate & Lyle), *Brit. Pat.* 1.543.168 (1979) [*Chem. Abstr.* **1979**, *91*, 193577d].
- [81] G. Jackson, M. R. Jenner, R. A. Khan, C. K. Lee, K. S. Mufti, G. D. Patel, and E. B. Rathbone, (Tate & Lyle), *Brit. Pat.* 2.104.063 (**1982**), *Eur. Pat. Appl.* EP 73.093 (**1983**) [*Chem. Abstr.* **1983**, *99*, 54127j].
- [82] (a) C. K. Lee (Tate & Lyle), *Brit. Pat.* 2.088.855 (1982), *Eur. Pat. Appl.* EP 50.952 (1982) [*Chem. Abstr.* **1982**, *97*, 145225q]. – (b) C. K. Lee (Tate & Lyle), *US Pat.* 4.405.654 (1983) [*Chem. Abstr.* **1984**, *100*, 33495b].
- [83] R. A. Khan, K. S. Mufti, and G. D. Patel (Tate & Lyle), *Brit. Pat.* 2.127.806, *Eur. Pat. Appl.* EP 103.479 (1984) [*Chem. Abstr.* **1984**, *101*, 23887n].
- [84] G. Jackson, M. R. Jenner, and R. A. Khan (Tate & Lyle), *Brit. Pat.* 2.101.989 (1982), *Eur. Pat. Appl.* EP 67.535 (1982) [*Chem. Abstr.* **1983**, *98*, 161107d].
- [85] (a) R. A. Khan and M. R. Jenner (Tate & Lyle), *Brit. Pat.* 2.037.561 (1980), *Eur. Pat. Appl.* EP 10.409 (1980) [*Chem. Abstr.* **1980**, *93*, 130944s]. – (b) R. A. Khan and M. R. Jenner (Tate & Lyle), *Brit. Pat.* 2.036.007 A (1980), *Eur. Pat. Appl.* EP 10.410 (1980) [*Chem. Abstr.* **1980**, *93*, 150590b].
- [86] (a) J. Reicherzer, *Die Zeit (München)*, No. 40 (**Sept. 26, 1991**), 31. – (b) Current Affairs – Sweetener News, *Zuckerindustrie (Berlin)* **1993**, *118*, 283.
- [87] (a) M. R. Jenner and D. Waite (Tate & Lyle PLC), *Brit. Pat.* 2.065.646 (1980), *Eur. Pat. Appl.* EP 30.804 (1981) [*Chem. Abstr.* **1981**, *95*, 169699g]. – (b) J. A. Kanters, R. L. Scherrenberg, B. R. Leeflang, J. Kroon, and M. Mathlouthi, *Carbohydr. Res.* **1988**, *180*, 175-182.
- [88] J. C. Christofides, D. B. Davies, J. A. Martin, and E. B. Rathbone, *J. Am. Chem. Soc.* **1986**, *108*, 5738-5743.
- [89] J. A. Kanters, G. Roelofsen, B. P. Alblas, and I. Meinders, *Acta Crystallogr., Sect. B*, **1977**, *33*, 665-672.
- [90] S. Takagi and G. A. Jeffrey, *Acta Crystallogr., Sect. B*, **1977**, *33*, 3510-3515.
- [91] R. S. Shallenberger and T. E. Acree, in: *Handbook of Sensory Physiology 4; Chemical Senses, Part 2 – Taste*, Springer Verlag, Berlin, **1971**, pp. 221-277.
- [92] See Ref. [21], most notably pp. 102-103.
- [93] R. S. Shallenberger, *Pure Appl. Chem.* **1978**, *50*, 1409-1420.

- [94] (a) B. Schneider, F. W. Lichtenthaler, G. Steinle, and H. Schiweck, *Liebigs Ann. Chem.* **1985**, 2443-2453. – (b) F. W. Lichtenthaler and S. Rönninger, *J. Chem. Soc., Perkin Trans. 2*, **1990**, 1489-1497.
- [95] (a) T. A. W. Koerner Jr., R. J. Voll, L. W. Cary, and E. S. Younathan, *Biochem. Biophys. Res. Commun.* **1978**, 82, 1273-1278. – (b) M. Jaseja, A. S. Perlin, and P. Dais, *Mag. Reson. Chem.* **1990**, 28, 283-289. – (c) S. J. Angyal, *Adv. Carbohydr. Chem. Biochem.* **1984**, 42, 15-68 **1991**, 49, 19-35; *Carbohydr. Res.* **1994**, 263, 1-11.
- [96] (a) R. S. Shallenberger, T. E. Acree, and W. E. Guild, *J. Food Sci.* **1965**, 30, 560-563. – (b) R. S. Shallenberger and M. G. Lindley, *Food Chem.* **1977**, 2, 145-153.
- [97] M. G. Lindley and G. G. Birch, *J. Sci. Food Agric.* **1975**, 26, 117-124.
- [98] R. J. Woods, V. H. Smith Jr., W. A. Szarek, and A. Farazdel, *J. Chem. Soc., Chem. Commun.* **1987**, 937-939.
- [99] R. J. Woods, W. A. Szarek, and V. H. Smith Jr., *J. Am. Chem. Soc.* **1990**, 112, 4732-4741.
- [100] R. J. Woods, W. A. Szarek, and V. H. Smith Jr., *Can. J. Chem.* **1991**, 69, 1917-1928.
- [101] G. G. Birch, S. Shamil, and Z. Shepard, *Experientia* **1986**, 42, 1232-1234.
- [102] In the case of fructose, the conformation of the 1-CH₂OH hydroxymethyl group is defined by two dihedral angles, the first referring to the O₁-C₁-C₂-O₅ torsion angle (*g* = *gauche*, *t* = *trans*), the second to O₁-C₁-C₂-C₃. The three staggered conformers are hence *gg*, *gt*, and *tg*.
- [103] W. A. Szarek, S. L. Korppi-Tommola, O. R. Martin, and V. H. Smith Jr., *Can. J. Chem.* **1984**, 62, 1506-1511.
- [104] C. K. Lee and G. G. Birch, *J. Pharm. Sci.* **1976**, 65, 1222-1225.
- [105] O. R. Martin, S. L. Korppi-Tommola, and W. A. Szarek, *Can. J. Chem.* **1982**, 60, 1857-1862.
- [106] Y. Tsuzuki and J. Yamazaki, *Biochem. Z.* **1953**, 323, 525-531; *J. Chem. Soc. Jpn.* **1953**, 74, 596-601.
- [107] M. G. Lindley, R. S. Shallenberger, and R. L. Whistler, *J. Food Sci.* **1976**, 41, 575-577.
- [108] (a) T. Suami, S. Ogawa, M. Takata, K. Yasuda, A. Suga, K. Takei, and Y. Uematsu, *Chem. Lett.* **1985**, 719-722. – (b) T. Suami, S. Ogawa, M. Takata, K. Yasuda, K. Takei, and A. Suga, *Bull. Chem. Soc. Jpn.* **1986**, 59, 819-821. – (c) T. Suami, *Pure Appl. Chem.* **1987**, 59, 1509-1520.
- [109] W. Janikovich, *J. Neurosci.* **1982**, 2, 49.
- [110] J. C. J. Bart, *J. Chem. Soc., B*, **1968**, 376-382; Y. Okaya, *Acta Crystallogr., Sect. B*, **1969**, 25, 2257-2263; G. Jovanovski and B. Kamenar, *Cryst. Struct. Comm.* **1982**, 11, 247.
- [111] E. F. Paulus, *Acta Crystallogr., Sect. B*, **1975**, 31, 1191-1193.
- [112] M. Hatada, J. Jancarik, B. Graves, and S.-H. Kim, *J. Am. Chem. Soc.* **1985**, 107, 4279-4282.
- [113] E. Benedetti, B. DiBlasio, V. Pavone, C. Pedone, W. D. Fuller, D. F. Mierke, and M. Goodman, *J. Am. Chem. Soc.* **1990**, 112, 8909-8912.
- [114] (a) H. Frühbeis, R. Klein, and H. Wallmeier, *Angew. Chem.* **1987**, 99, 413-428; *Angew. Chem. Int. Ed. Engl.* **1987**, 26, 403-419. – (b) W. C. Ripka and J. E. Blaney, *Topics in Stereochemistry* **1991**, 20, 1-85.
- [115] (a) H.-J. Schneider, *Angew. Chem.* **1991**, 103, 1419-1439; *Angew. Chem. Int. Ed. Engl.* **1991**, 30, 1417-1436. – (b) M. Delaage, in: *Molecular Recognition Mechanisms* (Ed.: M. Delaage), VCH Publ., Weinheim / New York, **1991**, pp. 1-14.
- [116] C. Tanford, *The Hydrophobic Effect: Formation of Micelles and Biological Membranes*, Wiley, New York, **1973**.

- [117] W. Blokzijl and J. B. F. N. Engberts, *Angew. Chem.* **1993**, *105*, 1610-1648; *Angew. Chem. Int. Ed. Engl.* **1993**, *32*, 1545-1579.
- [118] N. G. J. Richards, P. B. Williams, and M. S. Tute, *Intern. J. Quantum Chem., Quantum Biol. Symp.* **1991**, *18*, 299-316; *Intern. J. Quantum Chem.* **1992**, *44*, 219-233.
- [119] (a) J. Brickmann, in: *Software Development in Chemistry* (Ed.: C. Jochum), GDCh Publ., Frankfurt, **1994**, pp. 139-156. – (b) P. V. Pixner, W. Heiden, H. Merx, G. Moeckel, A. Moeller, and J. Brickmann, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1309-1319.
- [120] M. Mathlouthi and D. V. Luu, *Carbohydr. Res.* **1980**, *81*, 203-212.
- [121] M. Mathlouthi, *Carbohydr. Res.* **1981**, *91*, 113-123.
- [122] D. Cremer and J. A. Pople, *J. Am. Chem. Soc.* **1975**, *97*, 1354-1358.
- [123] G. A. Jeffrey and R. Taylor, *Carbohydr. Res.* **1980**, *81*, 182-183.
- [124] G. A. Jeffrey and J. H. Yates, *Carbohydr. Res.* **1979**, *74*, 319-322.
- [125] A. D. French, private communication.
- [126] A. D. French, *Carbohydr. Res.* **1989**, *188*, 206-211.
- [127] W. F. van Gunsteren and H. J. C. Berendsen, *Groningen Molecular Simulation (GROMOS) Library Manual*, Biomos, Nijenborgh 16, Groningen, The Netherlands, **1987**.
- [128] D. J. Heisterberg, *QTRFIT – Rigid Body Rotation and Fitting Program*, The Ohio Supercomputer Center, Columbus, Ohio 43212, **1991**.
- [129] P. Kollman, *Chem. Rev.* **1993**, *93*, 2395-2417.
- [130] M. J. Mitchel and A. McCammon, *J. Comput. Chem.* **1991**, *12*, 271-275.
- [131] (a) G. M. Torrie and J. P. Valleau, *Chem. Phys. Lett.* **1974**, *28*, 578-581; *J. Comput. Phys.* **1977**, *23*, 187-199; *J. Chem. Phys.* **1977**, *66*, 1402-1406. – (b) M. Mezei and D. L. Beveridge, *Ann. N.Y. Acad. Sci.* **1986**, *482*, 1-23.
- [132] A. E. Mark, S. P. van Helden, P. E. Smith, L. H. M. Janssen, and W. F. van Gunsteren, *J. Am. Chem. Soc.* **1994**, *116*, 6293-6302.
- [133] P. J. Bernal and W. A. Van Hook, *J. Chem. Thermodyn.* **1986**, *18*, 955-968; 969-978.
- [134] M. V. Kaulgud and S. S. Dhondge, *Indian J. Chem., Sect. A*, **1988**, *27*, 6-11.
- [135] W. Heiden, M. Schlenkrich, and J. Brickmann, *J. Comput.-Aided Mol. Des.* **1990**, *4*, 255-269.
- [136] W. F. van Gunsteren and H. J. C. Berendsen, *Angew. Chem.* **1990**, *102*, 1020-1055; *Angew. Chem. Int. Ed. Engl.* **1990**, *29*, 992-1023.
- [137] E. Reinefeld and K. D. Heincke, *Chem. Ber.* **1971**, *104*, 265-269.
- [138] C. Chauvin, K. Baczko, and D. Plusquellec, *Zuckerindustrie (Berlin)* **1992**, *117*, 476; *J. Org. Chem.* **1993**, *58*, 2291-2295.
- [139] F. W. Lichtenthaler, S. Immel, D. Martin, and V. Müller, *Starch / Stärke* **1992**, *44*, 445-456; and in: *Carbohydrates as Organic Raw Materials II* (Ed.: G. Descotes), VCH Publ., Weinheim / New York, **1993**, pp. 59-98, and references cited therein.
- [140] See Ref. [53], Chapter 13: *Hydrogen Bonding in Carbohydrates*, pp. 169-219; most notably pp. 183-185 and 198.
- [141] K. Yoshimoto and Y. Tsuda, *Chem. Pharm. Bull.* **1983**, *31*, 4324-4334.
- [142] (a) R. U. Lemieux, *Chem. Soc. Rev.* **1989**, *18*, 347-374. – (b) F. A. Quiocho, *Pure Appl. Chem.* **1989**, *61*, 1293-1306.
- [143] S. Delrot, N. Roques, G. Descotes, and J. Mentech, *Plant Physiol. Biochem.* **1991**, *29*, 25-29.
- [144] (a) P. Furet, A. Sele, and N. C. Cohen, *J. Mol. Graphics* **1988**, *6*, 182-189. – (b) J.-L. Fauchère, P. Quarendon, and L. Kaetterer, *J. Mol. Graphics* **1988**, *6*, 202-206.

- [145] (a) A. K. Ghose and G. M. Crippen, *J. Comput. Chem.* **1986**, *7*, 565-577. – (b) A. K. Ghose, A. Pritchett, and G. M. Crippen, *J. Comput. Chem.* **1988**, *9*, 80-90.
- [146] V. N. Viswanadhan, A. K. Ghose, G. R. Revankar, and R. K. Robins, *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 163-172.
- [147] (a) P. J. Card, W. D. Hitz, and K. G. Ripp, *J. Am. Chem. Soc.* **1986**, *108*, 158-161. – (b) W. D. Hitz, P. J. Card, and K. G. Ripp, *J. Biol. Chem.* **1986**, *261*, 11986-11991.
- [148] C. Chothia, *Nature* **1974**, *248*, 338-339.
- [149] (a) K. A. Sharp, A. Nicholls, R. F. Fine, and B. Honig, *Science* **1991**, *252*, 106-109. – (b) K. A. Sharp, A. Nicholls, R. Friedman, and B. Honig, *Biochemistry* **1991**, *30*, 9686-9697.
- [150] A. Ben-Naim and R. M. Mazo, *J. Phys. Chem.* **1993**, *97*, 10829-10834.
- [151] H. van der Wel, A. van der Heyden, and H. G. Peer, *Food Rev. Int.* **1987**, *3*, 193-268.
- [152] T. H. Grenby, *Progress in Sweeteners*, Elsevier Appl. Science, London / New York, **1989**.
- [153] D. E. Walter, F. T. Orthoefer, and G. E. DuBois *Sweeteners: Discovery, Molecular Design, and Chemoreception*, ACS Symposium Series #450, Am. Chem. Soc., Washington, D.C., **1991**.
- [154] G. G. Birch, J. A. Kanters, and M. Mathlouthi, *Sweet Taste Chemoreception*, Elsevier Appl. Science, London / New York, **1993**.
- [155] G. A. Jeffrey, *J. Mol. Struct.* **1995**, in press.
- [156] C. Meyer, S. Pérez, C. H. Du Penhoat, and V. Michon, *J. Am. Chem. Soc.* **1993**, *115*, 10300-10310.
- [157] R. W. W. Hoof, J. A. Kanters, and J. Kroon, *J. Comput. Chem.* **1991**, *12*, 943-947.
- [158] R. W. W. Hoof, J. A. Kanters, and J. Kroon, in: *Sweet Taste Chemoreception* (Eds.: M. Mathlouthi, J. A. Kanters, and G. G. Birch), Elsevier Appl. Science, London / New York, **1993**, pp. 11-19.
- [159] P. K. Dinda, I. T. Beck, W. A. Szarek, G. W. Hay, E. R. Ison, and D. M. Vyas, *Can. J. Physiol. Pharm.* **1982**, *60*, 652-654.
- [160] E. W. Deutsch and C. Hansch, *Nature* **1966**, *211*, 75.
- [161] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in FORTRAN – The Art of Scientific Computing*, Cambridge University Press, **1992**, 2nd Edition, pp. 650-664, most notably pp. 660-664.
- [162] S. Immel, U. Kreis, and F. W. Lichtenthaler, **1991**, unpublished results.
- [163] S. Immel, *CP_PCDS V2.00 – 2D- and 3D-Contouring Program for Polar Coordinate Data Sets*, Technische Hochschule Darmstadt, **1994**.
- [164] (a) H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, and H. J. Hermans, in: *Intermolecular Forces* (Ed.: B. Pullman), Reidel, Dordrecht, The Netherlands, **1981**, pp. 331-342; *Biopolymers* **1984**, *23*, 1513-1518.
- [165] R. H. Stote, D. J. States, and M. Karplus, *J. Chim. Phys.* **1991**, *88*, 2419-2433.
- [166] H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, A. Dinola, and J. R. Haak, *J. Chem. Phys.* **1984**, *81*, 3684-3690.
- [167] (a) J.-P. Ryckaert, G. Cicotti, and H. J. C. Berendsen, *J. Comput. Phys.* **1977**, *23*, 327-341. – (b) W. F. van Gunsteren and H. J. C. Berendsen, *Mol. Phys.* **1977**, *34*, 1311-1327.
- [168] T. F. Osberger, *Food Sci. Technol.* **1986**, *17*, 245-275.
- [169] J. E. Bujake, *Food Sci. Technol.* **1986**, *17*, 277-294.
- [170] R. S. Shallenberger, T. E. Acree, and C.-K. Lee, *Nature* **1969**, *221*, 555-556.
- [171] (a) H.-D. Belitz, H. Rohse, W. Stempf, H. Wieser, J. Gasteiger, and C. Hiller, *Lebensmittelchem. Gerichtl. Chem.* **1987**, *41*, 77-82; *Dev. Food. Sci.* **1988**, *17*, 49-62. –

- (b) H.-D. Belitz, H. Rohse, W. Stempfl, H. Wieser, J. Gasteiger, and C. Hiller, in: *Frontiers of Flavour* (Ed.: G. Charalambous), Elsevier Appl. Science, Amsterdam, **1988**, pp. 49-62.
- [172] G. G. Birch and S. Shamil, *Food Chem.* **1986**, *21*, 245-258.
- [173] S. Shamil and G. G. Birch, *Endeavour* **1990**, *14*, 191-193.
- [174] S. E. Kemp, G. G. Birch, M. O. Portmann, and M. Mathlouthi, *J. Sci. Food Agric.* **1990**, *51*, 97-107.
- [175] T. L. Mega, S. Cortes, and R. L. van Etten, *J. Org. Chem.* **1990**, *55*, 522-528.
- [176] W. A. Szarek, S. L. Korppi-Tommola, H. F. Shurvell, V. H. Smith Jr., and O. R. Martin, *Can. J. Chem.* **1984**, *62*, 1512-1518.
- [177] T. Suami and L. Hough, *J. Carbohydr. Chem.* **1992**, *11*, 953-967.
- [178] Y. Yano and M. Janado, *Trends Glycosci. Glycotechn.* **1990**, *2*, 156-167.
- [179] R. J. Woods, W. A. Szarek, and V. H. Smith Jr., *J. Chem. Soc., Chem. Commun.* **1991**, 334-337.
- [180] S. Ogawa, Y. Uematsu, S. Yoshida, N. Sasaki, and T. Suami, *J. Carbohydr. Chem.* **1987**, *6*, 471-478.
- [181] R. F. Brady Jr., *Carbohydr. Res.* **1970**, *15*, 35-40.
- [182] W. L. Glen, G. Myers, and G. A. Grant, *J. Chem. Soc.* **1951**, 2568-2572.
- [183] S. Shamil, G. G. Birch, M. Dinovi, and R. Rafka, *Food Chem.* **1989**, *32*, 171-188.
- [184] L.-X. Gan and R. L. Whistler, *Carbohydr. Res.* **1990**, *205*, 45-51.
- [185] W. A. Szarek, O. R. Martin, R. J. Rafka, and T. S. Cameron, *Can. J. Chem.* **1985**, *63*, 1222-1227.
- [186] (a) R. S. Shallenberger, *Food Chem.* **1983**, *12*, 89-107. – (b) R. J. Haefeli and D. Glaser, *Lebensm.-Wiss. Technol.* **1990**, *23*, 523-527. – (c) J. Buitenhuis and J. A. Kanters, *Food Chem.* **1991**, *40*, 109-112. – (d) T. Suami and L. Hough, *J. Carbohydr. Chem.* **1991**, *10*, 851-860; *Food Chem.* **1993**, *46*, 235-238.
- [187] (a) G. V. Levin (Biospherics, Inc.), *US Pat.* 4.262.032 (1981) [*Chem. Abstr.* **1981**, *95*, 78771h]. – (b) Biospherics, Inc., *Jpn. Kokai Tokyo Koho JP* 82.129.671 [*Chem. Abstr.* **1982**, *97*, 197120w].
- [188] S. M. Tarka Jr., C. A. Shively, J. L. Apgar, and K. L. Koch (Hershey Foods Corp.), *Eur. Pat. Appl. EP* 423.771 [*Chem. Abstr.* **1991**, *115*, 99324m].
- [189] See Chapter 2 for a detailed discussion.
- [190] S. Nordenson, S. Takagi, and G. A. Jeffrey, *Acta Crystallogr., Sect. B*, **1979**, *35*, 1005.
- [191] P. J. Goodford, *J. Med. Chem.* **1985**, *28*, 849-857.
- [192] (a) *Cambridge Crystallographic Data File*, Version 5.04, **1993**, data sets with missing coordinates and more recent structure determinations have been included if atomic coordinates are provided within the written publications. The structure ref.-codes are listed in the corresponding references. – (b) F. H. Allen, S. A. Bellard, M. D. Brice, B. A. Cartwright, A. Doubleday, H. Higgs, T. Hummelink, B. G. Hummelink-Peters, O. Kennard, W. D. S. Motherwell, J. R. Rodgers, and D. G. Watson, *Acta Crystallogr., Sect. B*, **1979**, *35*, 2331-2339. – (c) F. H. Allen, O. Kennard, and R. Taylor, *Acc. Chem. Res.* **1983**, *16*, 146-153.
- [193] I. Tvaroška and T. Bleha, *Adv. Carbohydr. Chem. Biochem.* **1989**, *47*, 45-123.
- [194] F.-J. Flath, *Ph.D. Thesis*, Technische Hochschule Darmstadt, **1993**.
- [195] A. de Bruyn, M. Anteunis, and G. Verhegge, *Bull. Soc. Chim. Belg.* **1974**, *83*, 475-476.
- [196] R. Lichtel, *Ph.D. Thesis*, Technische Hochschule Darmstadt, **1984**.
- [197] F. W. Lichtenthaler and F. Hoyer, *Carbohydr. Res.*, **1994**, *253*, 141-150.
- [198] J. E. Kilpatrick, K. E. Pitzer, and R. Spitzer, *J. Am. Chem. Soc.* **1947**, *69*, 2483-2488.
- [199] C. Altona and M. Sundaralingam, *J. Am. Chem. Soc.* **1972**, *94*, 8205-8212.

- [200] S. C. Harvey and M. Prabhakaran, *J. Am. Chem. Soc.* **1986**, *108*, 6128-6136.
- [201] A. D. French and V. Tran, *Biopolymers* **1990**, *29*, 1599-1611.
- [202] A. D. French, N. Mouhous-Riou, and S. Pérez, *Carbohydr. Res.* **1993**, *247*, 51-62.
- [203] J. Kopf and P. Köll, *Carbohydr. Res.* **1984**, *135*, 29-46.
- [204] A. Cossé-Barbi, D. G. Watson, and J. E. Dubois, *Tetrahedron Lett.* **1989**, *30*, 163-166.
- [205] K. S. Pitzer and W. E. Donath, *J. Am. Chem. Soc.* **1959**, *81*, 3213-3218.
- [206] L. A. Carreira, G. J. Jiang, W. B. Person, and J. N. Willis Jr., *J. Chem. Phys.* **1972**, *56*, 1440-1443.
- [207] J. R. Durig and D. W. Wertz, *J. Chem. Phys.* **1968**, *49*, 2118-2121.
- [208] T. Ikeda, R. C. Lord, T. B. Malloy Jr., and T. Ueda, *J. Chem. Phys.* **1972**, *56*, 1434-1439.
- [209] R. Davidson and P. A. Warsop, *J. Chem. Soc., Faraday Trans. 2*, **1972**, *68*, 1875-1889.
- [210] T. H. Chao and J. Laane, *J. Mol. Spectrosc.* **1978**, *70*, 357-360.
- [211] L. E. Baumann and J. Laane, *J. Phys. Chem.* **1988**, *92*, 1040-1051.
- [212] W. J. Adams, H. J. Geise, and L. S. Bartell, *J. Am. Chem. Soc.* **1970**, *92*, 5013-5019.
- [213] T. R. Ferguson and C. L. Beckel, *J. Chem. Phys.* **1973**, *59*, 1905-191.
- [214] D. Cremer and J. A. Pople, *J. Am. Chem. Soc.* **1975**, *97*, 1358-1367.
- [215] D. Cremer, *Isr. J. Chem.* **1983**, *23*, 72-84.
- [216] J. A. Boatz, M. S. Gordon, and R. L. Hilderbrandt, *J. Am. Chem. Soc.* **1988**, *110*, 352-358.
- [217] D. M. Ferguson and D. J. Raber, *J. Am. Chem. Soc.* **1989**, *111*, 4371-4378.
- [218] R. L. Rosas, C. Cooper, J. Laane, *J. Phys. Chem.* **1990**, *94*, 1830-1836.
- [219] D. M. Ferguson, I. R. Gould, W. A. Glauser, S. Schroeder, and P. A. Kollman, *J. Comput. Chem.* **1992**, *13*, 525-532.
- [220] S. D. Morley, D. E. Jackson, M. R. Saunders, and J. G. Vinter, *J. Comput. Chem.* **1992**, *13*, 693-703.
- [221] (a) J. A. Greenhouse and H. L. Strauss, *J. Chem. Phys.* **1969**, *50*, 124-134. – (b) W. J. Lafferty, D. W. Robinson, R. V. St. Louis, J. W. Russell, and H. L. Strauss, *J. Chem. Phys.* **1965**, *42*, 2915-2919.
- [222] G. G. Engerholm, A. C. Luntz, W. D. Gwinn, and D. O. Harris, *J. Chem. Phys.* **1969**, *50*, 2446-2457.
- [223] (a) H. M. Seip, *Acta Chem. Scand.* **1969**, *23*, 2741-2747. – (b) A. Almenningen, H. M. Seip, and T. Willadsen, *Acta Chem. Scand.* **1969**, *23*, 2748-2754.
- [224] (a) J. B. Lambert, J. J. Papay, E. S. Magyar, and M. K. Neuberger, *J. Am. Chem. Soc.* **1973**, *95*, 4458-4460. – (b) J. B. Lambert, J. J. Papay, S. A. Khan, K. A. Kappauf, and E. S. Magyar, *J. Am. Chem. Soc.* **1974**, *96*, 6112-6118.
- [225] I. O. C. Ekejiuba and H. E. Hallam, *J. Chem. Soc., Sect. B*, **1970**, 209-211.
- [226] J. R. Durig, J. M. Karriker, and W. C. Harries, *Spectrochim. Acta* **1971**, *27A*, 1955-1971.
- [227] (a) C. D. Hurd and W. H. Saunders Jr., *J. Am. Chem. Soc.* **1952**, *74*, 5324-5329. – (b) S. A. Barker, J. S. Brimacombe, A. B. Foster, D. H. Whiffen, and G. Zweifel, *Tetrahedron* **1959**, *7*, 10-18.
- [228] (a) J. S. Chickos, J. Y.-J. Uang, and T. A. Keiderling, *J. Org. Chem.* **1991**, *56*, 2594-2596. – (b) R. Curci, L. D'Accolti, M. Fiorentino, C. Fusco, W. Adam, M. E. González-Nuñez, and R. Mello, *Tetrahedron Lett.* **1992**, *33*, 4225-4228.
- [229] T. Lis, *Acta Crystallogr., Sect. C*, **1986**, *42*, 1745-1747 (FAVBOT).
- [230] N. Narendra, T. P. Seshadri, and M. A. Viswamitra, *Acta Crystallogr., Sect. C*, **1985**, *41*, 1612-1614 (DEFLAB).

- [231] (a) S. Cerrini, V. M. Coiro, D. Lamba, and G. M. B. Bisso, *Carbohydr. Res.* **1986**, *147*, 183-190 (COWDOH01). – (b) N. Narendra, T. P. Seshadri, and M. A. Viswamitra, *Acta Crystallogr., Sect. C*, **1985**, *41*, 31-34 (COWDOH).
- [232] L. Den Drijver, C. W. Holzapfel, M. S. van Dyk, and G. J. Kruger, *Carbohydr. Res.* **1987**, *161*, 65-73 (GAFVUE).
- [233] T. Taniguchi, M. Sawada, T. Tanaka, and T. Uchiyama, *Carbohydr. Res.* **1988**, *177*, 13-20 (SANXEK).
- [234] T. Taniguchi and T. Uchiyama, *Carbohydr. Res.* **1982**, *107*, 255-262 (BIVZAH).
- [235] F. W. Lichtenthaler and E. Cuny, unpublished results.
- [236] C. A. Beevers and W. Cochran, *Proc. R. Soc. London, Ser. A* **1947**, *190*, 257-272 (SUCNAB).
- [237] C. A. Accorsi, F. Bellucci, V. Bertolasi, V. Ferretti, and G. Gilli, *Carbohydr. Res.* **1989**, *191*, 105-116 (DINYOO10).
- [238] J. D. Oliver and L. C. Strickland, *Acta Crystallogr., Sect. C*, **1984**, *40*, 820-824 (ZZZSTI01).
- [239] Y. Nawata, K. Ochi, M. Shiba, K. Morita, and Y. Iitaka, *Acta Crystallogr., Sect. B*, **1981**, *37*, 246-249 (KSCOSF).
- [240] M. G. B. Drew, H. Lindseth, and R. Khan, *Carbohydr. Res.* **1979**, *71*, 35-42 (IPASUC).
- [241] J. Novotny, J. Ondracek, B. Kratochvil, and K. Capek, *Z. Kristallogr.* **1991**, *197*, 189-196 (KOJBOA).
- [242] T. Taga, E. Inagaki, Y. Fujimori, K. Fujita, and K. Hara, *Carbohydr. Res.* **1993**, *241*, 63-69.
- [243] L. Hough, L. V. Sinchareonkul, A. C. Richardson, F. Akhtar, and M. G. B. Drew, *Carbohydr. Res.* **1988**, *174*, 145-160 (SAFZII).
- [244] J. A. Kanters, R. L. Scherrenberg, B. R. Leeftang, J. Kroon, and M. Mathlouthi, *Carbohydr. Res.* **1988**, *180*, 175-182 (KANJOY).
- [245] W. Dreissig, and P. Luger, *Acta Crystallogr., Sect. B*, **1973**, *29*, 514-521 (IMATUL).
- [246] (a) G. A. Jeffrey, R. A. Wood, P. E. Pfeffer, and K. B. Hicks, *J. Am. Chem. Soc.* **1983**, *105*, 2128-2133; The crystal structure analysis of lactulose (**36**) revealed the presence of three disordered isomers of the reducing fructose residue in a ratio of approx. β -furanose : α -furanose : β -pyranose \approx 76 : 10 : 14; only the atomic coordinates of the major β -fructofuranose compound were provided and thus considered in this study (BOBKUY10). – (b) R. A. Wood, G. A. Jeffrey, P. E. Pfeffer, and K. B. Hicks, *Am. Cryst. Assoc., Ser.* **1982**, *10*, 18 (BOBKUY). – (c) G. A. Jeffrey, De-bin Huang, P. E. Pfeffer, R. L. Dudley, K. B. Hicks, and E. Nitsch, *Carbohydr. Res.* **1992**, *226*, 29-42.
- [247] T. Taga, E. Inagaki, Y. Fujimori, and S. Nakamura, *Carbohydr. Res.* **1993**, *240*, 39-45; The y/b-coordinate of C-2 of the fructofuranosyl residue (C-2") was erroneously given as 0.0323 instead of 0.7323.
- [248] D. Avenel, A. Neuman, and H. Gillier-Pandraud, *Acta Crystallogr., Sect. B*, **1976**, *32*, 2598-2605 (MELEZT01).
- [249] J. Becquart, A. Neuman, and H. Gillier-Pandraud, *Carbohydr. Res.* **1982**, *111*, 9-21 (MELEZT02).
- [250] D. C. Rohrer, *Acta Crystallogr., Sect. B*, **1972**, *28*, 425-433 (PLANTE10).
- [251] G. A. Jeffrey and Y. J. Park, *Acta Crystallogr., Sect. B*, **1972**, *28*, 257-267 (KESTOS).
- [252] V. Ferretti, V. Bertolasi, G. Gilli, and C. A. Accorsi, *Acta Crystallogr., Sect. C*, **1984**, *40*, 531-535 (CELGII).
- [253] K. Okuyama, K. Noguchi, M. Saitoh, S. Ohno, S. Fujii, M. Tsukada, H. Takeda, and T. Hidano, *Bull. Chem. Soc. Jpn.* **1993**, *66*, 374-379.

- [254] (a) H. M. Berman, *Acta Crystallogr., Sect. B*, **1970**, *26*, 290-299 (RAFINO). – (b) G. A. Jeffrey and De-bin Huang, *Carbohydr. Res.* **1990**, *206*, 173-182 (RAFINO01).
- [255] (a) R. Gilardi and J. L. Flippen-Anderson, *Acta Crystallogr., Sect. C*, **1987**, *43*, 806-808 (STACHY10). – (b) R. D. Gilardi and J. L. Flippen, *J. Am. Chem. Soc.* **1975**, *97*, 6264-6266 (STACHY).
- [256] G. A. Jeffery and De-Bin Huang, *Carbohydr. Res.* **1991**, *210*, 89-104 (STACHY01).
- [257] (a) M. Sawada, T. Tanaka, Y. Takai, T. Hanafusa, K. Hirotsu, T. Higuchi, M. Kawamura, and T. Uchiyama, *Chem. Lett.*, **1990**, 2011-2014 (VIPRAN). – (b) M. Sawada, T. Tanaka, Y. Takai, T. Hanafusa, T. Taniguchi, M. Kawamura, and T. Uchiyama, *Carbohydr. Res.* **1991**, *217*, 7-17.
- [258] J. A. Kanters, J. Buitenhuis, J. Kroon, M. Mathlouthi, J. H. van der Maas, and B. Lutz, *J. Crystallogr. Spectrosc. Res.* **1990**, *20*, 1-8 (KEMXOP).
- [259] M. J. Dianez, A. Lopez-Castro, and R. Marquez, *Acta Crystallogr., Sect. C*, **1988**, *44*, 657-660 (GEMYEC).
- [260] F. W. Lichtenthaler, unpublished data.
- [261] (a) P. Swaminathan, L. Anderson, and M. Sundaralingam, *Carbohydr. Res.* **1979**, *75*, 1-10 (DXSORF). – (b) S. T. Rao, P. Swaminathan, and M. Sundaralingam, *Carbohydr. Res.* **1981**, *89*, 151-154 (DXSORF10).
- [262] S. Takagi and G. A. Jeffrey, *Acta Crystallogr., Sect. B*, **1978**, *34*, 2932-2934 (DIPKGA).
- [263] R. S. Glass and P. L. Johnson, *Acta Crystallogr., Sect. B*, **1976**, *32*, 3129-3132 (PHISOR).
- [264] M. Levitt and A. Warshel, *J. Am. Chem. Soc.* **1978**, *100*, 2607-2613.
- [265] J. Raap, J. H. van Boom, H. C. van Lieshout, and C. A. G. Haasnoot, *J. Am. Chem. Soc.* **1988**, *110*, 2736-2743.
- [266] M. Sundaralingam, *J. Am. Chem. Soc.* **1971**, *93*, 6644-6647.
- [267] V. N. Bartenev, N. G. Kameneva, and A. A. Lipanov, *Acta Crystallogr., Sect. B*, **1987**, *43*, 275-280.
- [268] W. K. Olson, *J. Am. Chem. Soc.* **1982**, *104*, 270-278; 278-286.
- [269] W. Saenger, *Principles of Nucleic Acid Structure*, Springer Verlag, Berlin, **1984**.
- [270] (a) *Nucleic Acid Database Library*, **1993**. – (b) H. M. Berman, W. K. Olson, D. L. Beveridge, J. Westbrook, A. Gelbin, T. Demeny, S.-H. Hsieh, A. R. Srinivasan, and B. Schneider, *Biophys. J.* **1992**, *63*, 751-759.
- [271] C. Tosi and W. Saenger, *Chem. Phys. Lett.* **1982**, *90*, 277-281.
- [272] M. Karplus, *J. Chem. Phys.* **1959**, *30*, 11-15.
- [273] D. G. Streefkerk, M. J. A. De Bie, and J. F. G. Vliegthart, *Carbohydr. Res.* **1974**, *33*, 249-261.
- [274] (a) M. Karplus, *J. Am. Chem. Soc.* **1963**, *85*, 2870-2871. – (b) R. J. Abraham and K. G. R. Pachler, *Mol. Phys.* **1964**, *7*, 165-182. – (c) R. J. Abraham and G. Gatti, *J. Chem. Soc., Sect. B*, **1969**, 961-968. – (d) L. Phillips and V. Wray, *J. Chem. Soc., Perkin Trans. 2*, **1972**, 536-539.
- [275] C. A. G. Haasnoot, F. A. A. M. De Leeuw, and C. Altona, *Tetrahedron* **1980**, *36*, 2783-2792.
- [276] D. E. Itey, B. Fraser-Reid, *Can. J. Chem.* **1979**, *57*, 653-661.
- [277] L. Den Drijver, D. W. Holzapfel, M. S. van Dyk, and G. J. Kruger, *Carbohydr. Res.* **1987**, *161*, 65-73.
- [278] A. Boettcher, *Ph.D. Thesis*, Technische Hochschule Darmstadt, **1995**.
- [279] A. Bovali, G. Descotes, D. F. Ewing, A. Grouiller, J. Lefkidon, A.-D. Lespinasse, and G. Mackenzie, *J. Carbohydr. Chem.* **1992**, *11*, 159-169.

- [280] J. Defaye, H. Driguez, S. Poulet, R. Chambert, and M.-F. Petit-Glatron, *Carbohydr. Res.* **1984**, *130*, 299-315.
- [281] R. D. Guthrie, I. D. Jenkins, and R. Yamasaki, *Aust. J. Chem.* **1982**, *35*, 1003-1018; 1019-1029.
- [282] B. Erbing and B. Lindberg, *Acta Chem. Scand.* **1976**, *B30*, 12-14.
- [283] R. U. Lemieux and R. Nagarajan, *Can. J. Chem.* **1964**, *42*, 1270-1278.
- [284] A. L. Waterhouse, T. M. Calub, and A. D. French, *Carbohydr. Res.* **1991**, *217*, 29-42.
- [285] J. W. Timmermans, B. R. Leeflang, and H. Tournois, in: *Inulin and Inulin-Containing Crops* (Ed.: A. Fuchs), Elsevier Appl. Science, Amsterdam, **1993**, pp. 129-134.
- [286] J. Liu, A. L. Waterhouse, and N. J. Chatterton, *Carbohydr. Res.* **1993**, *245*, 11-19.
- [287] M. Anteunis, A. de Bruyn, and G. Verhegge, *Carbohydr. Res.* **1975**, *44*, 101-105.
- [288] D. A. Cumming and J. P. Carver, *Biochemistry* **1987**, *26*, 6664-6676.
- [289] S. J. Angyal, *Carbohydr. Res.* **1979**, *77*, 37-50.
- [290] B. Lesyng, W. Saenger, *Carbohydr. Res.* **1984**, *133*, 187-197.
- [291] E. C. Garrett and A. S. Serianni, *Carbohydr. Res.* **1990**, *206*, 183-191.
- [292] T. Vuorinen and A. S. Serianni, *Carbohydr. Res.* **1990**, *209*, 13-31.
- [293] A. S. Serianni and R. Barker, *J. Org. Chem.* **1984**, *49*, 3292-3300.
- [294] A. S. Serianni and D. M. Chipman, *J. Am. Chem. Soc.* **1987**, *109*, 5297-5303.
- [295] See Ref. [53], Chapter 13: *Hydrogen Bonding in Carbohydrates*, pp. 169-219; most notably pp. 172-178.
- [296] (a) F. W. Lichtenthaler and H. Lindner, *Liebigs Ann. Chem.* **1981**, 2372-2383. – (b) F. W. Lichtenthaler, *Dtsch. Zahnärztl. Z.* **1982**, *37*, S46-S49.
- [297] (a) G. E. Hawkes and D. Lewis, *J. Chem. Soc., Perkin Trans. 2*, **1984**, 2073-2078. – (b) D. G. Gillies and D. Lewis, *J. Chem. Soc., Perkin Trans. 2*, **1985**, 1155-1159. – (c) D. Lewis, *J. Chem. Soc., Perkin Trans. 2*, **1986**, 467-470; **1990**, 1349-1351. – (d) D. Lewis and S. Angyal, *J. Chem. Soc., Perkin Trans. 2*, **1989**, 1763-1765.
- [298] F. G. Gallwey, J. E. Hawkes, P. Haycock, and D. Lewis, *J. Chem. Soc., Perkin Trans. 2*, **1990**, 1979-1985.
- [299] S. J. Angyal, J. K. Saunders, C. T. Grainger, R. Le Fur, and P. G. Williams, *Carbohydr. Res.* **1986**, *150*, 7-21.
- [300] S. J. Angyal and R. Le Fur, *Carbohydr. Res.* **1980**, *84*, 201-209; **1984**, *126*, 15-26.
- [301] (a) M. van Duin, J. M. A. Baas, and B. van de Graaf, *J. Org. Chem.* **1986**, *51*, 1298-1302. – (b) J. P. Grigera, *J. Chem. Soc., Faraday Trans. 1*, **1988**, *84*, 2603-2608.
- [302] C. Müller, *Ph.D. Thesis*, Technische Hochschule Darmstadt, to be submitted.
- [303] (a) M. Barfield and D. M. Grant, *J. Am. Chem. Soc.* **1963**, *85*, 1899-1904. – (b) R. Cahill, R. C. Cookson, and T. A. Crabb, *Tetrahedron* **1969**, *25*, 4711-4735.
- [304] Y. D. Lee and H. S. Kim, *Biotechnol. Bioeng.* **1991**, *37*, 795-801.
- [305] F. Cramer, *Einschlussverbindungen*, Springer-Verlag, Berlin / Heidelberg, **1954**.
- [306] W. Saenger, *Angew. Chem.* **1980**, *92*, 343-361; *Angew. Chem. Int. Ed. Engl.* **1980**, *19*, 344-362.
- [307] R. J. Clarke, J. H. Coates, and S. F. Lincoln, *Adv. Carbohydr. Chem. Biochem.* **1988**, *46*, 205-249.
- [308] G. Wenz, *Angew. Chem.* **1994**, *106*, 851-870; *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 803-822.
- [309] For a comprehensive collection of invited papers dealing with various applications of cyclodextrins see: *Carbohydr. Res.* **1989**, Vol. 192.
- [310] For a number of reviews see: J. Szejtli: (a) *Starch / Stärke* **1977**, *29*, 26-33. – (b) *Pharmazie* **1980**, *35*, 779-787. – (c) *Pharm. Technol.* **1991**, *15*(6), 36-44. – (d) *Pharm. Technol.* **1991**, *15*(8), 24-38. – (e) *Starch / Stärke* **1980**, *32*, 386-391. –

- (f) *Starch / Stärke* **1987**, 39, 357-362. – (g) *Kontakte (Darmstadt)* **1988**, (1), 31-36. – (h) *Carbohydr. Polym.* **1990**, 12, 375-392. – (i) *Stud. Environ. Sci.* **1991**, 42, 387-397.
- [311] D. Sybilska, E. Smolková-Keulemansová, *Applications of Inclusion Compounds in Chromatography*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 6, pp. 229-243.
- [312] J. Szejtli, *Industrial Applications of Cyclodextrins*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 11, pp. 331-390.
- [313] See for example: J. Cully, H. R. Vollbrecht, and J. Wiesmueller, *Ger. Offen. DE 3,928,258* (**1991**) [*Chem. Abstr.* **1991**, 114, 205800e].
- [314] D. W. Griffiths and M. L. Bender, *Adv. Catal.* **1973**, 23, 209-261.
- [315] A. Deratani, G. Lelièvre, T. Maraldo, and B. Sébille, *Carbohydr. Res.* **1989**, 192, 215-222.
- [316] D. Duchene and D. Wouessidjewe, *J. Coord. Chem.* **1992**, 27, 223-236.
- [317] Y. Inoue, *Annu. Rep. NMR Spectrosc.* **1993**, 27, 59-101.
- [318] W. Saenger, *Structural Aspects of Cyclodextrins and their Inclusion Complexes*, in: *Inclusion Compounds (Structural Aspects of Inclusion Compounds formed by Organic Host Lattices)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 2, **1984**, Chapter 8, pp. 231-259.
- [319] (a) K. Harata, *Recent Advances in the X-ray Analysis of Cyclodextrin Complexes*, in: *Inclusion Compounds* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Oxford University Press, Oxford UK, Vol. 5, **1991**, Chapter 9, pp. 311-344. – (b) K. Harata, *X-Ray Structure of Cyclodextrin Inclusion Complexes*, in: *Report of the National Institute of Bioscience and Human-Technology*, Vol. 1, No. 2, **1993**, pp. 1-24.
- [320] T. Fujiwara, N. Tanaka, and S. Kobayashi, *Chem. Lett.* **1990**, 739-742 (SIYKOA).
- [321] To my knowledge, so far only one reliable proof of a guest-induced conformational transition of a pyranose ring system was found in the solid state structure of the heptakis(2,3,6-tri-*O*-methyl)- β -cyclodextrin *m*-iodo-phenol inclusion complex^[322]. Here, one glucose residue adopts a ⁰S₂ conformation (recalc. $Q = 0.722 \text{ \AA}$, $\theta = 86.7^\circ$, and $\phi = 323.6^\circ$). The distorted ²E ($\rightarrow 2,^5$ B) glucose conformation in an α -CD structure might originate from an error in the atomic coordinates (recalc. $Q = 0.538 \text{ \AA}$, $\theta = 68.0^\circ$, and $\phi = 114.9^\circ$)^[323].
- [322] K. Harata, F. Hirayama, H. Arima, K. Uekama, and T. Miyaji, *J. Chem. Soc., Perkin Trans. 2*, **1992**, 1159-1166.
- [323] B. Klingert and G. Rihs, *J. Chem. Soc., Dalton Trans.* **1991**, 2749-2760 (KOGKEW, KOGKIA, KOGKUM, and KOGLIB).
- [324] C. Morat and F. R. Taravel, *Bull. Magn. Res.* **1989**, 11, 321-323; *Tetrahedron Lett.* **1990**, 31, 1413-1416.
- [325] S. P. van Helden, M. J. van Drooge, A. J. Claessens, A. C. A. Jansen, and L. H. M. Janssen, *Carbohydr. Res.* **1991**, 215, 251-260.
- [326] Actually the inverse ratio of $d_{\text{max}}/d_{\text{min}}$ was used in this study^[325], but according to the definition used here the (theoretically possible) values range from 0.0 (extreme elliptical distortion) to 1.0 (perfect round-shape) rather than from 1.0 to infinity.
- [327] See Ref. [53], Chapter 18: *OH...O Hydrogen Bonding in Crystal Structures of Cyclic and Linear Oligoamyloses: Cyclodextrins, Maltotriose, and Maltohexaose*, pp. 309-350; most notably pp. 315-318.
- [328] T. Steiner and W. Saenger, *Carbohydr. Res.* **1994**, 259, 1-12.
- [329] B. Casu, M. Reggiani, G. G. Gallo, and A. Vigevani, *Tetrahedron* **1968**, 24, 803-821.
- [330] D. Rong and V. T. D'Souza, *Tetrahedron Lett.* **1990**, 31, 4275-4278.

- [331] H. Dodziuk and K. Nowinski, *J. Mol. Struct. (Theochem)* **1994**, *110*, 61-68.
- [332] K. B. Lipkowitz, *J. Org. Chem.* **1991**, *97*, 6357-6367.
- [333] J. E. H. Koehler, W. Saenger, and W. F. van Gunsteren, *Eur. Biophys. J.* **1987**, *15*, 197-210; *J. Mol. Biol.* **1988**, *203*, 241-250.
- [334] J. E. H. Koehler, W. Saenger, and W. F. van Gunsteren, *J. Biomol. Struct. Dyn.* **1988**, *6*, 182-198.
- [335] J. E. H. Koehler, W. Saenger, and W. F. van Gunsteren, *Eur. Biophys. J.* **1987**, *15*, 211-224; **1988**, *16*, 153-168.
- [336] (a) W. F. van Gunsteren, R. M. Brunne, A. E. Mark, and S. P. van Helden, in: *Molecular Aspects of Biotechnology: Computational Models and Theories* (Ed.: J. Bertrán), Kluwer Acad. Publ., Dordrecht, **1992**, pp. 105-122. – (b) S. P. van Helden, B. P. Eijck, and L. H. M. Janssen, *J. Biomol. Struct. Dyn.* **1992**, *9*, 1269-1283.
- [337] (a) P. C. Manor and W. Saenger, *J. Am. Chem. Soc.* **1974**, *96*, 3630-3639. – (b) W. Saenger, *Nature* **1979**, *279*, 343-344 (CHXAMH01). – (c) B. Klar, B. E. Hingerty, and W. Saenger, *Acta Crystallogr., Sect. B*, **1980**, *36*, 1154-1165 (CHXAMH02).
- [338] K. Lindner and W. Saenger, *Acta Crystallogr., Sect. B*, **1982**, *38*, 203-210 (CHXAMH03).
- [339] K. K. Chacko and W. Saenger, *J. Am. Chem. Soc.* **1981**, *103*, 1708-1715 (BANXUJ).
- [340] M. J. Gidley and S. M. Bociek, *J. Chem. Soc., Chem. Commun.*, **1986**, 1223-1226.
- [341] M. J. Gidley and S. Bociek, *Carbohydr. Res.* **1988**, *183*, 126-130.
- [342] (a) K. Lindner and W. Saenger, *Angew. Chem.* **1978**, *90*, 738-740; *Angew. Chem., Int. Ed. Engl.* **1978**, *17*, 694-695 (BCDEXD). – (b) J. J. Stezowski and J. M. MacLennan, *Am. Cryst. Assoc., Ser. 2*, **1980**, *7*, 24 (BCDEXD01). – (c) K. Lindner and W. Saenger, *Carbohydr. Res.* **1982**, *99*, 103-115.
- [343] T. Fujiwara, M. Yamazaki, Y. Tomizu, R. Tokuoka, K.-I. Tomita, T. Matsuo, H. Suga, and W. Saenger, *Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, **1983**, 181-187 [*Chem. Abstr.* **1983**, *98*, 178391q] (BCDEXD02 and BUVSEQ).
- [344] (a) C. Betzel, W. Saenger, B. E. Hingerty, and G. M. Brown, *J. Am. Chem. Soc.* **1984**, *106*, 7545-7557 (CUXCON). – (b) V. Zabel, W. Saenger, and S. A. Mason, *J. Am. Chem. Soc.* **1986**, *108*, 3664-3673 (CUXCON01).
- [345] J. A. Ripmeester, *Supramol. Chem.* **1993**, *2*, 89-91.
- [346] W. Saenger, C. Betzel, B. E. Hingerty, and G. M. Brown, *Nature* **1982**, *296*, 581-583; *Angew. Chem.* **1983**, *95*, 908-909; *Angew. Chem., Int. Ed. Engl.* **1983**, *22*, 883-884.
- [347] J. M. MacLennan and J. J. Stezowski, *Biochem. Biophys. Res. Commun.* **1980**, *92*, 926-932.
- [348] (a) K. Harata, *Chem. Lett.* **1984**, 641-644 (CIWMIE). – (b) *Bull. Chem. Soc. Jpn.* **1987**, *60*, 2763-2767 (CIWMIE10).
- [349] (a) V. Zabel, B. E. Hingerty, S. A. Mason, and W. Saenger, *Acta Crystallogr., Sect. A*, **1987**, *43*, C43. – (b) J. Ding, T. Steiner, V. Zabel, B. E. Hingerty, S. A. Mason, and W. Saenger, *J. Am. Chem. Soc.* **1991**, *113*, 8081-8089 (KOHBUJ).
- [350] M. Fathallah, F. Fotiadu, and C. Jaime, *J. Org. Chem.* **1994**, *59*, 1288-1293.
- [351] I. Furó, I. Pócsik, K. Tompa, R. Teeäär, and E. Lippmaa, *Carbohydr. Res.* **1987**, *166*, 27-33.
- [352] (a) T. Steiner, S. A. Mason, and W. Saenger, *J. Am. Chem. Soc.* **1990**, *112*, 6184-6190 (SIGHOF). – (b) **1991**, *113*, 5676-5687 (SIGHOF01 and SIGHOF02).
- [353] Y. Inoue and Y. Miyata, *Bull. Chem. Soc. Jpn.* **1981**, *54*, 809-816.
- [354] (a) D. J. Wood, F. E. Hruska, and W. E. Saenger, *J. Am. Chem. Soc.* **1977**, *99*, 1735-1740. – (b) M. Vincendon, *Bull. Soc. Chim. Fr. II*, **1981**, 129-134.

- [355] For details of the structure generation procedure for the δ -CD see Chapter 6, Appendix II.
- [356] H. Nomura, S. Koda, K. Matsumoto, and Y. Miyahara, *Stud. Phys. Theor. Chem.* **1983**, *27*, 151-163.
- [357] K. Lindner and W. Saenger, *Carbohydr. Res.* **1982**, *107*, 7-16 (BOBPIR).
- [358] K. Harata, *Bull. Chem. Soc. Jpn.* **1978**, *51*, 1644-1648 (ACDMSM).
- [359] K. Harata, *Bull. Chem. Soc. Jpn.* **1979**, *52*, 2451-2459 (ACDMFM and ACDPRO).
- [360] see for example: K. Harata: (a) *Bull. Chem. Soc. Jpn.* **1975**, *48*, 2409-2413 (CDEXIA10). – (b) **1976**, *49*, 2066-2072 (CDXBZS). – (c) **1977**, *50*, 1416-1424 (ACDHBA, ACDPNP). – (d) **1980**, *53*, 2782-2786 (CDNOAN). – (e) **1982**, *55*, 1367-1371 (BIJHOR).
- [361] D. Mentzafos, I. M. Mavridis, G. LeBas, G. Tsoucaris, *Acta Crystallogr., Sect. B*, **1991**, *47*, 746-757 (KOFJEU).
- [362] A. Rontoyianni, I. M. Mavridis, E. Hadjoudis, and A. J. M. Duisenberg, *Carbohydr. Res.* **1994**, *252*, 19-32.
- [363] I. M. Mavridis and E. Hadjoudis, *Carbohydr. Res.* **1992**, *229*, 1-15.
- [364] K. Harata, *Bull. Chem. Soc. Jpn.* **1984**, *57*, 2596-2599 (DIRVOP).
- [365] C. Jaime, J. Redondo, F. Sánchez-Ferrando, and A. Virgili, *J. Mol. Struct.* **1991**, *248*, 317-329.
- [366] J. A. Hamilton, *Carbohydr. Res.* **1985**, *142*, 21-37 (FASXUS).
- [367] S. Kamitori, K. Hirotsu, and T. Higuchi, *J. Chem. Soc., Chem. Commun.*, **1986**, 690-691 (DOCYID).
- [368] S. Kamitori, K. Hirotsu, and T. Higuchi, *J. Am. Chem. Soc.* **1987**, *109*, 2409-2414 (FEJFIJ and FEJFOP); *Bull. Chem. Soc. Jpn.* **1988**, *61*, 3825-3830 (SAJNAS).
- [369] H. Dodziuk, D. Sybilska, S. Miki, Z. Yoshida, J. Sitkowski, M. Asztemborska, A. Bielejewska, J. Kowalczyk, K. Duszczuk, and L. Stefaniak, *Tetrahedron* **1994**, *50*, 3619-3626.
- [370] Z.-I. Yoshida, H. Takekuma, S.-I. Takekuma, and Y. Matsubara, *Angew. Chem.* **1994**, *106*, 1658-1660; *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 1597-1599.
- [371] K. Freudenberg, E. Schaef, G. Dumpert, and T. Ploetz, *Naturwissenschaften* **1939**, *27*, 850-853.
- [372] For a detailed review see Ref. [307], pp. 219-233.
- [373] W. Saenger and M. Noltemeyer, *Chem. Ber.* **1976**, *109*, 503-517 (CDEXKR10 and CYDXKR10).
- [374] R. J. Bergeron, *Cycloamylose-Substrate Binding*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 12, pp. 391-443.
- [375] R. J. Bergeron and M. P. Meeley, *Bioorg. Chem.* **1976**, *5*, 197-202.
- [376] I. Tabushi, Y. Kiyosuke, T. Sugimoto, and K. Yamamura, *J. Am. Chem. Soc.* **1978**, *100*, 916-919.
- [377] R. J. Bergeron, M. A. Channing, G. J. Gibeily, and D. M. Pillor, *J. Am. Chem. Soc.* **1977**, *99*, 5146-5151.
- [378] R. I. Gelb, L. M. Schwartz, B. Cardelino, H. S. Fuhrmann, R. F. Johnson, and D. A. Laufer, *J. Am. Chem. Soc.* **1981**, *103*, 1750-1757.
- [379] R. I. Gelb, L. M. Schwartz, M. Radeos, and D. A. Laufer, *J. Phys. Chem.* **1983**, *87*, 3349-3354.
- [380] A. Leo, C. Hansch, and D. Elkins, *Chem. Rev.* **1971**, *71*, 525-616.
- [381] K. A. Connors and D. D. Pendergast, *J. Am. Chem. Soc.* **1984**, *106*, 7607-7614.
- [382] W. Broser and W. Lautsch, *Z. Naturforsch., Teil B* **1953**, *8*, 711-722.

- [383] B. Siegel and R. Breslow, *J. Am. Chem. Soc.* **1975**, *97*, 6869-6870.
- [384] A. Örstan and J. B. A. Ross, *J. Phys. Chem.* **1987**, *91*, 2739-2745.
- [385] K. A. Connors, M. J. Mulski, and A. Paulson, *J. Org. Chem.* **1992**, *57*, 1794-1798.
- [386] J. M. Schuette, T. T. Ndou, A. M. de la Peña, S. Mukundan Jr., and I. M. Warner, *J. Am. Chem. Soc.* **1993**, *115*, 292-298.
- [387] E. Grunwald, *J. Am. Chem. Soc.* **1986**, *108*, 5726-5731.
- [388] W. Jorgensen, J. Gao, and C. Ravimohan, *J. Phys. Chem.* **1985**, *89*, 3470-3473.
- [389] T. Endo, H. Takei, T. Isago, J.-I. Kato, M. M. Ito, K. Guro, K.-Y. Akiyama, Y. Nakajima, and H. Kataoka, *J. Am. Chem. Soc.* **1989**, *111*, 8166-8172.
- [390] D. H. Williams, *private communication*.
- [391] M. S. Searle, D. H. Williams, and U. Gerhard, *J. Am. Chem. Soc.* **1992**, *114*, 10697-10704.
- [392] M. S. Searle and D. H. Williams, *Bioorg. Med. Chem. Lett.* **1992**, *2*, 993-996.
- [393] M. S. Searle and D. H. Williams, *J. Am. Chem. Soc.* **1992**, *114*, 10690-10697.
- [394] M. Komiyama and M. L. Bender, *J. Am. Chem. Soc.* **1978**, *100*, 2259-2260.
- [395] P. Groves, M. S. Searle, M. S. Westwell, and D. H. Williams, *J. Chem. Soc., Chem. Commun.* **1994**, 1519-1520.
- [396] Y. Yamamoto, M. Onda, M. Kitagawa, Y. Inoue, and R. Chûjô, *Carbohydr. Res.* **1987**, *167*, C11-C16.
- [397] M. Kitagawa, H. Hoshi, M. Sakurai, Y. Inoue, and R. Chûjô, *Carbohydr. Res.* **1987**, *163*, C1-C3.
- [398] Y. Inoue, T. Okuda, Y. Miyata, and R. Chûjô, *Carbohydr. Res.* **1984**, *125*, 65-76.
- [399] T.-X. Lü, D.-B. Zhang, and S.-J. Dong, *J. Chem. Soc., Faraday Trans. 2*, **1989**, *85*, 1439-1445.
- [400] Y. Inoue, F.-H. Kuan, and R. Chûjô, *Carbohydr. Res.* **1987**, *159*, 1-10.
- [401] J. A. Ripmeester, C. I. Ratcliffe, and I. G. Cameron, *Carbohydr. Res.* **1989**, *192*, 69-81.
- [402] K. Harata, H. Uedaira, and J. Tanaka, *Bull. Chem. Soc. Jpn.* **1978**, *51*, 1627-1634 (ACDMNP).
- [403] M. Komiyama and H. Hirai, *Bull. Chem. Soc. Jpn.* **1981**, *54*, 828-831.
- [404] W. Saenger, K. Beyer and P. C. Manor, *Acta Crystallogr., Sect. B*, **1976**, *32*, 120-128 (CDEXIA01).
- [405] M. Noltemeyer and W. Saenger, *J. Am. Chem. Soc.* **1980**, *102*, 2710-2722 (CYDXLI10, CYDXTF, and ZZZANG10).
- [406] K. Harata, K. Uekama, M. Otagiri, F. Hirayama, and H. Ogino, *Bull. Chem. Soc. Jpn.* **1981**, *54*, 1954-1959 (BAJJAX).
- [407] K. Harata, *Bull. Chem. Soc. Jpn.* **1977**, *50*, 1259-1266 (ACDPRS).
- [408] K. Harata, K. Uekama, M. Otagiri, F. Hirayama, and Y. Ohtani, *Bull. Chem. Soc. Jpn.* **1985**, *58*, 1234-1238 (DEBGOG).
- [409] K. Harata, K. Uekama, M. Otagiri, and F. Hirayama, *Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, **1983**, 173-180 [*Chem. Abstr.* **1983**, *98*, 135604u] (BUPDEV).
- [410] W. J. James, D. French, and R. E. Rundle, *Acta Crystallogr.* **1959**, *12*, 385-389.
- [411] R. K. McMullan, W. Saenger, J. Fayos, and D. Mootz, *Carbohydr. Res.* **1973**, *31*, 211-227.
- [412] F. Cramer, U. Bergmann, P. C. Manor, M. Noltemeyer, and W. Saenger, *Liebigs Ann. Chem.* **1976**, 1169-1179.
- [413] M. Noltemeyer and W. Saenger, *Nature* **1976**, *259*, 629-632.
- [414] C. Betzel, B. Hingerty, M. Noltemeyer, G. Weber, W. Saenger, and J. A. Hamilton, *J. Inclusion Phenomena* **1983**, *1*, 181-191 (COCMIQ).

- [415] K. A. Murdoch, *Carbohydr. Res.* **1992**, 233, 161-174, and references cited therein.
- [416] T. L. Bluhm and P. Zugenmaier, *Carbohydr. Res.* **1981**, 89, 1-10.
- [417] H. Saito, J. Yamada, T. Yukumoto, H. Yajima, and R. Endo, *Bull. Chem. Soc. Jpn.* **1991**, 64, 3528-3537.
- [418] (a) F. F. Mikus, R. M. Hixon, and R. E. Rundle, *J. Am. Chem. Soc.* **1946**, 68, 1115-1121. – (b) L. Acker and G. Becker, *Starch/Stärke* **1971**, 23, 419-424. – (c) T. L.-G. Carlson, K. Larson, N. Dinh-Nguyen, and N. Krog, *Starch/Stärke* **1979**, 31, 222-224. – (d) K. Eberstein, R. Höpcke, G. Konieczny-Janda, and R. Stute, *Starch/Stärke* **1980**, 32, 397-404. – (e) R. Stute and G. Konieczny-Janda, *Starch/Stärke* **1983**, 35, 340-347. – (f) S. Raphaelides and J. Karkalas, *Carbohydr. Res.* **1988**, 172, 65-82. – (g) M. A. Rutschman and J. Solms, *Lebensm.-Wiss. Technol.* **1990**, 23, 84-87 [*Chem. Abstr.* **1990**, 113, 22322k].
- [419] R. Höpcke, *Stärke als Komplexbildner*, in: *Stärke – Schriftenreihe des Fonds der Chemischen Industrie*, Vol. 25, **1986**, pp. 34-42.
- [420] T. Cserhádi and J. Szejtli, *Carbohydr. Res.* **1992**, 224, 165-173.
- [421] T. Steiner, G. Koellner, and W. Saenger, *Carbohydr. Res.* **1992**, 228, 321-332.
- [422] R. Arad-Yellin, B. S. Green, M. Knossow, G. Tsoucaris, *Enantiomeric Selectivity of Host Lattices*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 9, pp. 263-295.
- [423] (a) J. A. Hamilton and L. Chen, *J. Am. Chem. Soc.* **1988**, 110, 5833-5841 (DUTLIN10). – (b) K. Uekama, F. Hirayama, T. Imai, M. Otagiri, and K. Harata, *Chem. Pharm. Bull.* **1983**, 31, 3363-3365 (CEDMUT).
- [424] (a) K. Kano, M. Tatsumi, and S. Hashimoto, *J. Org. Chem.* **1991**, 56, 6579-6585. – (b) H. Dodziuk, J. Sitkowski, L. Stefaniak, J. Jurczak, and D. Sybilska, *J. Chem. Soc., Chem. Commun.*, **1992**, 207-208.
- [425] D. W. Armstrong, T. J. Ward, R. D. Armstrong, and T. E. Beesley, *Science* **1986**, 232, 1132-1135.
- [426] K. Harata, K. Uekama, M. Otagiri, and F. Hirayama, *J. Inclusion Phenomena* **1984**, 2, 583-594.
- [427] (a) A. P. Croft and R. A. Bartsch, *Tetrahedron* **1983**, 39, 1417-1474. – (b) K. Koji, *Bioorg. Chem. Front.* **1993**, 3, 1-23.
- [428] I. Tabushi, *Tetrahedron* **1984**, 40, 269-292.
- [429] I. Tabushi, *Reactions of Inclusion Complexes formed by Cyclodextrins and their Derivatives*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 13, pp. 445-471.
- [430] R. Breslow, *Enzyme Models Related to Inclusion Compounds*, in: *Inclusion Compounds (Physical Properties and Applications)* (Eds.: J. L. Atwood, J. E. D. Davies, D. D. MacNicol), Academic Press, London, Vol. 3, **1984**, Chapter 14, pp. 473-508.
- [431] O. S. Tee, *Carbohydr. Res.* **1989**, 192, 181-195.
- [432] F. M. Menger and M. A. Dulany, *Tetrahedron Lett.* **1985**, 26, 267-270.
- [433] K. Harata, K. Uekama, M. Otagiri, and F. Hirayama: (a) *Bull. Chem. Soc. Jpn.* **1982**, 55, 407-410 (BEYLOG). – (b) **1982**, 55, 3904-3910 (BUDKEQ). – (c) *Chem. Lett.* **1983**, 1807-1810 (CECMAY and CECMEC). – (d) **1987**, 60, 497-502 (CECMAY10 and CECMEC10). – (e) *Nippon Kagaku Kaishi (J. Chem. Soc. Jpn.)*, **1983**, 173-180 [*Chem. Abstr.* **1983**, 98, 135604u] (BUPDIZ). – (f) K. Harata, K. Uekama, M. Otagiri, F. Hirayama, and Y. Sugiyama, *Bull. Chem. Soc. Jpn.* **1982**, 55, 3386-3389 (BOHWUQ). – (g) K. Harata, *J. Chem. Soc., Perkin Trans. 2*, **1990**, 799-804 (JEJWOK and JEJXAX).

- [434] (a) K. Harata, K. Uekama, M. Otagiri, and F. Hirayama, *Bull. Chem. Soc. Jpn.* **1983**, *56*, 1732-1736 (CAMPIP). – (b) K. Harata, K. Uekama, T. Imai, F. Hirayama, and M. Otagiri, *J. Inclusion Phenomena* **1984**, *1*, 279-293 (CAMPIP10 and COYXET10). – (c) *Chem. Lett.* **1984**, 1549-1552 (COYXAP and COYXET). – (d) *J. Inclusion Phenomena* **1988**, *6*, 443-460 (COYXAP10 and COYXET20).
- [435] Y. Yamamoto, M. Onda, Y. Takahashi, Y. Inoue, and R. Chûjô, *Carbohydr. Res.* **1987**, *170*, 229-234.
- [436] W. A. König, *Carbohydr. Res.* **1989**, *192*, 51-60.
- [437] J. Nishijo, M. Yasuda, M. Nagai, and M. Sugiura, *Chem. Pharm. Bull.* **1994**, *42*, 761-767.
- [438] M. Komiyama, H. Yamamoto, and H. Hirai, *Chem. Lett.* **1984**, 1081-1084.
- [439] European Research Conference on Supramolecular Chemistry, *Molecular Recognition from Biology to Materials*, held in Mainz, Germany, 11-16 August 1994.
- [440] D. French, *Adv. Carbohydr. Chem.* **1957**, *12*, 189-260.
- [441] (a) A. O. Pulley and D. French, *Biochem. Biophys. Res. Commun.* **1961**, *5*, 11-15. – (b) D. French, A. O. Pulley, J. A. Effenberger, M. A. Rougvie, and M. Abdullah, *Arch. Biochem. Biophys.* **1965**, *111*, 153-160.
- [442] T. Nakagawa, K. Ueno, M. Kashiwa, and J. Watanabe, *Tetrahedron Lett.* **1994**, *35*, 1921-1924.
- [443] M. Mori, *Ph.D. Thesis*, University of Tokyo, **1991**; mentioned in Ref. [444].
- [444] H. Kuyama, T. Nukada, Y. Nakahara, and T. Ogawa, *Tetrahedron Lett.* **1993**, *34*, 2171-2174.
- [445] M. Mori, Y. Ito, and T. Ogawa, *Tetrahedron Lett.* **1989**, *30*, 1273-1276; *Carbohydr. Res.* **1989**, *192*, 131-146.
- [446] M. Mori, Y. Ito, J. Uzawa, and T. Ogawa, *Tetrahedron Lett.* **1990**, *31*, 3191-3194.
- [447] M. Kawamura, T. Uchiyama, T. Kuramoto, Y. Tamura, and K. Mizutani, *Carbohydr. Res.* **1989**, *192*, 83-90.
- [448] T. Uchiyama, in: *Stud. Plant Sci. (Inulin and Inulin-Containing Crops)* (Ed.: A. Fuchs) **1993**, *3*, 143-148.
- [449] P. R. Sundararajan and V. S. R. Rao, *Carbohydr. Res.* **1970**, *13*, 351-358.
- [450] The solid state structures of different crystal forms of non-complexed α -CD (**4**)^[337-339] revealed asymmetric distortions, which are not retained in (aqueous) solution. For statistical reasons and to obtain a general overview of the conformational features of **4**, its inclusion complexes were included into the geometry analysis^[333,334].
- [451] Experimental proof for the slight flattening at C-4 in **3** may be derived from the ^1H - ^1H -NMR coupling constants of its peracetate synthesized recently^[442], which with $J_{3,4} \approx 7.6$ and $J_{4,5} \approx 8.3$ Hz are smaller than those usually found in the cyclodextrins ($J_{3,4} \approx J_{4,5} \approx 9.0 - 9.5$ Hz)^[452]. In contrast to previous predictions based on early theoretical considerations^[440,449], no indication of glucose chair / boat transitions in **3** could be obtained from NMR data^[442] and the calculations.
- [452] A. F. Casy and A. D. Mercer, *Magn. Res. Chem.* **1988**, *26*, 765-774.
- [453] H. Vollhardt, *Diploma Thesis*, Technische Hochschule Darmstadt, **1991**.
- [454] (a) S. Reiling, *Ph.D. Thesis*, Technische Hochschule Darmstadt, **1994**. – (b) S. Reiling, M. Schlenkrich, and J. Brickmann, *J. Comput. Chem.* **1995**, submitted for publication.
- [455] (a) S. Reiling, M. Schlenkrich, P. A. Bopp, J. Brickmann, *J. Comput. Chem.* **1995**, in press. – (b) S. Reiling, J. Brickmann, *Macromol. Chem. (Theory and Simulations)* **1995**, in press.
- [456] A. T. Brünger, *Annu. Rev. Phys. Chem.* **1991**, *42*, 197-205.
- [457] In both force fields, hydrogen bonding is treated exclusively as an electrostatic interaction, no special energy terms are added to account for H-bonds. The significantly

- higher charges of the modified CHARMM force field^[454] (approx. atomic charges of -OH: -0.66 and +0.43, acetal oxygens -0.36, carbons +0.20, and ring protons +0.09) in contrast to PIMM91 (partial charges of all oxygens -0.32 – -0.35, carbon +0.10 – +0.20, hydroxyl-H +0.20, and C-H +0.00 – +0.10) lead to increased H-bond interaction energies in the former^[45].
- [458] L. Verlet, *Phys. Rev.* **1967**, *159*, 98-103.
- [459] (a) B. R. Brooks, R. E. Bruccoleri, B. D. Olafson, D. J. States, S. Swaminathan, and M. Karplus, *J. Comput. Chem.* **1983**, *4*, 187-217. – (b) L. Nilsson and M. Karplus, *J. Comput. Chem.* **1986**, *7*, 591-616.
- [460] (a) S. M. Kast, K. Nicklas, H.-J. Bär, and J. Brickmann, *J. Chem. Phys.* **1994**, *100*, 566-576. – (b) S. M. Kast, J. Brickmann, *J. Chem. Phys.* **1995**, to be published.
- [461] (a) S. Houdier and P. J. A. Vottéro, *Carbohydr. Res.* **1993**, *248*, 377-384. – (b) *Angew. Chem.* **1994**, *106*, 365-367; *Angew. Chem. Int. Ed. Engl.* **1994**, *33*, 354-356.
- [462] P. M. Collins and M. H. Ali, *Tetrahedron Lett.* **1990**, *31*, 4517-4520.
- [463] A recent computational study in favor of symmetry breaking as an energy minimizing factor in cyclodextrins^[332] suffers from an unjustified overestimation of the overall puckering of the macrocycles caused by strong intramolecular hydrogen bonding effects. A more detailed discussion of these aspects is contained in Chapter 6.
- [464] The apparent molar volume of α -CD has been determined by density measurements in aqueous solutions^[356] to be $\Phi_V \approx 1010 \text{ \AA}^3$, which is in close agreement with the computed volume; this indicates that water penetrates the central cavity easily.
- [465] C. J. Pedersen, *J. Am. Chem. Soc.* **1967**, *89*, 2495-2496; 7017-7036.
- [466] J. W. H. M. Uiterwijk, S. Harkema, and D. Feil, *J. Chem. Soc., Perkin Trans. 2*, **1987**, 721-731.
- [467] N. Yoshie, H. Hamada, S. Takada, and Y. Inoue, *Chem. Lett.* **1993**, 353-356.
- [468] T. Uchiyama, M. Kawamura, T. Uragami, and H. Okuno, *Carbohydr. Res.* **1993**, *241*, 245-248.
- [469] Y. Takai, Y. Okumura, S. Takahashi, M. Sawada, M. Kawamura, and T. Uchiyama, *J. Chem. Soc., Chem. Commun.* **1993**, 53-54.
- [470] Y. Takai, Y. Okumura, T. Tanaka, M. Sawada, S. Takahashi, M. Shiro, M. Kawamura, and T. Uchiyama, *J. Org. Chem.* **1994**, *59*, 2967-2975.
- [471] K. Esau, *Pflanzenanatomie*, G. Fischer Verlag, Stuttgart, **1969**.
- [472] St. v. Nárday-Szabó, *Liebigs Ann. Chem.* **1928**, *465*, 299-304.
- [473] J. R. Katz and T. B. van Itallie, *Z. Physik. Chem. (A)*, **1930**, *150*, 90-99.
- [474] R. S. Bear, *J. Am. Chem. Soc.* **1942**, *64*, 1388-1392.
- [475] B. Meyer, *Stärke – Struktur und Eigenschaften*, in: *Stärke – Schriftenreihe des Fonds der Chemischen Industrie*, Vol. 25, **1986**, pp. 3-15.
- [476] A. Buléon, F. Duprat, F. P. Booy, and H. Chanzy, *Carbohydr. Polymers* **1984**, *4*, 161-173.
- [477] R. Stute, *Vergleichende Betrachtungen von Stärken verschiedenen pflanzlichen Ursprungs*, in: *Stärke – Schriftenreihe des Fonds der Chemischen Industrie*, Vol. 25, **1986**, pp. 16-33.
- [478] H.-C. H. Wu and A. Sarko, *Carbohydr. Res.* **1977**, *54*, C3-C6.
- [479] A. Sarko and H.-C. H. Wu, *Starch / Stärke* **1978**, *30*, 73-78.
- [480] H.-C. H. Wu and A. Sarko, *Carbohydr. Res.* **1978**, *61*, 7-25.
- [481] H.-C. H. Wu and A. Sarko, *Carbohydr. Res.* **1978**, *61*, 27-40.
- [482] A. Imberty, H. Chanzy, S. Pérez, A. Buléon, and V. Tran, *J. Mol. Biol.* **1988**, *201*, 365-378.
- [483] D. L. Wild and J. M. V. Blanshard, *Carbohydr. Polym.* **1986**, *6*, 121-143.

- [484] A. Buléon, M. M. Delage, J. Brisson, and H. Chanzy, *Int. J. Biol. Macromol.* **1990**, *12*, 25-33.
- [485] W. T. Winter and A. Sarko, *Biopolymers* **1974**, *13*, 1461-1482.
- [486] B. Zaslow and R. L. Miller, *J. Am. Chem. Soc.* **1961**, *83*, 4378-4381.
- [487] J. Brisson, H. Chanzy, and R. Vuong, *Food Hydrocolloids* **1987**, *1*, 523-525.
- [488] J. Brisson, H. Chanzy, and W. T. Winter, *Biol. Macromol.* **1991**, *13*, 31-39.
- [489] W. T. Winter and A. Sarko, *Biopolymers* **1974**, *13*, 1447-1460.
- [490] R. Cleven, C. van den Berg, and L. van der Plas, *Starch / Stärke* **1978**, *30*, 223-228.
- [491] G. Rappenecker and P. Zugenmaier, *Carbohydr. Res.* **1981**, *89*, 11-19.
- [492] A. Sarko and R. H. Marchessault, *J. Am. Chem. Soc.* **1967**, *89*, 6454-6462.
- [493] T. L. Bluhm, G. Rappenecker, and P. Zugenmaier, *Carbohydr. Res.* **1978**, *60*, 241-250.
- [494] A. Sarko and A. Biloski, *Carbohydr. Res.* **1980**, *79*, 11-21.
- [495] S. A. Foord and E. D. T. Atkins, *Biopolymers* **1989**, *28*, 1345-1365.
- [496] (a) S. Arnott and W. E. Scott, *J. Chem. Soc., Perkin Trans. 2*, **1972**, 324-335. – (b) A. D. French and V. G. Murphy, *Carbohydr. Res.* **1973**, *27*, 391-406.
- [497] A. D. French and V. G. Murphy, *Polymers* **1977**, *18*, 489-494.
- [498] P. Dais, *Carbohydr. Res.* **1987**, *160*, 73-93.
- [499] J. Szejtli, *ACS Symp. Ser.* **1991**, *458*, 2-10 [*Chem. Abstr.* **1991**, *115*, 29776m].
- [500] S. Kitamura, T. Okoamoto, Y. Nakata, T. Hayashi, and T. Kuge, *Biopolymers* **1987**, *26*, 537-548.
- [501] E. S. Stevens and B. K. Sathyanarayana, *J. Am. Chem. Soc.* **1989**, *111*, 4149-4154.
- [502] E. Takusagawa, R. A. Jacobson, *Acta Crystallogr., Sect. B*, **1978**, *34*, 213-218.
- [503] M. E. Gress, G. A. Jeffrey, *Acta Crystallogr., Sect. B*, **1977**, *33*, 2490-2495.
- [504] I. Tanaka, N. Tanaka, T. Ashida, M. Kakudo, *Acta Crystallogr., Sect. B*, **1976**, *32*, 155-160.
- [505] S. S. C. Chu, G. A. Jeffrey, *Acta Crystallogr.* **1967**, *23*, 1038-1049.
- [506] (a) W. Hinrichs, G. Büttner, M. Steifa, C. Betzel, V. Zabel, B. Pfannenmüller, and W. Saenger, *Science* **1987**, *238*, 205-208. – (b) W. Hinrichs and W. Saenger, *J. Am. Chem. Soc.* **1990**, *112*, 2789-2796.
- [507] R. Viebahn-Haensler, *Ger. Offen.* **1991**, DE 4.100.782 [*Chem. Abstr.* **1992**, *117*, 137686g].
- [508] M. M. Colin and H. Gaultier de Claubry, *Ann. Chim.* **1814**, *90*, 87-100.
- [509] For some reports of historical interest see: (a) A. Lottermoser, *Z. Angew. Chem.* **1924**, *37*, 84-85. – (b) H. D. Murray, *J. Chem. Soc. London* **1925**, *127*, 1288-1294. – (c) K. H. Meyer and P. Bernfeld, *Helv. Chim. Acta* **1941**, *24*, 389-392.
- [510] (a) R. E. Rundle and R. R. Baldwin, *J. Am. Chem. Soc.* **1943**, *65*, 554-558. – (b) R. E. Rundle and D. French, *J. Am. Chem. Soc.* **1943**, *65*, 558-561. – (c) R. E. Rundle and D. French, *J. Am. Chem. Soc.* **1943**, *65*, 1707-1710. – (d) R. E. Rundle and F. C. Edwards, *J. Am. Chem. Soc.* **1943**, *65*, 2200-2203. – (e) R. E. Rundle, *J. Am. Chem. Soc.* **1947**, *69*, 1769-1772.
- [511] (a) F. L. Bates, D. French, and R. E. Rundle, *J. Am. Chem. Soc.* **1943**, *65*, 142-148. – (b) R. R. Baldwin, R. S. Bear, and R. E. Rundle, *J. Am. Chem. Soc.* **1944**, *66*, 111-115. – (c) R. E. Rundle, J. F. Foster, and R. R. Baldwin, *J. Am. Chem. Soc.* **1944**, *66*, 2116-2120.
- [512] (a) R. E. Rundle, *J. Chem. Phys.* **1947**, *15*, 880. – (b) R. S. Stein and R. E. Rundle, *J. Chem. Phys.* **1948**, *16*, 195-207.
- [513] C. D. West, *J. Chem. Phys.* **1947**, *15*, 689; **1951**, *19*, 1432.
- [514] (a) R. J. Hach and R. E. Rundle, *J. Am. Chem. Soc.* **1951**, *73*, 4321-4324. – (b) J. M. Reddy, K. Knox, and M. B. Robin, *J. Chem. Phys.* **1964**, *40*, 1082-1089.

- [515] (a) J. F. Foster and D. Zucker, *J. Phys. Chem.* **1952**, *56*, 170-173. – (b) J. F. Foster and E. Paschall, *J. Am. Chem. Soc.* **1952**, *74*, 2105-2106. – (c) E. Paschall and J. F. Foster, *J. Am. Chem. Soc.* **1953**, *75*, 1177-1180; 1181-1183.
- [516] (a) F. W. Schneider, C. L. Cronan, and S. K. Podder, *J. Phys. Chem.* **1968**, *72*, 4563-4568. – (b) C. L. Cronan and F. W. Schneider, *J. Phys. Chem.* **1969**, *73*, 3990-4004.
- [517] (a) J. A. Thoma and D. French, *J. Am. Chem. Soc.* **1960**, *82*, 4144-4147. – (b) J. M. Bailey and W. J. Whelan, *J. Biol. Chem.* **1961**, *236*, 969-973. – (c) T. Handa and H. Yajima, *Biopolymers* **1979**, *18*, 873-886; **1980**, *19*, 723-740. – (d) B. Pfannenmüller, H. Mayerhöfer, R. C. Schulz, *Macromol. Chem.* **1969**, *121*, 147-158; *Biopolymers* **1971**, *10*, 243-261.
- [518] M. B. Senior and E. Hamori, *Biopolymers* **1973**, *12*, 65-78.
- [519] B. Pfannenmüller, *Carbohydr. Res.* **1978**, *61*, 41-52.
- [520] (a) C. T. Greenwood, *Adv. Carbohydr. Chem.* **1956**, *11*, 335-393. – (b) J. F. Kennedy, *Adv. Carbohydr. Chem. Biochem.* **1974**, *29*, 305-405.
- [521] (a) F. R. Dintzis and A. C. Beckwith, *Macromolecules* **1976**, *9*, 471-478. – (b) F. R. Dintzis, R. Tobin, and A. C. Beckwith, *Macromolecules* **1976**, *9*, 478-482.
- [522] (a) M. Tasumi, *Chem. Lett.* **1972**, 75-78. – (b) M. E. Heyde, L. Rimai, R. G. Kilponen, and D. Gill, *J. Am. Chem. Soc.* **1972**, *94*, 5222-5227. – (c) R. C. Teitelbaum, S. L. Ruby, and T. J. Marks, *J. Am. Chem. Soc.* **1978**, *100*, 3215-3217; **1980**, *102*, 3322-3328.
- [523] T. Hirai, M. Hirai, S. Hayashi, and T. Ueki, *Macromolecules* **1992**, *25*, 6699-6702.
- [524] (a) W. Banks, C. T. Greenwood, and D. D. Muir, *Starch / Stärke* **1971**, *23*, 118-124. – (b) M. S. Karve and N. R. Kale, *Starch / Stärke* **1992**, *44*, 19-21.
- [525] M. K. Pal and P. K. Pal, *Macromol. Chem.* **1989**, *190*, 2929-2938.
- [526] M. B. Robin, *J. Chem. Phys.* **1964**, *40*, 3369-3377.
- [527] B. S. Ehrlich and M. Kaplan, *J. Chem. Phys.* **1969**, *51*, 603-606.
- [528] R. Bersohn and I. Isenberg, *J. Chem. Phys.* **1961**, *35*, 1640-1643.
- [529] W. L. Peticolas, *Nature* **1963**, *197*, 898-899.
- [530] H. Murakami, *J. Chem. Phys.* **1954**, *22*, 367-374; **1955**, *23*, 1979.
- [531] (a) S. Ono, S. Tsuchihashi, and T. Takashi, *J. Am. Chem. Soc.* **1953**, *75*, 3601-3602. – (b) T. Kuge and S. Ono, *Bull. Chem. Soc. Jpn.* **1960**, *33*, 1269-1270; 1273-1278.
- [532] S. Ono, T. Watanabe, K. Ogawa, and N. Okazaki, *Bull. Chem. Soc. Jpn.* **1965**, *38*, 643-648.
- [533] J. C. Thompson and E. Hamori, *J. Phys. Chem.* **1972**, *75*, 272-280.
- [534] A. Cesáro, J. C. Benegas, and D. R. Ripoli, *J. Phys. Chem.* **1986**, *90*, 2787-2791.
- [535] M. Minick, K. Fotta, and A. Khan, *Biopolymers* **1991**, *31*, 57-63.
- [536] G. A. Gilbert, J. V. R. Marriott, *Trans. Faraday Soc.* **1948**, *44*, 84-93.
- [537] T. Handa, H. Yajima, and T. Kajiura, *Biopolymers* **1980**, *19*, 1723-1741.
- [538] (a) W. Banks, C. T. Greenwood, and K. M. Khan, *Carbohydr. Res.* **1971**, *17*, 25-33. – (b) A. Cesáro, E. Jerian, and S. Saule, *Biopolymers* **1980**, *19*, 1491-1506. – (c) T. Handa, H. Yajima, T. Yamamura, T. Ishii, and H. Aikawa, *Stärke / Starch* **1980**, *32*, 194-197.
- [539] F. Cramer, *Naturwissenschaften* **1951**, *38*, 188.