STRUCTURAL CHEMISTRY

Volume 73 (2017)

Supporting information for article:

Structural characterization, gelation ability, and energy-framework analysis of two bis(long-chain ester)-substituted 4,4′-biphenyl compounds

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Supplementary Material

Structural characterization, gelation ability and energy framework analysis of two bis (long-chain ester)-substituted 4,4'-biphenyl compounds

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Table S1. Pertinent CCDC 4,4'-biphenol references

Refcode	CCDC identifier	Reference	dihedral angle between rings
COBLAG	139753	C.Glidewell, G.Ferguson, R.M.Gregson, A.J.Lough, *Acta Crystallographica,Section C: Crystal Structure Communications*, 1999, 55, 2133-2136. DOI: 10.1107/S0108270199010434	180, -155.5, 180
COZZEX	730429	D.R.Weyna, T.Shattock, P.Vishweshwar, M.J.Zaworotko, *Crystal Growth and Design*, 2009, 9, 1106-1123. DOI: 10.1021/cg800936d	-180
CUTYEV	141641	R.M.Gregson, C.Glidewell, G.Ferguson, A.J.Lough, *Acta Crystallographica,Section B: Structural Science*, 2000, 56, 39-57. DOI: 10.1107/S0108768199006072	180, -143.5 (monodeprot.)
CUVNAI	141648	C.Glidewell, G.Ferguson, R.M.Gregson, C.F.Campana, *Acta Crystallographica,Section B: Structural Science*, 2000, 56, 68-84. DOI: 10.1107/S0108768199009714	15.7, 170.8, -172, 167.7, -175.4 -179.6 (deprot.)
ECELON	1148485	S.Ahn, B.M.Kariuki, K.D.M.Harris, *Crystal Growth and Design*, 2001, 1, 107-111. DOI: 10.1021/cg000010b	172.1
ECELON01	163762	S.Ahn, B.M.Kariuki, K.D.M.Harris, *Crystal Growth and Design*, 2001, 1, 107-111. DOI: 10.1021/cg000010b	145.2

HAJQUF	241603	R.Kuroda, K.Higashiguchi, S.Hasebe, Y.Imai, *CrystEngComm*, 2004, 6, 464-468. DOI: 10.1039/b408971e	179.5
KEWZUI	636008	J.A.Bis, O.L.McLaughlin, P.Vishweshwar, M.J.Zaworotko, *Crystal Growth and Design*, 2006, 6, 2648-2650. DOI: 10.1021/cg060516f	-144.6
KEXBAR	636010	J.A.Bis, O.L.McLaughlin, P.Vishweshwar, M.J.Zaworotko, *Crystal Growth and Design*, 2006, 6, 2648-2650. DOI: 10.1021/cg060516f	-180, -164
KIHYUW	655973	J.A.Bis, P.Vishweshwar, D.Weyna, M.J.Zaworotko, *Molecular Pharmaceutics*, 2007, 4, 401-416. DOI: 10.1021/mp070012s	-180
LIPXUD	134767	G.Ferguson, C.Glidewell, E.S.Lavender, *Acta Crystallographica,Section B: Structural Science*, 1999, 55, 591-600. DOI: 10.1107/S0108768199002657	-180
LIQQAD	137120	W.Jaunky, M.W.Hosseini, J.M.Planeix, A.De Cian, N.Kyritsakas, J.Fischer, *Chemical Communications*, 1999, 2313-2314. DOI: 10.1039/a906728k	150
NISLOQ	131948	G.Ferguson, C.Glidewell, R.M.Gregson, P.R.Meehan, I.L.J.Patterson, *Acta Crystallographica,Section B: Structural Science*, 1998, 54, 151-161. DOI: 10.1107/S0108768197010148	139.6
NISLUW	131949	G.Ferguson, C.Glidewell, R.M.Gregson, P.R.Meehan, I.L.J.Patterson CCDC 131949: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/cc4f9f8	-142.5, -164.4
NISMAD	131950	G.Ferguson, C.Glidewell, R.M.Gregson, P.R.Meehan, I.L.J.Patterson, *Acta Crystallographica, Section B: Structural Science*, 1998, 54, 151, DOI: 10.1107/S0108768197010148	180
QOVHUF	730430	D.R.Weyna, T.Shattock, P.Vishweshwar, M.J.Zaworotko, *Crystal Growth and Design*, 2009, 9, 1106-1123. DOI: 10.1021/cg800936d	180
TEHNAW	607931	J.A.Bis, P.Vishweshwar, R.A.Middleton, M.J.Zaworotko, *Crystal Growth and Design*, 2006, 6, 1048-1053. DOI: 10.1021/cg0680024 J.A.Bis, P.Vishweshwar, D.Weyna, M.J.Zaworotko, *Molecular Pharmaceutics*, 2007, 4, 401-416. DOI: 10.1021/mp070012s	180

TEHNAW01	607932	J.A.Bis, P.Vishweshwar, R.A.Middleton, M.J.Zaworotko, *Crystal Growth and Design*, 2006, 6, 1048-1053. DOI: 10.1021/cg0680024 J.A.Bis, P.Vishweshwar, D.Weyna, M.J.Zaworotko, *Molecular Pharmaceutics*, 2007, 4, 401-416. DOI: 10.1021/mp070012s	-160, -140.3
WISQAQ	144373	C.Glidewell, G.Ferguson, R.M.Gregson, A.J.Lough, *Acta Crystallographica,Section B: Structural Science*, 2000, 56, 287-298. DOI: 10.1107/S0108768199014032	180, 161.5 (monode-prot.)

Figure S1. ^{1}H NMR spectrum of BBO6A in DMSO-d_6

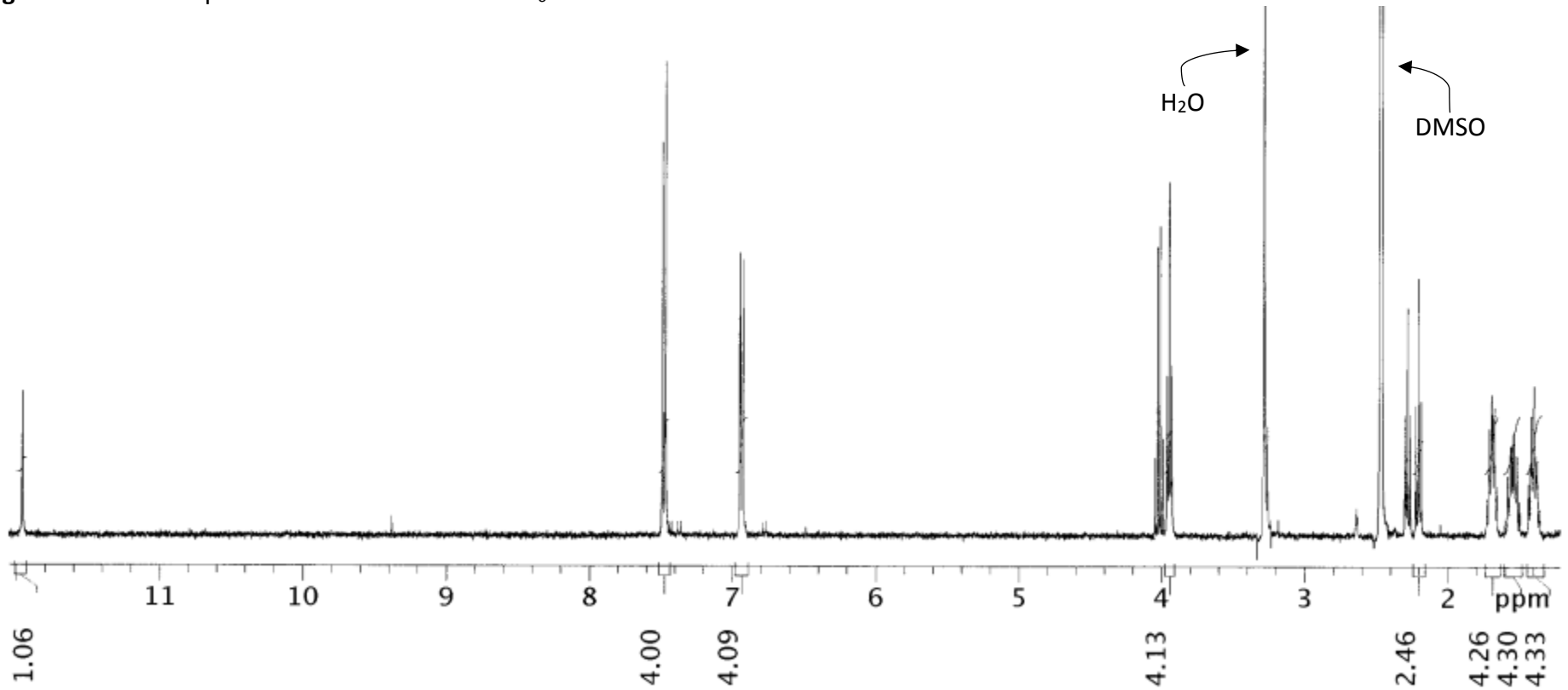

Figure S2. ^{1}H NMR spectrum of BBO6-Me in $CDCl_3$

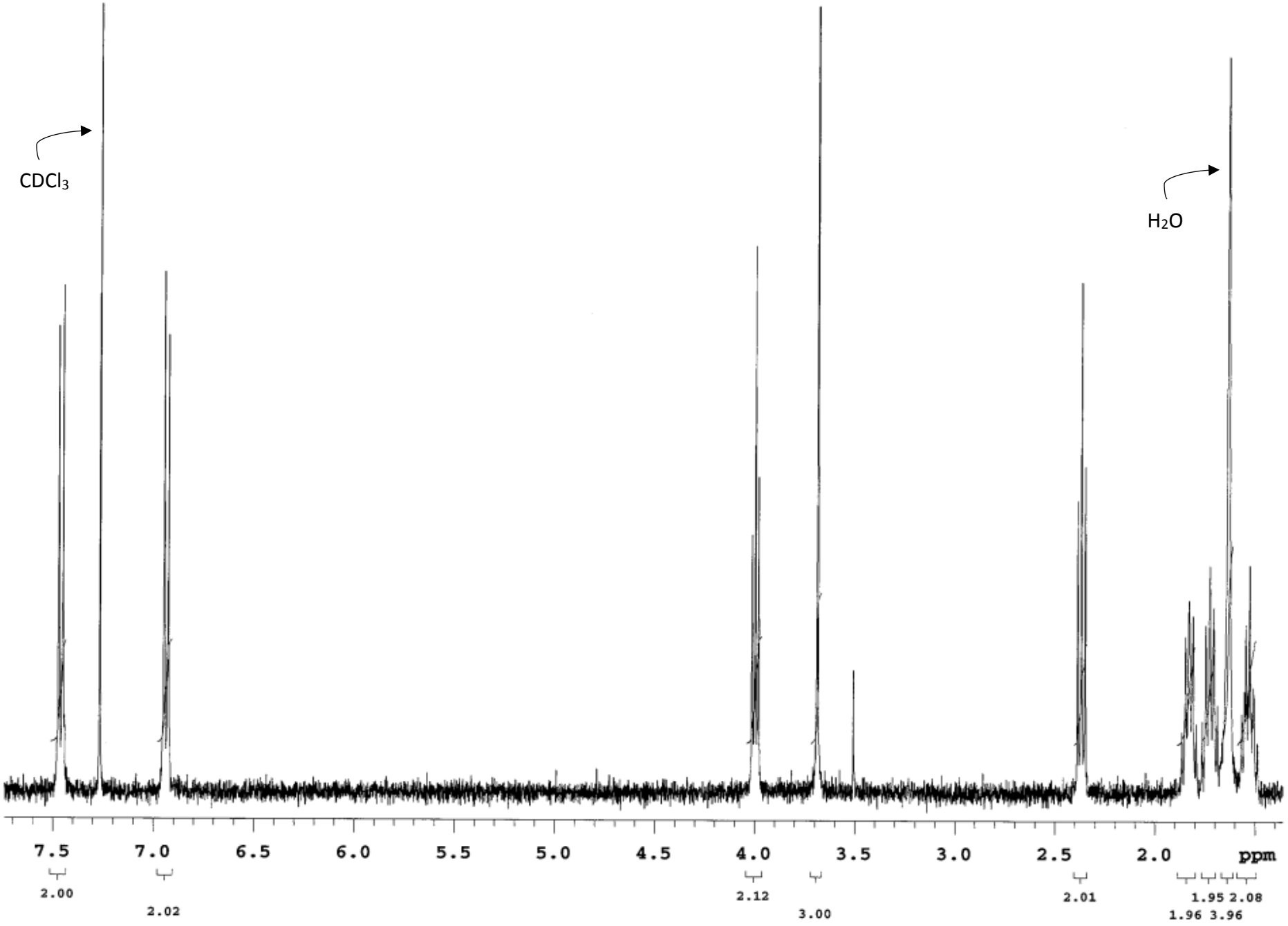

Figure S3. ^{1}H NMR spectrum of BBO6-Et in DMSO-d_6