STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 71 (2015)

Supporting information for article:

Structural and energy insights on solid-state complexes with trimethoprim: a combined theoretical and experimental investigation

Anaelle Tilborg, Andrea Carletta and Johan Wouters

Table S1 C-O bond lengths (fumaric acid molecules in Figure 1)

Bond numbering (Figure 1)	**C-O lenthgs (Å)**
1	1.300(2)
2	1.219(2)
3	1.236(2)
4	1.263(2)
5	1.302(2)
6	1.218(2)
7	1.235(2)
8	1.266(3)

Table S2 C-O bond lengths (fumaric acid molecules in Figure 1)

Metallic or counter-anion partners	**Structure CSD refcodes**
Cu	COHDOS (Naldini *et al.*, 1984)
	HAGRUD (Raj *et al.*, 2003)
	KUJFOL (Habib *et al.*, 2009)
	LOBFAK01 (Maddileti *et al.*, 2015)
	LOBFAK (Ajibade *et al.*, 2008)
	TUKPAR (Habib *et al.*, 2009)
	VEWSUL (Demartin *et al.*, 1990)
Co	CIBDIA (Demartin *et al.*, 1983)
	CIBDIA01 (Madhupriya *et al.*, 2014)
	LOBFEO (Ajibade *et al.*, 2008)
Cd	BEHNEH (Thomas Muthiah *et al.*, 1999)
	UGIZEP (Simo *et al.*, 2000)
Ni	DEPBEG (Ajibade *et al.*, 2006)
Rh	FEMFEI (Zoroddu *et al.*, 1987)
Zn	UGIZAL (Simo *et al.*, 2000)
Sulfate	CABYIO (Thomas Muthiah *et al.*, 2001)
Perchlorate	IDILUC (Thomas Muthiah *et al.*, 2002)
Chloride	TMPHCL01 (Nakai *et al.*, 1984)
tetrafluoroborate	VAYTUL (Hemamalini *et al.*, 2005)

Table S3 CSD structures involving trimethoprim and sulfonamides derivatives.

Structure name (CSD refcode)	Formula	Space group	Lattice parameters (Å)	Lattice parameters (°)	Cell volume	Z	R (%)
Cocrystals							
SMZTMP (Giuseppetti et al., 1980) (sulfamethoxazole)	$C_{14}H_{18}N_4O_3$, $C_{10}H_{11}N_3O_3S$	*Pbca*	a 12.055(5) b 24.476(1) c 17.4223(1)	α 90.00 β 90.00 γ 90.00	5140.5(9)	8	5.40
RIWLOY (Sardone et al., 1997) (sulfadimidine monohydrate)	$C_{14}H_{18}N_4O_3$, 2($C_{12}H_{14}N_4O_2S$), H_2O	*P2₁/n*	a 11.075(1) b 9.268(1) c 40.170(5)	α 90.00 β 94.05(1) γ 90.00	4112.8(8)	4	4.90
RASSUZ (Bettinetti et al., 1997) (sulfadimidine methanol solvate)	$C_{14}H_{18}N_4O_3$, $C_{12}H_{14}N_4O_2S$, CH_4O	$P\bar{1}$	a 7.812(1) b 12.000(1) c 17.161(1)	α 78.92(2) β 84.32(2) γ 72.23(2)	1502.0(3)	2	4.10
QASHEX (Bettinetti et al., 2000) (sulfamethoxy pyridazine)	$C_{14}H_{18}N_4O_3$, $C_{11}H_{12}N_4O_3S$	*P2₁/c*	a 12.499(1) b 24.993(1) c 9.393(1)	α 90.00 β 93.163(1) γ 90.00	2929.7(9)	4	5.73
Salts							
QASHIB (Bettinetti et al., 2000) (sulfamethoxy pyridazine sesquihydrate)	$C_{14}H_{19}N_4O_3^+$, $C_{11}H_{11}N_4O_3S^-$, 1.5(H_2O)	*C2/c*	a 42.4543(8) b 6.5404(1) c 20.9017(4)	α 90.00 β 100.291(7) γ 90.00	5710.3(6)	8	4.79
SMZTMP01(Nakai et al., 1984) (sulfamethoxazole)	$C_{14}H_{19}N_4O_3^+$, $C_{10}H_{10}N_3O_3S^-$	*Pbca*	a 12.058(2) b 24.479(6) c 17.427(4)	α 90.00 β 90.00 γ 90.00	5143.8(9)	8	5.70
HEKRUK	$C_{14}H_{19}N_4O_3^+$,	*P2₁/c*	a 14.768(3)	α 90.00	2649.2(3)	4	3.19

(Giuseppetti et al., 1994) (sulfametrole)	$C_9H_9N_4O_3S_2^-$		b 15.133(4) c 12.818(3)	β 112.36(2) γ 90.00			

Table S4 CSD other cocrystals structures involving trimethoprim.

Structure name (CSD refcode)	Formula	Space group	Lattice parameters (Å)	Lattice parameters (°)	Cell volume	Z	R (%)
Cocrystals							
GOLDOC (Ton et al., 2010 & 2014) (3,3-tetramethyleneglutarimide)	$C_{14}H_{18}N_4O_3$, $C_9H_{13}NO_2$	$P\bar{1}$	a 9.674(2) b 14.638(3) c 17.910(4)	α 94.71(3) β 98.15(3) γ 108.72(3)	2355.6(4)	4	9.40
BEXVOP (Shimizu et al., 1982) (saccharine monohydrate)	$C_{14}H_{18}N_4O_3$, $C_7H_5NO_3$, H_2O	$P\bar{1}$	a 9.152(9) b 11.487(6) c 12.674(9)	α 89.81(5) β 103.97(7) γ 113.95(6)	1174.9(2)	2	8.20
BIGCUP (Shimizu et al., 1982) (barbital)	$C_{14}H_{18}N_4O_3$, $C_8H_{12}N_2O_3$	*C2/c*	a 12.509(10) b 16.532(7) c 22.627(29)	α 90.00 β 94.56(13) γ 90.00	4664.4(2)	8	7.30
LIBCOQ (Delori et al., 2011) (2-aminoterephthalic acid)	$C_{14}H_{18}N_4O_3$, $C_8H_7NO_4$	$P2_1/c$	a 9.1977(1) b 8.2553(1) c 23.7783(4)	α 90.00 β 96.193(1) γ 90.00	1794.9(4)	2	5.61
GIGQIX (Thomas Muthiah et al., 2007) (barbituric acid monohydrate)	$C_{14}H_{18}N_4O_3$, $C_4H_4N_2O_3$, H_2O	$P\bar{1}$	a 7.558(3) b 24.955(3) c 5.742(2)	α 95.28(3) β 111.89(3) γ 89.83(3)	1000.0(8)	2	7.14

TOSGOZ (Ton, 2015) (glutarimide)	$C_{14}H_{18}N_4O_3$, $C_5H_7NO_2$	*P2₁/n*	a 8.774(2) b 17.046(3) c 14.168(3)	α 90.00 β 102.04(3) γ 90.00	2072.3(8)	4	4.11
TOSGUF (Ton, 2015) (3,3-dimethylglutarimide)	$C_{14}H_{18}N_4O_3$, $C_7H_{11}NO_2$	$P\bar{1}$	a 7.361(2) b 12.032(2) c 14.132(3)	α 109.59(3) β 92.48(3) γ 99.14(3)	1157.9(3)	2	3.75

Table S5 CSD salt structures with coformers similar to fumaric acid.

Structure name (CSD refcode)	Formula	Space group	Lattice parameters (Å)	Lattice parameters (°)	Cell volume	Z	R (%)
Salts							
YECNEA (Trask et al., 2006) (succinate)	$C_{14}H_{19}N_4O_3^+$, $0.5(C_4H_4O_4^{2-})$	*C2/c*	a 17.343(4) b 11.672(2) c 16.835(3)	α 90.00 β 91.95(3) γ 90.00	3405.8(9)	8	3.90
QOVROJ (Franklin et al., 2009) (DL-malate)	$C_{14}H_{19}N_4O_3^+$, $0.5(C_4H_4O_5^{2-})$	*P2₁/c*	a 12.9850(3) b 9.3038(2) c 15.6815(3)	α 90.00 β 111.065(1) γ 90.00	1767.8(8)	2	4.50
QIKDIX (Prabakaran et al., 2001) (hemimaleate)	$C_{14}H_{19}N_4O_3^+$, $C_4H_3O_5^-$	*P2₁/n*	a 28.485(2) b 12.964(3) c 5.413(2)	α 90.00 β 93.27(3) γ 90.00	1995.6(6)	4	6.51
HAMYIE (Hemamalini et al., 2004) (hemimalonate)	$C_{14}H_{19}N_4O_3^+$, $C_3H_3O_4^-$	$P\bar{1}$	a 8.4851(2) b 8.6566(2) c 13.6425(3)	α 106.360(3) β 91.712(2) γ 92.950(3)	959.1(9)	2	5.40
CACBOY (Robert et al., 2001) (hemiglutarate)	$C_{14}H_{19}N_4O_3^+$, $C_5H_7O_4^-$	$P\bar{1}$	a 12.017(2) b 10.090(3) c 8.804(4)	α 84.430(3) β 94.900(3) γ 104.590(3)	1026.1(4)	2	4.80

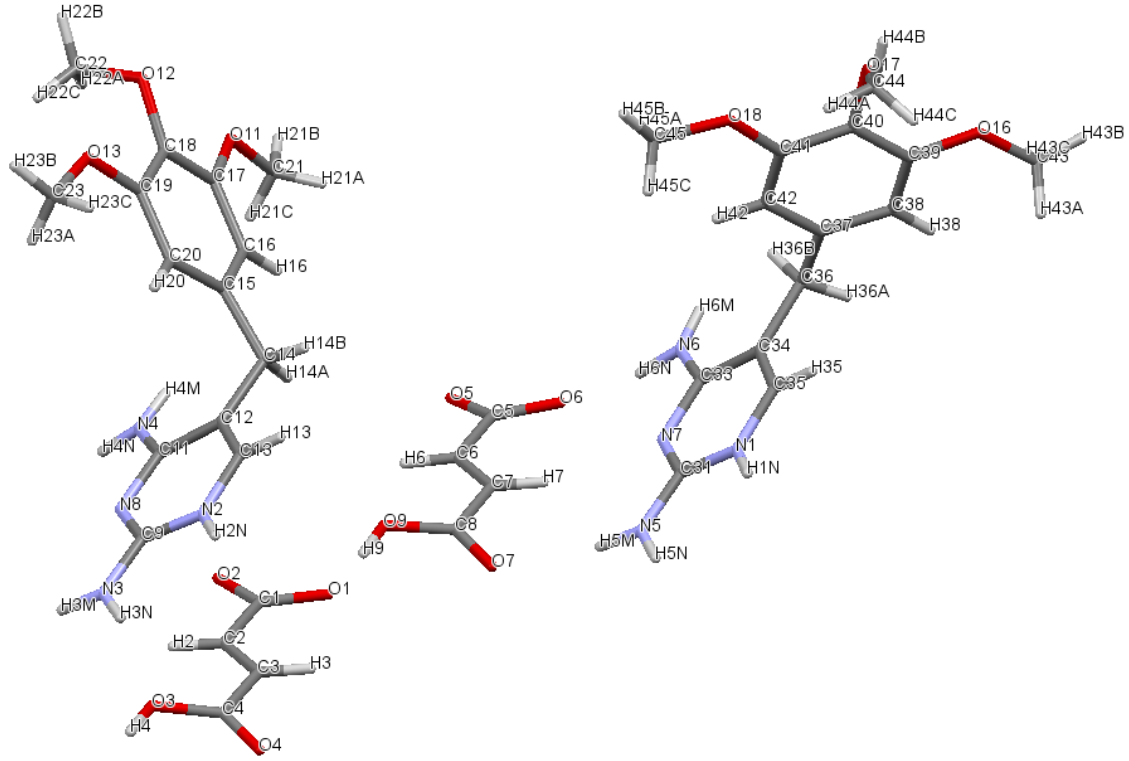

Figure S1 Numbering of atoms in the asymmetric unit for $TRIMH^{+}/FA^{-}$.

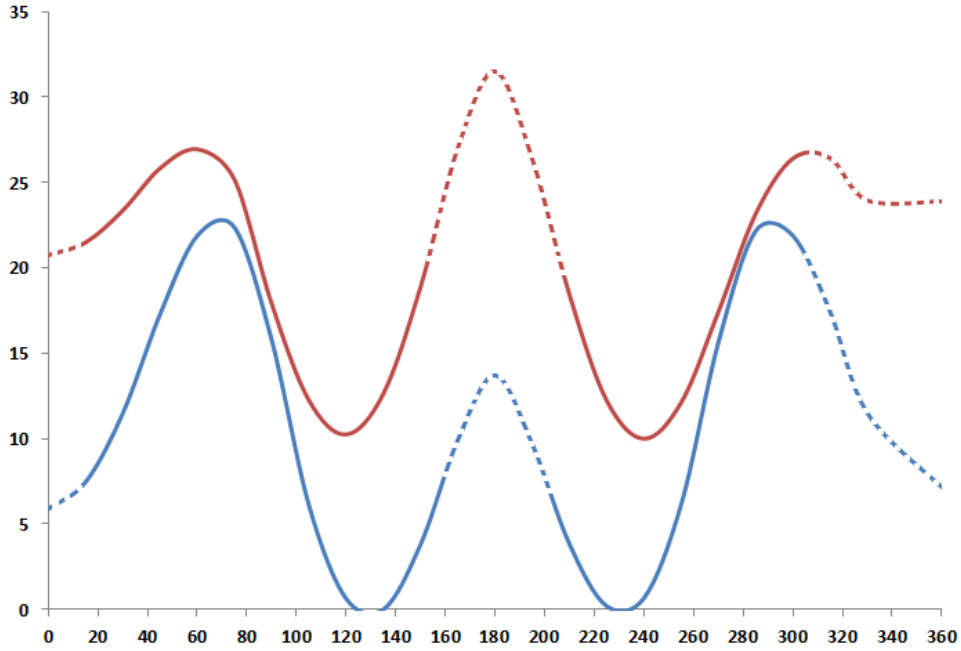

Figure S2 Comparison for 1D conformational scan of T1 for protonated and non-protonated form of TRIM. The two curves fit nicely, allowing the inclusion of neutral structures in the comparison with theoretical results from 2D conformational scan (T1 and T2 torsion angles). Dotted parts represented the blank areas in the 2D conformational scan, not considered because of sterical hindrance.