

SUPPLEMENTARY MATERIAL for

Crystal Packing in *vicinal* Diols $C_nH_m(OH)_2$

BY CAROLYN PRATT BROCK

Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055, USA

EMAIL address: CPBROCK@UKY.EDU

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Synopsis: A survey of the O-H \cdots O bonds in *vic*-diols $C_nH_m(OH)_2$ reveals a variety of patterns. The space-group frequencies are anomalous for the half of the *vic*-diols that form full, or almost full, sets of O-H \cdots O bonds.

Material Included: Spreadsheet giving information about the 71 *vic*-diol structures included in the survey.

Tabulation of vic-diol Structures CnHm(OH)2:

REFCODE	Type	Spc Grp #	SpcGrp Name	Z'	SS ?	no - 1?	Rng Siz; # mult bnds, fused rngs	Stereo-chem	Pattern	nD	design ation	Link sym	dim ers?	dim er sym m	Inter OH...O Bonding	avg inter	Inter O...O Distances	Other	R	T	H xyz?	H xyz ref?
NOZKES	1	19	P212121	1	0	1	NA	NA	3D net	3	3a		0	NA	2/2	2	2.71, 2.73	could have -1 imposed but doesn't	0.052	130	1	1
BACKAR	2.2	14	P21/c	1	1	0	6; 2	trans	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.69, 2.71		0.074	RT	1	1
BOPRIH10	2.2	14	P21/c	2	0	0	6; 1	cis	dimer columns	1	1b	T(a) [-1 + -1]	1	-1	2/2; 2/2	2	2.68 - 2.82 (4)	A...A and B...B dimers	0.053	RT	1	1
BUCHDO	2.2	2	P-1	2	1	0	6; 0	cis	tetramer stacks	1	1f	? [-1]	1	-1	2/3; 1/2	2	2.76 - 2.89 (4)		0.063	RT	1	1
CIZYOZ	2.2	2	P-1	2	1	0	5; 1	cis	tetramer stacks	1	1f	T(c) [-1*2]	1	-1	2/3; 1/2	2	2.82 - 3.06 (4)		0.046	RT	1	1
DHXBAN	2.2	14	P21/c	1	1	0	6; 2	trans	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.75, 2.84		0.069	RT	1	1
DHXCAM	2.2	80	I41	2	1	1	5; 1	trans	ladder (double)	1	1h		0	NA	2/2; 2/2	2	2.66 - 2.88 (4)	2 OH..OH.. chains around 4(1) axis;	0.047	RT	0	NA
DOXBZA	2.2	86	P42/n	1	1	0	6; 2	trans	dimer stacks	1	1c	42(c) [2(c)] (?)	1	2	2/2	2	2.80, 2.80	pi stacking?	0.059	RT	1	1
FILJIT	2.2	2	P-1	6	1	0	6; 0	trans	dimer ribbons/stacks; ladder	1	1x		1	-1, 1	6*(2/2)	2	2.69 - 2.83 (24)	very complicated pattern (Z'=6)	0.075	173	1	1
JAJSOC	2.2	15	C2/c	1	1	0	5; 2	trans	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.76, 2.78		0.042	RT	1	1
MBZAOX10	2.2	14	P21/a	2	1	0	6; 2	cis	dimer ribbons	1	1a	T(c) [1]	1	1	2/2; 2/2	2	2.69 - 2.88 (4)	pi...pi interactions; pseudo -1 in dimer	0.050	RT	1	1
NADNIP	2.2	19	P212121	1	1	1	6; 2	trans	variant of linked chains	2	2b		0	NA	2/2	2	2.70, 2.77		0.059	RT	1	1
TETRD001	2.2	4	P21	2	1	1	6; 1	trans	dimer nets	2	2a		1	1	2/2; 1/3	2	2.82 - 2.92 (4)	pi...pi interactions?	0.031	RT	1	1
TITKIQ	2.2	2	P-1	0.5	0	0	NA	NA	none	NA	NA	NA	NA	NA	0/0	0		no O...O < 4.0	0.053	183	1	1
VABVAV	2.2	4	P21	1	1	1	NA	NA	simple chain	1	1i	21(b)	0	NA	1/1	1	2.78+R8	no other O...O < 3.4; possible intra H bond	0.033	RT	1	1
VABVEZ	2.2	14	P21/c	0.5	0	0	NA	NA	linked chains	2	2b		0	NA	2/2	2	2.80		0.045	RT	1	1
YACROJ	2.2	2	P-1	2	0	0	5; 2	cis	tetramer stacks	1	1f	T(a) [-1*2]	1	-1	2/2; 1/3	2	2.85, 2.86, 2.90, 3.06	one long bond (no H positions)	0.040	178	0	NA
YIPSIZ	2.2	61	Pbca	1	1	0	6; 2	trans	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.67, 2.68		0.051	RT	1	1
ZENMUA	2.2	2	P-1	1	1	0	6; 3	trans	ladder	1	1h	-1(z+1/2) [-1]	1	-1	2/2	2	2.70, 2.72	weak pi stacking?	0.045	RT	1	1
ZZZKPE01	2.2	61	Pbca	1	1	0	6; 0	trans	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.73, 2.78		0.035	RT	1	1
ZZZKPE03	2.2	152	P3121	1	1	1	6; 0	trans	3D dimer network	3	3b	??? [2(ab)]	1	2	2/2	2	2.75, 2.79	dimers on C2	0.025	215	1	1
ZZZPSA01	2.2	61	Pbca	1	0	0	6; 0	cis	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.76, 2.78		0.033	RT	1	1
ACAVIJ	3	88	I41/a	1	1	0	6; 2	cis	simple chain	1	1i	41©	0	NA	1/1	1	2.756	no other O...O < 3.4	0.044	RT	1	1

BOWDUM	3	19	P212121	2	1	1	5; 1	trans	partially linked dimers	1	1g	T(c) [1]	1	1	1/2, 1/2	1.5	2.74, 2.81, 2.83	0.096	RT	0	NA
DXTHBP	3	14	P21/c	1	1	0	6; 3	cis	dimer ribbons	1	1a	T(b) [-1]	1	-1	2/2	2	2.71, 2.72	0.052	RT	0	NA
HINFIT	3	14	P21/n	1	1	0	NA	NA	chelate chains	1	1e		0	NA	1/3	2	2.93, 3.01	0.082	RT	1	1
ISCOMD	3	19	P212121	1	1	1	5; 2	cis	simple chain	1	1i	21(a)	0	NA	1/1	1	2.82	0.069	RT	1	1
LIMJEW	3	14	P21/c	1	1	0	8; 2	trans	simple chain	1	1i	cglide(b)	0	NA	1/1	1	2.89	0.042	150	1	0
NUMTUK	3	144	P31	1	1	1	6; 1	cis	chelate chains	1	1e		0	NA	1/3	2	2.71, 3.14	0.040	RT	1	0
POSMIT	3	14	P21/n	1	1	0	NA	NA	dimers	0	0a	[-1]	1	-1	1/1	1	2.93	0.050	RT	1	1
POS MOZ	3	4	P21	1	1	1	NA	NA	simple chain	1	1i	21(b)	0	NA	1/1	1	2.84	0.043	RT	1	0
TIVFUZ	3	154	P3221	1	1	1	6; 2	cis	simple chain	1	1i	21(ab)	0	NA	1/1	1	2.73	0.042	RT	1	0
XAPVAL	3	14	P21/c	1	1	0	NA	NA	dimers	0	0a	[-1]	1	-1	1/1	1	2.89	0.039	RT	1	1
YUYXAR	3	171	P62	2	1	1	NA	NA	tetramer	0	0x		0	NA	2/2, 1/2	1.75	2.78, 2.79, 2.80, 2.87	0.055	RT	1	0
YUYXEV	3	45	lba2	1	1	0	NA	NA	none	NA	NA	NA	0	NA	0/0	0		0.035	RT	1	1
ZEBVAD	3	19	P212121	1	1	1	5; 1	cis	simple chain	1	1i	21(c)	0	NA	1/1	1	2.68	0.063	RT	0	NA
ZESPES	3	2	P-1	1	1	0	6; 2	cis	dimer ribbons	1	1a	T(a) [-1]	1	-1	2/2	2	2.71, 2.71	0.043	130	1	0
ZOTBUF	3	4	P21	2	1	1	NA	NA	variant of simple chain	1	1i	T(a) [1]	0	NA	1/1, 2/0	1	2.78, 2.84	0.045	RT	1	1
ZOTCAM	3	14	P21/c	1	1	0	NA	NA	dimers	0	0a	[-1]	1	-1	1/1	1	2.92	0.045	RT	1	1
BEXJET	4	20	C2221	1	1	1	6; 1	cis	simple chain	1	1i	2(a) [2(b)]	0	NA	1/1	1	2.80, 2.80	0.035	RT	0	NA
BHPHOL	4	19	P212121	1	1	1	NA	NA	none	NA	NA	NA	0	NA	0/0	0		0.033	RT	1	1
BUHDAJ	4	86	P42/n	1	1	0	NA	NA	dimer ribbons	1	1a	42(c) [2(c)]	1	2	2/2	2	2.72, 2.79, 2.95	0.062	RT	0	NA
CIXWIP	4	4	P21	1	1	1	5; 1	cis	simple chain	1	1i	21(b)	0	NA	1/1	1	2.82	0.069	RT	1	0
CIZTIO	4	14	P21/a	1	1	0	5; 2	trans	simple chain	1	1i	aglide(b)	0	NA	1/1	1	2.88	0.046	RT	1	1
CSNLRA	4	182	P6322	1	1	1	NA	NA	paired layers	2	2x	2(ab) [3(c)]	0	NA	1/2	1.5	2.78, 3.15	0.062	RT	0	NA
DIJWUO10	4	1	P1	3	1	1	NA	NA	dimer/trimers	1	1d	T(a) [1 +]	1	1	2/2, 2/2, 2/2	2	2.80 - 3.06 (6)	0.064	RT	1	0
DODECB	4	2	P-1	1	1	0	5; 5	cis	simple chain	1	1i	T(b) [-1]	0	NA	1/1	1	2.71, 2.75	0.065	RT	0	NA
EDAROQ	4	19	P212121	1	1	1	7; 1	cis	simple chain	1	1i	21(b)	0	NA	1/1	1	2.84	0.046	RT	1	1
FECVIS	4	29	Pca21	1	0	0	(5; 1)(5; 2)	cis	simple chain	1	1i	21(c)	0	NA	1/1	1	2.78	0.073	RT	1	0
FODZED	4	2	P-1	1	1	0	8; 2	trans	simple chain	1	1i	T(c) [-1]	0	NA	1/1	1	2.85, 2.90	0.046	RT	1	0
FUJREH	4	14	P21/n	1.5	0	0	NA	NA	dimers/trimers	1	1d	T(a) [-1 + -1(1/2)]	1	-1	2/2, 2/2	2	2.77, 2.80, 2.82	0.052	RT	1	1
FUTZOJ	4	19	P212121	1	1	1	NA	NA	none	NA	NA	NA	0	NA	0/0	0		0.038	RT	0	NA

HOMQOP	4	15	C2/c	1.5	0	0	6; 4	cis	trimers	0	0x	[2(b)]	0	NA	1/0, 1/1	0.75	2.70	no other O...O < 3.4	0.077	RT	0	NA
HORCUM	4	19	P212121	2	1	1	NA	NA	simple chain (ABA..)	1	1i	21(b) [1]	0	NA	1/1, 1/1	1	2.75, 2.80	no other O...O < 3.4; possible intra H bond	0.058	RT	1	0
JAGGAZ	4	19	P212121	1	1	1	NA	NA	simple chain	1	1i	21(b)	0	NA	1/1	1	2.85	no other O...O < 3.4; possible intra H bond	0.043	RT	1	1
MTCDOL	4	29	Pca21	1	1	0	4; 2	cis	simple chain	1	1i	aglide(b)	0	NA	1/1	1	2.71	no other O...O < 3.4; possible intra H bond	0.034	RT	1	0
NUTSAW	4	33	Pha21	1	1	0	NA	NA	simple chain	1	1i	aglide(b)	0	NA	1/1	1	2.94	no other O...O < 3.4	0.044	180	1	0
PINCOL	4	15	C2/c	2	0	0	NA	NA		2	2x	?? [-1]	1	-1	2/2, 2/2, 2/2	2	2.82 - 2.86 (4)		0.063	RT	0	NA
VEHGOE	4	14	P21/n	1	0	0	NA	NA	simple chain	1	1i	T(b)	0	NA	1/1	1	2.84	no other O...O < 3.4	0.072	228	1	0
WEVSAR	4	2	P-1	1	0	0	NA	NA	simple chain (ABA..)	1	1i	T(a-c) [-1(1/2) + -1(1/2)]	0	NA	1/1, 1/1	1	2.86	no other O...O < 3.4	0.041	173	1	0
WEZDOU	4	4	P21	2	1	1	7; 2	cis	simple chains (AA..., BB..)	1	1i	2*{ 21(b) }	0	NA	1/1, 1/1	1	2.76, 2.77	no other O...O < 3.4; possible intra H bond	0.045	RT	1	1
WEZDUA	4	4	P21	2	1	1	5; 1	cis	simple chain (ABA..)	1	1i	T(c) [1]	0	NA	1/1, 1/1	1	2.79, 2.79	no other O...O < 3.4 if ignore comp disor	0.067	RT	1	0
WOVDIU	4	2	P-1	1	1	0	5; 1	trans	simple chain (ABA..)	1	1i	T(a)	0	NA	1/1	1	3.04	no other O...O < 3.4	0.048	RT	1	0
WOVDOA	4	14	P21/c	2	1	0	6; 2	trans	dimer ribbons	1	1a	T(c) [-1 + -1]	1	-1	2/2, 2/2	2	2.78, 2.83, 2.84(2)	dimers are AA or BB	0.065	RT	1	0
ZIVCEM	4	2	P-1	2	1	0	NA	NA	dimer ribbons	1	1a	T(a) [-1 + -1]	1	-1	2/2, 2/2	2	2.72 (2), 2.78 (2)	dimers are AA or BB	0.043	RT	1	1
ZIWVEG	4	15	C2/c	3	0	0	5; 0	cis	dimer ribbons	1	1a	T(a-c) { -1 } [1 + -1]	1	-1, 1	2/2, 2/2, 2/2	2	2.76 - 2.89 (5)	dimers are AB and CC	0.058	RT	0	NA
ZIXCOY	4	19	P212121	1	1	1	5; 1	cis	simple chain	1	1i	21(b)	0	NA	1/1	1	2.87	no other O...O < 3.4; possible intra H bond	0.055	RT	1	1
ZOSNEA	4	2	P-1	1	1	0	NA	NA	partially linked dimers	1	1g	T(a) [-1]	1	-1	1/2	1.5	2.78, 2.89	no other O...O < 3.4	0.048	RT	o	NA
CATCOL12	A	14	P21/c	1	0	0	6; 6	NA	dimer nets	2	2a	?? [-1]	1	-1	2/2	2	2.82, 2.80		0.038	RT	1	1
COXRUC	A	88	I41/a	1	0	0	6; 6	NA	chelate chains	1	1e		0	NA	1/3	2	3.19, 3.22		0.065	RT	1	1
VOGSEP	A	61	Pcab	2	0	0	6; 6	NA	partially linked dimers	1	1g	T(a) [1]	1	1	1/2; 1/2	1.5	2.74, 2.78, 3.04		0.032	RT	1	1