SUPPLEMENTARY MATERIAL for

Crystal Packing in vicinal Diols C_nH_m(OH)_2

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Synopsis: A survey of the O-H···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···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:

<table>
<thead>
<tr>
<th>REFCODE</th>
<th>SpcGrp Name</th>
<th>SpcGrp #</th>
<th>Type</th>
<th>Z'</th>
<th>SS</th>
<th>Rng Siz; mult bnds, fused rngs</th>
<th>Spc</th>
<th>Grp #</th>
<th>Designation</th>
<th>Link Sym</th>
<th>Inter OH…O Bonding</th>
<th>avg Inter O…O Distances</th>
<th>Other Remarks</th>
<th>R</th>
<th>T</th>
<th>Hxyz ref?</th>
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<td>NA</td>
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<td>0</td>
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<td>1i</td>
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<td>γ (°)</td>
<td>V (Å³)</td>
<td>D (g/cm³)</td>
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<td>PINCOL 4 15 C2/c 2 0 0 NA NA simple chain 2 2x ?? [-1] 1 -1 2/2, 2/2, 2/2 2 2.82 - 2.86 (4) possible intra H bond 0.063 RT 0 NA</td>
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<td>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 possible intra H bond 0.045 RT 1 1</td>
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<td>WOVDOA 4 14 P21/c 2 1 0 6:2 trans dimer ribbons 1 1a T(c) [1 - 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</td>
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