

Molecular Structures of Ribonucleotide Reductase Inhibitors: 3,4-Dihydroxybenzohydroxamic Acid Monohydrate and Pivalohydroxamic Acid

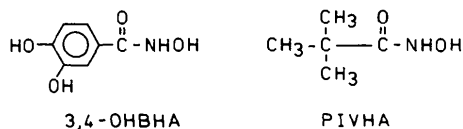
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Abstract. $C_7H_7NO_4 \cdot H_2O$ (3,4-OHBHA): $M_r = 187.16$, orthorhombic, $P2_12_12_1$, $a = 18.070$ (5), $b = 4.0228$ (9), $c = 10.695$ (3) Å, $V = 777.4$ (4) Å³ at 105 K, $Z = 4$, $D_m(293\text{ K}) = 1.56$, $D_x = 1.598$ (1) Mg m⁻³, $\lambda(\text{Mo K}\alpha) = 0.71073$ Å, $\mu = 0.129$ mm⁻¹, $F(000) = 392$. $C_5H_{11}NO_2$ (PIVHA): $M_r = 117.15$, orthorhombic, $Pbcn$, $a = 11.230$ (6), $b = 12.000$ (4), $c = 9.964$ (7) Å, $V = 1342.7$ (5) Å³ at 105 K, $Z = 8$, $D_m(293\text{ K}) = 1.095$, $D_x = 1.158$ (1) Mg m⁻³, $\lambda(\text{Mo K}\alpha) = 0.71073$ Å, $\mu = 0.083$ mm⁻¹, $F(000) = 512$. Final $R = 0.032$ for 2007 unique observed reflections for 3,4-OHBHA and 0.041 for 1161 unique observed reflections for PIVHA. In both compounds the conformation of HO–NH–C=O is synperiplanar (sp). The molecule of 3,4-OHBHA is roughly planar, and the crystals are stabilized by a system of H bonds including the water molecules. The voluminous molecules of PIVHA are more loosely packed in the crystals as rows of H-bonded tetramers. The conformations of PIVHA and similar compounds are compared with the conformations of pivalamide as found by molecular-mechanics calculations.

Introduction. A series of compounds (analogues of hydroxyurea, $H_2NCONHOH$) has been tested for inhibitory action on the enzyme ribonucleotide reductase and the molecular mechanism of action of the compounds has been established (Kjøller Larsen, Sjöberg & Thelander, 1982). The dihydroxybenzene derivative 3,4-OHBHA was one of the most potent



compounds, far more potent (on mammalian enzyme) than hydroxyurea, whereas the aliphatic hydroxamic acid PIVHA (2,2-dimethylpropanohydroxamic acid) was essentially inactive. Both of the compounds were found to possess the one-electron oxidizability necessary for activity (Larsen, 1980; Elford, van't Riet, Wampler, Lin & Elford, 1981), and the lack of activity

of PIVHA is probably due to the bulky *tert*-butyl group, which prevents the hydroxamic acid group from reacting with the free-radical group present in the subunit B2 of the enzyme (Kjøller Larsen *et al.*, 1982). Structure determinations of the compounds have been performed in order to obtain precise information on the geometry of a very active as well as an inactive compound. X-ray structure determination of the subunit B2 of ribonucleotide reductase from *E. coli* has been initiated (Joelson, Uhlin, Eklund, Sjöberg, Hahne & Karlsson, 1984).

Experimental. 3,4-OHBHA and PIVHA prepared as previously described (Kjøller Larsen *et al.*, 1982). Crystals of 3,4-OHBHA suitable for X-ray work obtained by slow evaporation from a solution in a mixture of aqueous ethanol and ethyl acetate, of PIVHA from a solution in a mixture of ethyl acetate and chloroform. D_m measured by flotation. Crystals of 3,4-OHBHA $0.10 \times 0.35 \times 0.35$ mm and of PIVHA $0.12 \times 0.20 \times 0.42$ mm chosen for data collection on Enraf–Nonius CAD-4 diffractometer equipped with graphite monochromator and Nonius low-temperature device. Temperature kept at about 105 K and estimated to be correct within ± 5 K. Temperature kept constant within 0.5 K. Cell dimensions determined by least-squares fit of angular settings of 18 reflections. Intensities measured using ω - 2θ scan method for θ values up to 35° for 3,4-OHBHA ($0 \leq h \leq 30$, $-6 \leq k \leq 6$, $0 \leq l \leq 17$) and 30° for PIVHA ($0 \leq h \leq 15$, $-16 \leq k \leq 16$, $0 \leq l \leq 14$). Three standard reflections measured every 75 reflections showed no significant variations. Intensities of 4807 reflections measured for 3,4-OHBHA, 2447 of which unique ($R_{int} = 0.02$), 2007 reflections with $I_o > 2.0\sigma(I_o)$ considered observed. Intensities of 3700 reflections measured for PIVHA, 1950 of which unique ($R_{int} = 0.03$), 1161 reflections with $I \geq 2.0\sigma(I_o)$ considered observed. No absorption corrections made. Structures solved by direct methods using MULTAN80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Full-matrix least-squares refinements of positional parameters of all atoms, with anisotropic temperature factors for non-H atoms and isotropic temperature factors for H atoms. All H atoms located in difference Fourier maps.

Table 1. Fractional atomic coordinates (x and $z \times 10^5$, $y \times 10^4$ for 3,4-OHBHA; $\times 10^4$ for PIVHA) and equivalent isotropic thermal parameters (\AA^2)
$$B_{eq} = \frac{1}{3} \sum_i \sum_j B_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	B_{eq}
3,4-OHBHA				
C(1)	20765 (5)	2207 (3)	76261 (9)	0.82
C(2)	25724 (5)	1228 (3)	66902 (9)	0.88
C(3)	33165 (5)	1987 (3)	68002 (9)	0.86
O(3)	37939 (4)	1037 (3)	58739 (8)	1.34
C(4)	35737 (5)	3695 (3)	78561 (9)	0.84
O(4)	43202 (4)	4225 (2)	79146 (8)	1.03
C(5)	30834 (6)	4702 (3)	87796 (9)	0.96
C(6)	23339 (6)	3993 (3)	86607 (9)	0.91
C(7)	12882 (5)	1209 (3)	74717 (9)	0.86
O(7)	10473 (4)	-14 (2)	64881 (8)	1.17
N(8)	8510 (5)	1781 (3)	84705 (9)	0.97
O(9)	1386 (4)	429 (2)	84438 (8)	1.08
O(10)	51747 (5)	3872 (2)	56237 (8)	1.03
PIVHA				
C(1)	6695 (1)	-195 (1)	2093 (2)	1.03
O(1)	6342 (1)	84 (1)	3238 (1)	1.29
N(1)	6352 (1)	353 (1)	1009 (1)	1.05
O(2)	5575 (1)	1253 (1)	1123 (1)	1.19
C(2)	7496 (1)	-1211 (1)	1892 (1)	1.21
C(3)	8340 (2)	-1310 (2)	3085 (2)	2.05
C(4)	8229 (2)	-1143 (2)	600 (2)	1.95
C(5)	6671 (2)	-2225 (1)	1857 (2)	2.35

Quantity minimized $\sum w(|F_o| - k|F_c|)^2$, where $w = 1.0/[\sigma^2(F_o) + 0.0005(F_o)^2]$ for 3,4-OHBHA and $w = 1.0/[\sigma^2(F_o) + 0.001(F_o)^2]$ for PIVHA. Av. and max. Δ/σ in final refinement cycles 0.07 and 0.4, respectively, for both structures. Final $R = 0.032$, $wR = 0.040$, $S = 1.3$, $\Delta\rho$ fluctuations $\pm 0.3 \text{ e \AA}^{-3}$ (on benzene ring occasionally 0.5 e \AA^{-3}) for 3,4-OHBHA. For PIVHA final $R = 0.041$, $wR = 0.053$, $S = 1.2$, $\Delta\rho$ fluctuations $\pm 0.3 \text{ e \AA}^{-3}$. Scattering factors for H those of Stewart, Davidson & Simpson (1965), for O, N and C those of Cromer & Mann (1968). Programs used in refinement from XRAY76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976).

Discussion. The final atomic parameters of 3,4-OHBHA and PIVHA are listed in Table 1.* Bond lengths and angles are given in Table 2. The atom-numbering schemes, molecular conformations and packing arrangements are shown in Figs. 1 and 2.

3,4-OHBHA. The molecule is not quite planar, the average deviation from the least-squares plane through all C, N and O atoms being 0.09 (3) \AA , but still rather flat, *i.e.* with a thickness of less than 3.5 \AA , as found for similar potent inhibitors of ribonucleotide reductase (*cf.*

Kj\o ller Larsen *et al.*, 1982). The deviations from planarity are predominantly due to twists in the hydroxamic acid group, as reflected in the torsion angles given in Table 2. The conformation of HO-NH-C=O is *sp* (synperiplanar) as in salicylohydroxamic acid (Larsen, 1978), where the torsion angle O(7)-C(7)-N(8)-O(9) is 6.3 (5) $^\circ$. This conformation is often found in crystal structures of hydroxamic acids. The conformation of the hydroxamic group is probably determined by the possibilities for hydrogen bonding. Bond lengths and angles of 3,4-OHBHA seem to be quite normal and similar to those of *e.g.* salicylohydroxamic acid. A comparison of the molecular geometry and dimensions of hydroxamic acids as found in crystal structures will be given in another report.

Table 2. Bond lengths (\AA), bond angles ($^\circ$), selected torsion angles ($^\circ$) and hydrogen-bond geometry (\AA , $^\circ$)

3,4-OHBHA				
C(1)-C(2)	1.400 (1)	C(5)-C(6)	1.390 (2)	
C(2)-C(3)	1.384 (1)	C(6)-C(1)	1.399 (2)	
C(3)-O(3)	1.368 (1)	C(1)-C(7)	1.489 (1)	
C(3)-C(4)	1.401 (1)	C(7)-O(7)	1.240 (1)	
C(4)-O(4)	1.367 (1)	C(7)-N(8)	1.348 (1)	
C(4)-C(5)	1.387 (1)	N(8)-O(9)	1.398 (1)	
C(1)-C(2)-C(3)	119.94 (9)	C(5)-C(6)-C(1)	120.12 (9)	
C(2)-C(3)-C(4)	119.93 (9)	C(6)-C(1)-C(2)	119.82 (9)	
C(2)-C(3)-O(3)	119.31 (9)	C(6)-C(1)-C(7)	122.97 (8)	
O(3)-C(3)-C(4)	120.76 (8)	C(2)-C(1)-C(7)	117.20 (9)	
C(3)-C(4)-C(5)	120.34 (9)	C(1)-C(7)-N(8)	115.25 (9)	
C(3)-C(4)-O(4)	116.14 (8)	C(1)-C(7)-O(7)	122.46 (9)	
O(4)-C(4)-C(5)	123.51 (9)	O(7)-C(7)-N(8)	122.28 (9)	
C(4)-C(5)-C(6)	119.82 (9)	C(7)-N(8)-O(9)	117.19 (9)	
C(6)-C(1)-C(7)-N(8)	-7.9 (2)	O(7)-C(7)-N(8)-O(9)	10.7 (2)	
Hydrogen bonding				
<i>A</i> -H... <i>B</i>	<i>A</i> ... <i>B</i>	H... <i>B</i>	\angle A-H... <i>B</i>	Symmetry code for <i>B</i>
O(3)-H(3)...O(10)	2.756 (1)	1.93 (3)	168 (2)	x, y, z
O(4)-H(4)...O(10)	2.602 (1)	1.81 (2)	164 (2)	$-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$
N(8)-H(8)...O(3)	2.882 (2)	2.10 (2)	153 (2)	$-x+\frac{1}{2}, -y, z+\frac{1}{2}$
O(9)-H(9)...O(7)	2.821 (1)	2.10 (2)	148 (2)	$-x, y+\frac{1}{2}, -z+\frac{1}{2}$
O(9)-H(9)...O(9)	2.894 (1)	2.25 (2)	136 (2)	$-x, y+\frac{1}{2}, -z+\frac{1}{2}$
O(10)-H(10)...O(7)	2.793 (1)	1.98 (2)	169 (2)	$x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$
O(10)-H(10)...O(4)	2.813 (1)	2.02 (2)	165 (2)	$-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$
Short distances				
O(10)...O(9)	2.958 (1)			$-x+\frac{1}{2}, -y, z-\frac{1}{2}$
O(10)...O(4)	2.900 (1)			x, y, z
PIVHA				
N(1)-O(2)	1.393 (2)	C(2)-C(3)	1.525 (3)	
N(1)-C(1)	1.322 (2)	C(2)-C(4)	1.530 (3)	
C(1)-O(1)	1.253 (2)	C(2)-C(5)	1.530 (2)	
C(1)-C(2)	1.528 (2)			
C(1)-N(1)-O(2)	120.1 (1)	C(1)-C(2)-C(4)	112.6 (1)	
N(1)-C(1)-O(1)	121.2 (1)	C(1)-C(2)-C(5)	106.3 (1)	
N(1)-C(1)-C(2)	117.5 (1)	C(3)-C(2)-C(4)	109.0 (1)	
O(1)-C(1)-C(2)	121.2 (1)	C(3)-C(2)-C(5)	109.4 (1)	
C(1)-C(2)-C(3)	109.0 (1)	C(4)-C(2)-C(5)	110.4 (1)	
O(2)-N(1)-C(1)-O(1)	-0.6 (2)	O(1)-C(1)-C(2)-C(4)	-156.2 (1)	
O(1)-C(1)-C(2)-C(3)	-35.1 (2)	O(1)-C(1)-C(2)-C(5)	82.7 (2)	
Hydrogen bonding				
<i>A</i> -H... <i>B</i>	<i>A</i> ... <i>B</i>	H... <i>B</i>	\angle A-H... <i>B</i>	Symmetry code for <i>B</i>
O(2)-H(2)...O(1)	2.647 (2)	1.74 (2)	171 (2)	$-x+1, y, -z+\frac{1}{2}$
N(1)-H(1)...O(1)	2.810 (3)	2.01 (3)	164 (2)	$x, -y, z-\frac{1}{2}$

* Lists of structure factors, anisotropic thermal parameters, H-atom positions, bonds and angles involving H atoms, and deviations from least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43599 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The crystal structure of 3,4-OHBHA is stabilized by hydrogen bonds and van der Waals interactions, *cf.* Table 2 and Fig. 1. The water molecule, which is surrounded by five O atoms in a hydrophilic channel in the structure, is donor for two and acceptor for two hydrogen bonds, thereby connecting four different hydroxamic acid molecules. In addition, the hydroxamic acid molecules are connected by a three-centred (bifurcated) H bond, O(9)—H(9)···O(7), O(9)—H(9)···O(9).

PIVHA. The conformation of HO—NH—C=O is *sp* as also found in a thorium complex with PIVHA as a ligand (Smith & Raymond, 1981). The hydroxamic acid moiety is nearly planar with an average deviation of 0.014 (5) Å from the least-squares plane through C(1), C(2), N(1), O(1) and O(2) [0.007 (3) Å in the Th complex]. All three C—CH₃ bonds are twisted out of the hydroxamic acid plane as reflected in the O=C—C—C torsion angles given in Table 2. This conformation of PIVHA presents the apparently most favourable steric conditions, *i.e.* least overlap of ligands. In the Th complex of PIVHA one of the C—CH₃ bonds eclipses the C=O bond, the corresponding O=C—C—C torsion angle being 0.3 (3)°. The C—H bonds of the

three CH₃ groups in PIVHA are all in nearly staggered (*sc*, synclinal) conformations (C—C—C—H torsion angles have been deposited).

A study of the geometry of 16 *N*-pivaloyl derivatives of small peptides from the Cambridge Structural Database (January 1986 release; Allen *et al.*, 1979) showed that in most of these structures one of the C—CH₃ bonds is nearly eclipsed by the C=O bond of the amide group, the O=C—C—C torsion angles being $\pm(1.1-22.7)^\circ$. In four of the structures one of the C—CH₃ bonds nearly eclipses the C—N bond with O=C—C—C torsion angles of $\pm(167.1-178.6)^\circ$, while only one of the 16 structures occupies nearly the same conformation as that observed in PIVHA, *i.e.* with an O=C—C—C torsion angle of 32.3 (3)°.

Calculation of the potential-energy variation with the O=C—C—C torsion angle in pivalamide using the empirical force-field program MM2 (Burkert & Allinger, 1982) and the amide parameters of Karlsson, Lijefors & Sandström (1977) showed global minima (19.97 kJ mol⁻¹) when a C—CH₃ bond eclipses the C=O bond and maxima when a C—CH₃ bond eclipses the C—N bond (28.88 kJ mol⁻¹). Most of the structures investigated, but not PIVHA, thus crystallize close to the energetically most favourable conformation of the *tert*-butyl moiety. A similar tendency of steric interaction between one of the C—C bonds of a *tert*-butyl moiety and a C=N or a C=C bond has been observed by others, *cf.* Huige, Spek & de Boer (1985).

The diameter of the *tert*-butyl group is about 6 Å (5.92 Å calculated as the sum of the maximum deviations of H atoms from the hydroxamic acid plane plus 2×1.1 Å, van der Waals radius of H), and thus the thickness of the molecule is far beyond that allowed (about 3.5 Å) for potent inhibitors of ribonucleotide reductase of the type under study (Kjøller Larsen *et al.*, 1982).

Also bond lengths and angles of PIVHA have been compared with those of the 16 above-mentioned *N*-pivaloyl peptides, which all have e.s.d.'s for C—C bonds less than 0.01 Å, and are without disorder of the *tert*-butyl group (eight structures were discarded). The carbonyl bond in PIVHA is longer and the C—N bond shorter than in most of the pivaloyl peptides, in which the mean value of these bonds is 1.230 (2) and 1.347 (3) Å, respectively, indicating more π -electron delocalization in PIVHA and in the Th complex of PIVHA, where the lengths of these bonds were 1.262 (5) and 1.316 (5) Å, respectively. In most of the *N*-pivaloyl peptides, the C—C bond attached to the carbonyl C atom is longer [mean 1.535 (3) Å] than the other three C—C bonds [mean 1.519 (5) Å], whereas these bonds are of essentially equal length in PIVHA. The C—C angles of PIVHA are less distorted (range 109.0–112.6°) than in the structures with eclipsed bonds (range 99.8–115.2°), probably due to less steric hindrance, *cf.* Huige *et al.* (1985).

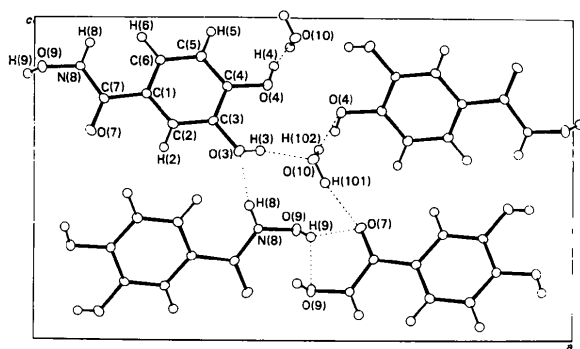


Fig. 1. The structure of 3,4-OHBHA viewed along the *b* axis, and drawn by ORTEP (Johnson, 1970).

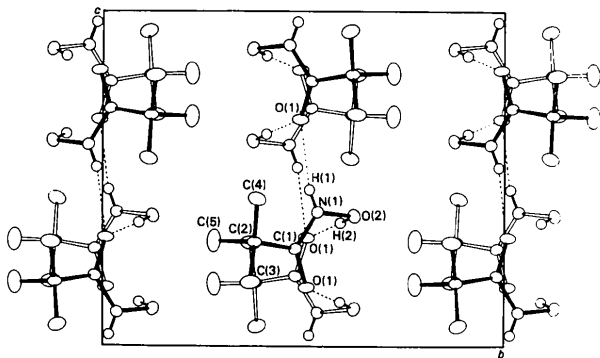


Fig. 2. The structure of PIVHA viewed along the *a* axis, and drawn by ORTEP (Johnson, 1970).

The molecules of PIVHA are packed in the crystal as rows of hydrogen-bonded tetramers. The dimensions of the hydrogen bonds are given in Table 2 and illustrated in Fig. 2, in which the H atoms of the *tert*-butyl groups are omitted for clarity.

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Bis(η^5 -cyclopentadienyl)bis(dicarbonylcobaltio)tritelluridimolybdenum

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Abstract. $[(\eta^5\text{-C}_5\text{H}_5)_2\text{Mo}_2(\mu_4\text{-Te})(\mu_3\text{-Te})_2\text{Co}_2(\text{CO})_4]$, $\text{C}_{14}\text{H}_{10}\text{Co}_2\text{Mo}_2\text{O}_4\text{Te}_3$, $M_r = 934.8$, triclinic, $P\bar{1}$, $a = 7.744$ (3), $b = 10.269$ (5), $c = 13.373$ (5) Å, $\alpha = 86.07$ (4), $\beta = 96.69$ (3), $\gamma = 108.35$ (3)°, $V = 1002.0$ (7) Å³, $Z = 2$, $D_x = 3.098$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71073$ Å, $\mu = 72.7$ cm⁻¹, $F(000) = 840$, 295 K, $R = 4.03\%$ for 2688 reflections with $F_o \geq 3\sigma(F_o)$ and 181 parameters. The compound is structurally similar to its sulfur analogue. The two cyclopentadienyl rings are nearly parallel and perpendicular to the Mo-Mo vector, 2.754 (1) Å. Nearly parallel to the cyclopentadienyl rings is a plane bisecting the Mo-Mo

vector containing the pentagonally arranged units, $\mu_3\text{-Te}$, $\mu_4\text{-Co}(\text{CO})_2$, $\mu_4\text{-Te}$, $\mu_4\text{-Co}(\text{CO})_2$, $\mu_3\text{-Te}$; there is no $(\mu_3\text{-Te})-(\mu_3\text{-Te})$ ring closure [Te...Te 3.605 (1) Å].

Experimental. Black brick-shaped crystals (0.17 × 0.22 × 0.26 mm) obtained from the reaction of $\text{Co}_4\text{Te}_2(\text{CO})_{11}$ and $(\eta^5\text{-C}_5\text{H}_5)_2\text{Mo}_2(\text{CO})_6$ (Bogan, 1986). Nicolet *R3m/μ*, ω scans; lattice parameters from 25 reflections, $21 \leq 2\theta \leq 28^\circ$, least-squares fit; empirical ellipsoidal absorption correction, seven reflections, 10° increments, $T_{\max}/T_{\min} = 0.502/0.252$; 2θ max. = 48° ($h = \pm 9$, $k = \pm 12$, $l = +16$); standard reflections $\bar{4}15$,

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