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2-{[Tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one and its 6-hydroxy and 6-methoxy derivatives

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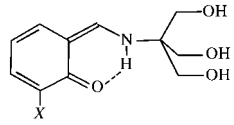
The title compounds, 2-{[tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one, $C_{11}H_{15}NO_4$, (I), 6-hydroxy-2-{[tris(hydroxymethyl)methyl]aminomethylene}-cyclohexa-3,5-dien-1(2*H*)-one, $C_{11}H_{15}NO_5$, (II), and 6-methoxy-2-{[tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one, $C_{12}H_{17}NO_5$, (III), adopt the keto–amine tautomeric form, with the formal hydroxy H atom located on the N atom, and the NH group and oxo O atom display a strong intramolecular N—H···O hydrogen bond. The N—H···O hydrogen-bonded rings are almost planar and coupled with the cyclohexadiene rings. The carbonyl O atoms accept two other H atoms from the alcohol groups of adjacent molecules in (I), and one from the alcohol and one from the phenol group in (II), but from only one alcohol H atom in (III).

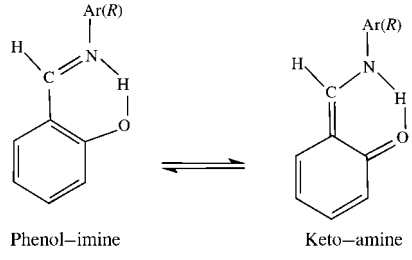
Comment

There is considerable interest in Schiff base ligands and their complexes with regard to their striking antitumour activities (Zhou *et al.*, 2000). Among them, *o*-hydroxy Schiff base ligands and their complexes derived from the reaction of *o*-hydroxyaldehydes with aniline have been extensively studied (Steward & Lingafelter, 1959; Calligaris *et al.*, 1972; Maslen & Waters, 1975) and a number of these compounds have been used as models for biological systems (Costamagna *et al.*, 1992, 1998). *o*-Hydroxy Schiff bases exist as enol (Yıldız *et al.*, 1998; Elmalı *et al.*, 1998, 1999; Elmalı & Elerman, 1998; Dey *et al.*, 2001; Ünver, Yıldız *et al.*, 2002; Yang & Vittal, 2003) or keto (Ünver, Kabak *et al.*, 2002; Hökelek *et al.*, 2000), or as enol/keto mixtures (Nazır *et al.*, 2000; Szady-Chelmienicecka *et al.*, 2001; Ogawa & Harada, 2003) as a result of H-atom transfer from the hydroxy O atom to the N atom. Such H-atom tautomerism plays an important role in many fields of chemistry and especially biochemistry (Zollinger, 1991; Hem *et al.*, 2002). Molecules giving tautomers by intramolecular H-atom transfer are often used as laser dyes, in high-energy radiation detectors, in molecular memory storage devices, as fluorescent probes and as polymer protectors (Sytnik & Del Valle, 1995; Nagaoka *et al.*, 1983). Many *o*-hydroxyarylidene anilines, being relatively simple in structure and exhibiting intramolecular H-atom transfer, have, therefore, attracted considerable attention from both experimental (Kownacki *et al.*, 1994; Grabowska *et al.*, 1994; Guha *et al.*, 2000; Ogawa *et al.*, 2001) and theoretical (Zgierski & Grabowska, 2000) points of view. *N*-Substituted *o*-hydroxyimines have been reported to display thermo- and photochromism in the solid state by H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). In the course of our ongoing studies of the synthesis and structural characterization of polyhydroxyazomethine derivatives, the title compounds, *viz.* (I), (II) and (III), have been synthesized and we report their crystal structures here.



(I) X = H
(II) X = OH
(III) X = OCH_3

As shown below, *o*-hydroxyarylidene Schiff bases display two possible tautomeric forms, namely, phenol–imine and keto–amine. In the solid state, the keto–amine tautomer has been found in naphthaldimine (Hökelek *et al.*, 2000; Ünver, Kabak *et al.*, 2002), while the phenol–imine tautomer is found in salicylaldimine Schiff bases (Kaitner & Pavlović, 1996; Yıldız *et al.*, 1998; Elmalı *et al.*, 1998, 1999; Elmalı & Elerman, 1998; Dey *et al.*, 2001; Yang & Vittal, 2003; Karadayı *et al.*, 2003). Compounds (I), (II) and (III) are polyhydroxysalicylaldimines and the present X-ray investigation indicates that the keto–amine tautomer is favoured over the phenol–imine tautomer. The crystal structure of (I) has been reported several times, most recently by Cungen *et al.* (2000) at room temperature.



Phenol–imine Keto–amine

Fig. 1 shows the hydrogen-bonded structure of (I), determined at 208 K, and the atom-numbering scheme. Selected bond distances and angles are listed in Table 1. Compound (I) has strong intramolecular N—H···O [N···O = 2.6181 (14) Å] and intermolecular O—H···O [mean = O···O 2.700 Å]

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hydrogen bonds. Such strong intramolecular N···O hydrogen bonds are a common feature of *o*-hydroxysalicylidene systems (Nazır *et al.*, 2000; Yıldız *et al.*, 1998). The sum of the van der Waals radii of oxygen and nitrogen is 3.07 Å (Bondi, 1964), and the intramolecular hydrogen bond in (I) is shorter than this. Apart from the intramolecular hydrogen bond, (I) displays strong intermolecular O···O hydrogen bonds (Table 2). It has been reported (Pizzala *et al.*, 2000) that these hydrogen bonds are indeed characterized by relatively short O···O distances (shorter than the sum of the van der Waals radii of two O atoms of 3.04 Å).

The salicylidene ring bond lengths in (I) follow the alternating sequence C1—C2 > C2—C3 > C3—C4 < C4—C5 > C5—C6 < C6—C1. Compound (I) exists primarily as the keto–amine tautomer, as indicated by the C2—O1, C1—C7, C7—N and C1—C2 bond lengths (Table 1). These bonds are 1.356 (3), 1.448 (3), 1.270 (3) and 1.288 (4) Å, respectively, in the phenol–imine tautomer of 1,8-bis(*N*-2-oxyphenylsalicylidene)-3,6-dioxaoctane (Yıldız *et al.*, 1998), and 1.286 (3), 1.441 (3), 1.297 (3) and 1.436 (3) Å, respectively, in the keto–amine tautomer of 4-[(3-chlorophenyl)diazenyl]-2-{[tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one (Odabaşoğlu *et al.*, 2003). Our investigation shows

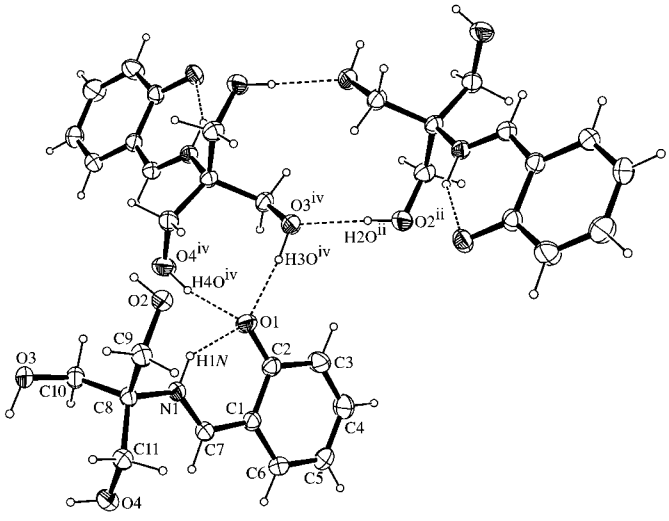

Figure 1
A view of the molecule of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids [symmetry codes: (ii) $1-x$, $y+\frac{1}{2}$, $\frac{3}{2}-z$; (iv) x, $\frac{1}{2}-y$, $z+\frac{1}{2}$].

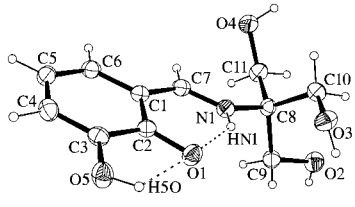

Figure 2
A view of the molecule of (II), with the atom-numbering scheme and 50% probability displacement ellipsoids.

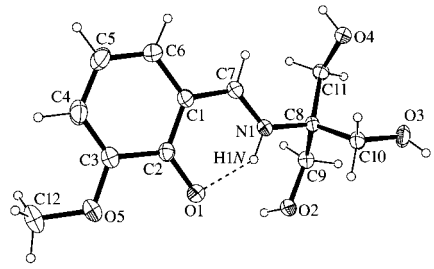

Figure 3
A view of the molecule of (III), with the atom-numbering scheme and 50% probability displacement ellipsoids.

that there is an elongation of C7—N1 compared with the normal value for a C=N double bond (Yıldız *et al.*, 1998), and of C1—C2, C2—C3, C4—C5 and C6—C1 compared with the normal values for a salicylidene ring (Elmalı & Elerman, 1998). Furthermore, the formal hydroxy H atom is located on atom N1, thus confirming a preference for the keto–amine tautomer (the quinoid form) in the solid state. Formation of the quinoid form results in electron-localization distortion and so the C3—C4 and C5—C6 bonds are shortened in comparison with their normal values in a salicylidene ring. The N—H···O hydrogen-bonded ring in (I) is almost planar and coupled with the cyclohexadiene ring, with an N1—C7—C1—C2 torsion angle of 0.3 (2)°.

Molecular views of (II) and (III), and their numbering schemes, are shown in Figs. 2 and 3, respectively, and selected bond distances and angles are listed in Tables 3 and 5, respectively. The structures of (II) and (III) are similar to that of (I), with small differences for some bond lengths due to the OH and CH_3O groups attached to the cyclohexadiene ring (Tables 3 and 5). The O1—C2 bond lengths of 1.2968 (17) Å in (II) and 1.2892 (18) Å in (III) are somewhat shorter than the value of 1.3025 (16) Å in (I). Compound (II) has two strong intramolecular hydrogen bonds [N···O = 2.5851 (16) Å and O···O = 2.7000 (15) Å; Table 4].

Compounds (II) and (III), like compound (I), have strong intermolecular O···O hydrogen bonds (Tables 4 and 6). Atom O1 in (I) accepts two other H atoms from the alcohol groups of adjacent molecules, *viz*. O1···O3^{iv} and O1···O4^{iv} [symmetry code: (iv) $x, \frac{1}{2}-y, z+\frac{1}{2}$]. In (II), atom O1 accepts one H atom from an alcohol group, O1···O3^{ii} [symmetry code: (ii) $2-x, -y, -z$], and one from the phenol group, O1···O5, but in (III), atom O1 accepts only one alcohol H atom, O1···O4^{iii} [symmetry code: (iii) $\frac{1}{2}-x, \frac{1}{2}+y, z$].

The N—H···O hydrogen-bonded rings in (II) and (III) are almost planar-coupled with the cyclohexadiene rings, with N1—C7—C1—C2 torsion angles of 3.63 (1) and 0.8 (2)°, respectively (Tables 3 and 5).

Experimental

For compound (I), a solution of tris(hydroxymethyl)aminomethane (2.42 g, 20 mmol) in butan-1-ol (75 ml) was added to a solution of salicylaldehyde (2.44 g, 20 mmol) in butan-1-ol (75 ml). The mixture

was stirred under reflux and the water produced in the reaction was distilled out. The resulting yellow precipitate was filtered off and recrystallized from ethyl alcohol by slow evaporation, and well shaped crystals of (I) were obtained. Compounds (II) and (III) were synthesized and crystallized using exactly the same procedure as for (I), using 2,3-dihydroxybenzaldehyde in the case of (II) and 2-hydroxy-3-methoxybenzaldehyde for (III), but recrystallization was carried out from acetonitrile for (III) instead of ethyl alcohol. Yield: 95%, m.p. 422–423 K for (I), 90%, m.p. 415–417 K for (II), and 95%, m.p. 454–455 K for (III).

Compound (I)

Crystal data

$C_{11}H_{15}NO_4$
M_r = 225.24
Monoclinic, $P2_1/c$
a = 10.4437 (9) Å
b = 8.7029 (7) Å
c = 12.6147 (11) Å
β = 101.801 (2)°
V = 1122.32 (16) Å^3
Z = 4
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 986 reflections
θ = 2.8–26.6°
μ = 0.10 mm^{-1}
T = 208 (2) K
Prism, colourless
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
12 824 measured reflections
2701 independent reflections
2226 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.0°
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.111
S = 1.10
2701 reflections
206 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.3161P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

O1—C2	1.3025 (16)	C1—C7	1.4290 (18)
N1—C7	1.2952 (18)	C2—C3	1.4158 (19)
N1—C8	1.4741 (16)	C3—C4	1.369 (2)
C1—C6	1.4113 (19)	C4—C5	1.401 (2)
C1—C2	1.4276 (18)	C5—C6	1.368 (2)
C6—C1—C7	118.64 (12)	O1—C2—C1	121.22 (12)
C2—C1—C7	121.22 (12)	N1—C7—C1	123.15 (12)
O1—C2—C3	121.89 (12)		
C6—C1—C2—O1	178.12 (12)	C2—C1—C7—N1	0.3 (2)

Table 2
Hydrogen-bonding geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1	0.915 (17)	1.865 (17)	2.6181 (14)	138.1 (15)
O2—H2O···O3^{i}	0.84 (2)	1.89 (2)	2.7314 (15)	177 (2)
O3—H3O···O1^{ii}	0.91 (2)	1.74 (2)	2.6426 (14)	172 (2)
O4—H4O···O1^{ii}	0.86 (2)	1.90 (2)	2.7254 (15)	161 (2)

Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$.

Compound (II)

Crystal data

$C_{11}H_{15}NO_5$
M_r = 241.24
Monoclinic, $P2_1/c$
a = 9.6807 (17) Å
b = 11.793 (2) Å
c = 9.8373 (18) Å
β = 106.110 (3)°
V = 1078.9 (3) Å^3
Z = 4
D_x = 1.485 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 560 reflections
θ = 2.5–29.3°
μ = 0.12 mm^{-1}
T = 223 (2) K
Prism, colourless
0.25 × 0.25 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
T_{min} = 0.971, T_{max} = 0.988
6019 measured reflections
2258 independent reflections
1972 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.6°
$h = -12 \rightarrow 10$
$k = -14 \rightarrow 13$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.103
S = 1.09
2258 reflections
214 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.326P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 3
Selected geometric parameters (Å, °) for (II).

O1—C2	1.2968 (17)	C1—C7	1.428 (2)
O5—C3	1.3737 (18)	C2—C3	1.4277 (19)
N1—C7	1.2943 (19)	C3—C4	1.366 (2)
N1—C8	1.4730 (17)	C4—C5	1.410 (2)
C1—C6	1.415 (2)	C5—C6	1.370 (2)
C1—C2	1.4258 (19)		
C6—C1—C7	120.08 (13)	O1—C2—C3	119.21 (13)
C2—C1—C7	119.50 (13)	N1—C7—C1	121.74 (13)
O1—C2—C1	124.00 (13)		
C7—C1—C2—O1	0.9 (2)	C2—C1—C7—N1	−3.5 (2)

Table 4
Hydrogen-bonding geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1	0.89 (2)	1.84 (2)	2.5851 (16)	140.0 (18)
O2—H2O···O3^{i}	0.84 (2)	1.91 (3)	2.7465 (16)	171 (2)
O3—H3O···O1^{ii}	0.88 (2)	1.83 (2)	2.6910 (15)	167 (2)
O4—H4O···O5^{iii}	0.84 (2)	1.95 (3)	2.7652 (17)	167 (2)
O5—H5O···O2^{ii}	0.87 (3)	2.02 (3)	2.8193 (17)	153 (2)
O5—H5O···O1	0.87 (3)	2.27 (2)	2.7000 (15)	110.3 (19)

Symmetry codes: (i) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$; (ii) $2-x, 1-y, 1-z$; (iii) $x, y, z-1$.

Compound (III)

Crystal data

$C_{12}H_{17}NO_5$
M_r = 255.27
Orthorhombic, *Pbca*
a = 10.6464 (7) Å
b = 10.7749 (7) Å
c = 20.8540 (13) Å
V = 2392.2 (3) Å^3
Z = 8
D_x = 1.418 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 720 reflections
θ = 2.2–27.6°
μ = 0.11 mm^{-1}
T = 213 (2) K
Needle, colourless
0.30 × 0.30 × 0.03 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
T_{min} = 0.968, T_{max} = 0.997
12 603 measured reflections
2744 independent reflections
2241 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.5°
$h = -6 \rightarrow 13$
$k = -13 \rightarrow 14$
$l = -26 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.105
S = 1.07
2744 reflections
231 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.9405P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 5
Selected geometric parameters (Å, °) for (III).

O1—C2	1.2892 (18)	C1—C2	1.431 (2)
O5—C3	1.3684 (19)	C2—C3	1.440 (2)
N1—C7	1.2962 (19)	C3—C4	1.364 (2)
N1—C8	1.4685 (18)	C4—C5	1.405 (3)
C1—C7	1.417 (2)	C5—C6	1.360 (3)
C1—C6	1.421 (2)		
C7—C1—C6	118.89 (14)	O1—C2—C3	121.20 (13)
C7—C1—C2	120.37 (13)	N1—C7—C1	122.73 (14)
O1—C2—C1	122.85 (13)		
C7—C1—C2—O1	7.3 (2)	C2—C1—C7—N1	−0.8 (2)

Table 6
Hydrogen-bonding geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1	0.91 (2)	1.85 (2)	2.6125 (16)	139.7 (18)
O2—H2O···O4^{i}	0.84 (2)	1.92 (2)	2.7549 (16)	170 (2)
O3—H3O···O2^{ii}	0.83 (2)	1.91 (2)	2.7280 (17)	171 (2)
O4—H4O···O1^{iii}	0.85 (2)	1.91 (2)	2.7359 (16)	163 (2)
O4—H4O···O5^{iii}	0.85 (2)	2.47 (2)	3.0346 (16)	124.1 (17)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$; (ii) $2 - x, -y, 1 - z$; (iii) $\frac{3}{2} - x, \frac{1}{2} + y, z$.

All H atoms were refined freely. For (I), C—H = 0.938 (19)–1.011 (17) Å and U_{iso}(H) = 0.022 (4)–0.056 (6) Å^2, for (II), C—H = 0.974 (17)–1.007 (18) Å and U_{iso}(H) = 0.025 (4)–0.057 (7) Å^2, and for (III), C—H = 0.95 (2)–1.02 (2) Å and U_{iso}(H) = 0.021 (4)–0.047 (6) Å^2.

For all compounds, data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1432). Services for accessing these data are described at the back of the journal.

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