

In (IV), however, the C4 substituent is hydroxy and the angle spreading found in (I) and (II) has all but vanished. These differences are probably less the result of the steric properties of the O-methyl substituents in (I) and (II) than of the intramolecular H...O5 link observed in (IV). In (I), for example, the O4...O5 distance of 2.810 (3) Å is close to the usual 2.8 Å O...O contact distance, whereas the corresponding 2.56 (1) Å value in (IV) is substantially shorter.

The crystal packing is ordinary. There are no intermolecular contacts less than the sum of the appropriate van der Waals radii.

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Structures of 1*H*-Indole-3-ethylene-3'-methoxysalicylalimine (3'-Meo-salTPA) and 3-[3'-Azapentyl-3'-en-4'-(2''-hydroxyphenyl)]indole (OHAPH-TPA)

BY P. MARTIN ZARZA, P. GILL,* M. C. DÍAZ GONZÁLEZ AND M. G. MARTIN REYES

Departamento de Química Inorgánica, Universidad de La Laguna, Tenerife, Canary Islands, Spain

J. M. ARRIETA

Departamento de Química, Facultad de Ciencias, Universidad del País Vasco, Apartado 644, Bilbao, Spain

V. NASTOPOULOS AND G. GERMAIN

Unité de Chimie Physique Moléculaire et de la Cristallographie, Université de Louvain, Place Louis Pasteur 1, 1348 Louvain-la-Neuve, Belgium

AND T. DEBAERDEMAEKER

Sektion für Röntgen- und Elektronenbeugung, Universität Ulm, D-7900 Ulm, Federal Republic of Germany

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Abstract. 3'-Meo-salTPA, systematic name 2-[2-(1*H*-indol-3-yl)ethyliminomethyl]-6-methoxyphenol, C₁₈H₁₈N₂O₂, *M_r* = 294.34, triclinic, *P* $\bar{1}$, *a* = 11.932 (2), *b* = 11.590 (3), *c* = 11.401 (4) Å, α = 89.94 (2), β = 101.44 (2), γ = 101.24 (2)°, *V* = 1514 (1) Å³, *Z* = 4, *D_x* = 1.29, *D_m* = 1.30 Mg m⁻³, *F*(000) = 624, λ (Mo *K*α) = 0.71069 Å, μ = 0.92 mm⁻¹, room temperature, final *R* = 0.0505, *wR* = 0.0597 for 1809 observed reflections. OHAPH-TPA, systematic name 2-[1-[2-(1*H*-indol-3-yl)ethylimino]ethyl]phenol, C₁₈H₁₈N₂O, *M_r* = 278.36, monoclinic,

*P*2₁/*a*, *a* = 10.018 (2), *b* = 14.669 (4), *c* = 10.015 (2) Å, β = 90.54 (2)°, *V* = 1472 (1) Å³, *Z* = 4, *D_x* = 1.26, *D_m* = 1.29 Mg m⁻³, *F*(000) = 592, λ (Mo *K*α) = 0.71069 Å, μ = 0.44 mm⁻¹, final *R* = 0.0962, *wR* = 0.1174 for 1490 observed reflections. The two structures are compared and some structural features are emphasized. The C7A–C8A bond length for both compounds is shorter than a normal aromatic C–C bond. Both structures also show intramolecular and intermolecular hydrogen bonds, the first between the phenolic H and the N of the imino group and the second between the indolic N–H and the phenolic O of the other molecule.

* Author to whom correspondence should be addressed.

Introduction. Tryptamine (1*H*-indole-3-ethanamine) is able to condense aromatic carbonyl compounds as previously described (Rodríguez, Medina de la Rosa, Gili, Martín Zarza, Martín Reyes, Medina & Díaz González, 1987). In this work we have examined the crystal structures of the products obtained for the first time by condensation of tryptamine with 3-methoxysalicylaldehyde and with *ortho*-hydroxyacetophenone. The compounds obtained are respectively 3'-Meo-salTPA and OHAPH-TPA. These compounds are ligands that form complexes with transition metals (Martín Reyes, Gili, Martín Zarza, Medina Ortega & Díaz González, 1986) and the structures are compared with those of similar compounds previously described.

Experimental. 3'-Meo-salTPA was obtained as a yellow precipitate upon mixing and refluxing ethanol solutions of tryptamine and 3-methoxysalicylaldehyde. After filtering and washing with ethanol, the compound was recrystallized from ethanol. Yellow prismatic crystals, crystal *ca* 0.15 × 0.16 × 0.30 mm, cell parameters by least squares from the setting angles of 15 reflections ($10 < 2\theta < 25^\circ$); 5336 independent reflections measured, ω scan up to $2\theta = 50^\circ$. One standard reflection measured every 50 reflections showed only random deviation from its mean intensity. 1809 reflections with $I \geq 2.5\sigma(I)$ were considered observed and included in the refinement; index range $h -12, +11$; $k -13, +13$; $l 0, +13$. $\sum w(\Delta F)^2$ minimized, anisotropic thermal parameters for non-H atoms. H positions determined by difference Fourier synthesis, refined with an overall isotropic temperature factor. Final $R = 0.0505$ and $wR = 0.0597$, $w = [\sigma^2(F) + 0.009202F^2]^{-1}$; max. and min. electron densities in final difference map 0.17, -0.21 e \AA^{-3} .

OHAPH-TPA was obtained in a similar manner by mixing and refluxing equimolar ethanol solutions of tryptamine and *ortho*-hydroxyacetophenone. Yellow prismatic crystals of OHAPH-TPA were obtained by recrystallization from ethanol. Unit-cell parameters were determined by a least-squares analysis of 2θ values for 15 reflections ($10 < 2\theta < 25^\circ$) measured with the diffractometer from a crystal *ca* 0.20 × 0.15 × 0.25 mm. Intensity measurements were made for 2585 independent reflections of which 1490 were considered observed with $I \geq 2.5\sigma(I)$ and included in the refinement. Index range $h -11, +11$; $k 0, +17$; $l 0, +11$. ω scans up to $2\theta = 50^\circ$. One standard reflection measured every 50 reflections showed only random deviation from its mean intensity. $\sum w(\Delta F)^2$ minimized, anisotropic thermal parameters for non-H atoms. H positions determined by difference Fourier synthesis, refined with an overall isotropic temperature factor. Final $R = 0.0962$ and $wR = 0.1174$, $w = 2.6399 \times [\sigma^2(F) + 0.002198F^2]^{-1}$. Max. and min. electron densities in final difference map 0.46, -0.37 e \AA^{-3} . The high value of R is due to the poor quality of the single crystal.

For both compounds intensity data were measured with an automated Philips PW1100 four-circle computer-controlled diffractometer; graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$, was used. Lorentz and polarization but not absorption corrections were made. The structures were solved by direct methods (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and Fourier synthesis (Stewart, Kundell & Baldwin, 1970). Torsion angles, planes and dihedral angles were calculated by the *PARST* program (Nardelli, 1982). Scattering factors from *International Tables for X-ray Crystallography* (1974). Least-squares refinement with *SHELX76* (Sheldrick, 1976). The experimental densities were determined by pycnometry.

Discussion. Table 1 list the final atomic parameters and their estimated standard deviations, following the numbering schemes of Figs. 1 and 2.* Table 2 gives bond angles and bond lengths. Selected torsion angles for both compounds are listed in Table 3. Stereoviews of the molecule are given in Figs. 3 and 4.

Some interesting structural data can be observed in these results; for example, the lengths of the C7A–C8A bond are 1.38 (1) and 1.37 (1) Å for 3'-Meo-salTPA and OHAPH-TPA, respectively, similar in both cases to that found for the compound salTPA [1.36 (1) Å] (Rodríguez *et al.*, 1987) and are slightly shorter than the expected value for a normal aromatic C–C bond (1.395 Å). This shortening of the bond has also been observed in tryptamine hydrochloride, a radiation protector (Wakahara, Fujiwara & Tomita, 1973).

The N12A–C13A bond corresponding to the imino group of 3'-Meo-salTPA and salTPA (Rodríguez *et al.*, 1987) is 1.27 (1) Å, similar to that found for OHAPH-TPA, and indicates a double bond for the –C=N group.

The distance O20A–C19A for 3'-Meo-salTPA is 1.29 (1) Å, which is shorter than in the case of salTPA [1.34 (1) Å] and indicates double-bond character for the C–O group. The value found for this same group in the case of OHAPH-TPA is 1.31 (1) Å, which is intermediate between values in 3'-Meo-salTPA and salTPA.

The N12A–C13A–C14A bond angle for 3'-Meo-salTPA is 123.6 (6)° while this same angle is 118.5 (7)° for OHAPH-TPA. This decrease can be explained by the steric impediment caused by the methyl group.

The majority of the torsion angles for 3'-Meo-salTPA are to be found between 0 and 180° as in the

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44563 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

case of salTPA (Rodriguez *et al.*, 1987). The C7A–C10A–C11A–N12A torsion angle is 60.2 (7)°, and the C7B–C10B–C11B–N12B torsion angle is –62.6 (7)°, indicating a synclinal disposition through the C10–C11 bonds (Klyne & Prelog, 1960). The indole groups of 3'-Meo-salTPA in molecules *A* and *B* form a dihedral angle of 90.0 (1)°.

In OHAPH-TPA it is observed that the indole and phenol rings are to be found on different planes, forming a dihedral angle of approximately 70°. On the other hand, the system formed by the imino group (N12–C13), the oxygen (O21) and the phenyl group is not located on the same plane. The torsion angle for C7–C10–C11–N12 of OHAPH-TPA is 68.2 (9)°.

Table 1. Fractional atomic coordinates ($\times 10^4$) with *e.s.d.*'s in parentheses and B_{eq} values (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	B_{eq}
3'-Meo-salTPA				
C1A	1444 (6)	3697 (6)	5431 (6)	6.02
C2A	958 (6)	4423 (7)	6070 (7)	7.83
C3A	1627 (7)	5268 (6)	6932 (7)	7.18
C4A	2821 (6)	5430 (5)	7206 (5)	5.67
C5A	3331 (6)	4703 (5)	6582 (5)	4.75
C6A	2667 (5)	3846 (5)	5692 (5)	4.61
C7A	3488 (5)	3344 (4)	5225 (5)	4.60
C8A	4583 (5)	3866 (5)	5846 (5)	5.11
N9A	4486 (5)	4678 (4)	6666 (4)	5.08
C10A	3175 (5)	2403 (5)	4221 (5)	5.63
C11A	4184 (6)	2177 (5)	3692 (5)	5.61
N12A	5069 (5)	1792 (4)	4585 (4)	4.91
C13A	6166 (6)	2028 (5)	4630 (6)	5.30
C14A	6994 (5)	1679 (5)	5566 (5)	4.78
C15A	8195 (6)	1971 (5)	5531 (6)	6.37
C16A	9001 (6)	1661 (6)	6424 (7)	7.13
C17A	8651 (6)	1035 (5)	7382 (6)	5.96
C18A	7504 (6)	751 (5)	7444 (6)	4.98
C19A	6614 (6)	1059 (5)	6535 (5)	4.56
C20A	5525 (3)	798 (3)	6589 (3)	5.32
C21A	7074 (3)	151 (4)	8347 (3)	5.75
C22A	7881 (6)	–330 (6)	9205 (6)	7.40
C1B	1281 (6)	–1674 (7)	8204 (8)	8.15
C2B	1682 (8)	–1075 (9)	7340 (11)	10.49
C3B	1232 (10)	–223 (10)	6701 (9)	10.82
C4B	2422 (8)	37 (7)	6868 (7)	7.92
C5B	3045 (7)	–562 (5)	7721 (6)	5.60
C6B	2502 (6)	–1412 (5)	8408 (6)	5.60
C7B	3394 (6)	–1824 (5)	9218 (5)	5.04
C8B	4442 (5)	–1216 (5)	8981 (5)	5.27
N9B	4231 (5)	–459 (4)	8089 (4)	5.50
C10B	3219 (5)	–2703 (5)	10141 (6)	6.38
C11B	4290 (6)	–2786 (5)	11071 (6)	6.76
N12B	5196 (6)	–3156 (4)	10540 (5)	5.95
C13B	6286 (7)	–2931 (5)	11009 (5)	6.02
C14B	7143 (6)	–3276 (5)	10452 (5)	5.21
C15B	8316 (7)	–3020 (6)	11028 (6)	7.54
C16B	9142 (7)	–3330 (6)	10508 (7)	7.99
C17B	8836 (5)	–3957 (6)	9394 (7)	6.66
C18B	7692 (5)	–4210 (5)	8809 (5)	5.00
C19B	6795 (5)	–3873 (4)	9315 (5)	4.67
C20B	5720 (3)	–4122 (3)	8764 (3)	5.77
C21B	7280 (3)	–4814 (4)	7720 (4)	6.22
C22B	8099 (6)	–5278 (6)	7196 (6)	7.87
OHAPH-TPA				
C1	–58 (7)	5856 (6)	3149 (7)	4.79
C2	–461 (8)	6724 (6)	3333 (8)	5.08
C3	308 (8)	7308 (6)	4104 (8)	5.36
C4	1472 (9)	7047 (6)	4699 (8)	5.35
C5	1866 (7)	6171 (6)	4535 (7)	4.53
C6	1142 (7)	5528 (5)	3748 (7)	4.26
C7	1837 (7)	4623 (6)	3742 (7)	4.62
C8	2937 (7)	4776 (8)	4536 (8)	5.87
N9	2986 (6)	5687 (6)	5016 (6)	6.01
C10	1463 (8)	3784 (6)	2959 (9)	5.70
C11	1862 (7)	3850 (6)	1502 (9)	5.11
N12	3327 (6)	3835 (4)	1393 (7)	4.52
O13	3980 (8)	3814 (5)	306 (8)	4.21
C14	3244 (9)	3859 (6)	–1006 (9)	6.01
C15	5409 (7)	3721 (4)	378 (7)	3.97
C16	6203 (9)	3643 (5)	–805 (8)	4.97
C17	7543 (9)	3520 (6)	–755 (9)	5.73
C18	8174 (8)	3466 (6)	462 (9)	5.28
C19	7484 (7)	3531 (5)	1651 (8)	4.86
C20	6080 (7)	3665 (5)	1631 (7)	4.03
C21	5435 (5)	3718 (4)	2760 (5)	5.69

Table 2. Bond distances (\AA) and angles ($^\circ$) with *e.s.d.*'s in parentheses

3'-Meo-salTPA		3'-Meo-salTPA	
C2A–C1A	1.39 (1)	C2B–C1B	1.37 (1)
C6A–C1A	1.41 (1)	C6B–C1B	1.40 (1)
C3A–C2A	1.40 (1)	C3B–C2B	1.37 (1)
C4A–C3A	1.37 (1)	C4B–C3B	1.37 (1)
C5A–C4A	1.40 (1)	C5B–C4B	1.38 (1)
C6A–C5A	1.42 (1)	C6B–C5B	1.40 (1)
N9A–C5A	1.37 (1)	N9B–C5B	1.38 (1)
C7A–C6A	1.42 (1)	C7B–C6B	1.42 (1)
C8A–C7A	1.38 (1)	C8B–C7B	1.39 (1)
C10A–C7A	1.52 (1)	C10B–C7B	1.48 (1)
N9A–C8A	1.36 (1)	N9B–C8B	1.36 (1)
C11A–C10A	1.51 (1)	C11B–C10B	1.51 (1)
N12A–C11A	1.45 (1)	N12B–C11B	1.47 (1)
C13A–N12A	1.27 (1)	C13B–N12B	1.28 (1)
C14A–C13A	1.42 (1)	C14B–C13B	1.42 (1)
C15A–C14A	1.42 (1)	C15B–C14B	1.40 (1)
C19A–C14A	1.42 (1)	C19B–C14B	1.42 (1)
C16A–C15A	1.36 (1)	C16B–C15B	1.35 (1)
C17A–C18A	1.40 (1)	C17B–C18B	1.41 (1)
C18A–C17A	1.36 (1)	C18B–C17B	1.37 (1)
C19A–C18A	1.43 (1)	C19B–C18B	1.43 (1)
O21A–C18A	1.37 (1)	O21B–C18B	1.38 (1)
O20A–C19A	1.29 (1)	O20B–C19B	1.29 (1)
C22A–C21A	1.42 (1)	C22B–C21B	1.43 (1)
C1A–C2A–C3A	123.0 (7)	C11A–N12A–C13A	126.3 (5)
C2A–C3A–C4A	121.5 (7)	N12A–C13A–C14A	123.6 (6)
C3A–C4A–C5A	116.6 (6)	C13A–C14A–C19A	119.8 (6)
C4A–C5A–N9A	129.1 (5)	C13A–C14A–C15A	119.5 (5)
C4A–C5A–C6A	122.8 (6)	C15A–C14A–C19A	120.6 (6)
C6A–C5A–N9A	108.1 (5)	C14A–C15A–C16A	120.4 (6)
C1A–C6A–C5A	119.4 (6)	C15A–C16A–C17A	120.2 (7)
C5A–C6A–C7A	106.0 (5)	C16A–C17A–C18A	120.6 (6)
C1A–C6A–C7A	134.5 (6)	C17A–C18A–O21A	125.1 (6)
C6A–C7A–C10A	124.7 (5)	C17A–C18A–C19A	121.8 (6)
C6A–C7A–C8A	107.4 (5)	C19A–C18A–O21A	113.1 (6)
C8A–C7A–C10A	127.9 (6)	C14A–C19A–C18A	116.3 (6)
C7A–C8A–N9A	109.5 (5)	C18A–C19A–O20A	122.2 (5)
C5A–N9A–C8A	108.9 (5)	C14A–C19A–O20A	121.5 (5)
C7A–C10A–C11A	115.5 (5)	C18A–O21A–C22A	116.7 (5)
C10A–C11A–N12A	111.8 (5)		
OHAPH-TPA			
C1–C2	1.35 (1)	C10–C11	1.52 (1)
C1–C6	1.42 (1)	N12–C13	1.27 (1)
C2–C3	1.38 (1)	C13–C14	1.50 (1)
C3–C4	1.36 (1)	C13–C15	1.44 (1)
C4–C5	1.35 (1)	C15–C16	1.44 (1)
C5–C6	1.42 (1)	C15–C20	1.42 (1)
C5–N9	1.41 (1)	C16–C17	1.35 (1)
C6–C7	1.50 (1)	C17–C18	1.37 (1)
C7–C8	1.37 (1)	C18–C19	1.38 (1)
C7–C10	1.50 (1)	C19–C20	1.42 (1)
C8–N9	1.42 (1)	C20–O21	1.31 (1)
C2–C1–C6	121.0 (8)	C10–C11–N12	200.0 (7)
C1–C2–C3	119.7 (8)	C11–N12–C13	125.7 (7)
C2–C3–C4	122.8 (8)	N12–C13–C15	118.5 (7)
C3–C4–C5	117.6 (8)	N12–C13–C14	119.6 (7)
C4–C5–N9	132.0 (8)	C14–C13–C15	121.7 (7)
C4–C5–C6	123.2 (7)	C13–C15–C20	120.8 (6)
C6–C5–N9	104.8 (7)	C13–C15–C16	121.6 (7)
C1–C6–C5	115.7 (7)	C16–C15–C20	117.5 (7)
C5–C6–C7	110.8 (6)	C15–C16–C17	122.4 (7)
C1–C6–C7	133.5 (7)	C16–C17–C18	119.3 (8)
C6–C7–C10	127.8 (7)	C17–C18–C19	122.1 (8)
C6–C7–C8	102.9 (7)	C18–C19–C20	120.0 (7)
C8–C7–C10	129.1 (7)	C15–C20–C19	118.7 (6)
C7–C8–N9	112.0 (7)	C19–C20–O21	119.5 (6)
C5–N9–C8	109.5 (6)	C15–C20–O21	121.7 (6)
C7–C10–C11	112.5 (7)		

$$B_{eq} = \frac{1}{3} \pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

corresponding to a synclinal disposition through the C10–C11 bond, analogous to that found for 3'-Meo-salTPA.

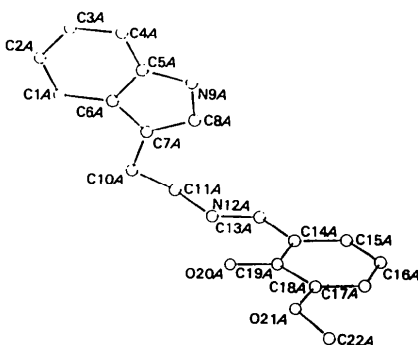


Fig. 1. View of the 3'-Meo-salTPA molecule.

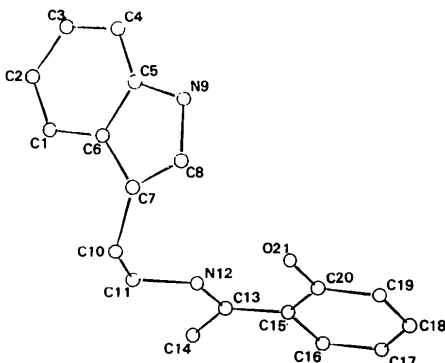


Fig. 2. View of the OHAPH-TPA molecule.

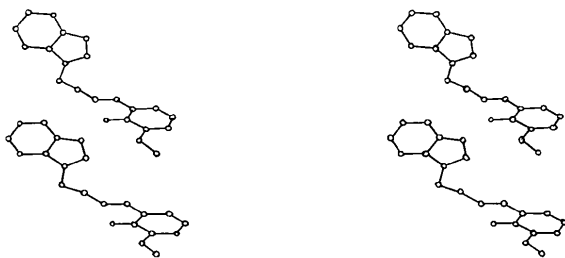


Fig. 3. A perspective view of the structure of 3'-Meo-salTPA.

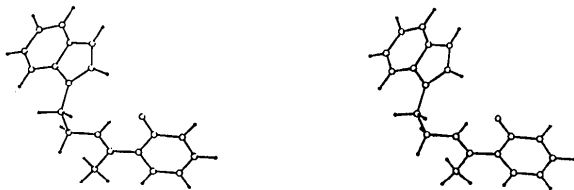


Fig. 4. View of the OHAPH-TPA molecule drawn with *PLUTO* (Motherwell & Clegg, 1978).

Table 3. Selected torsion angles ($^{\circ}$)

3'-Meo-salTPA			
C7A–C10A–C11A–N12A	+60.2 (7)	C11A–N12A–C13A–C14A	+176.4 (6)
C7B–C10B–C11B–N12B	–62.6 (7)	C11B–N12B–C13B–C14B	–178.2 (6)
C10A–C11A–N12A–C13A	–145.9 (6)	C8A–C7A–C10A–C11A	–12.2 (9)
C10B–C11B–N12B–C13B	+155.6 (6)	C8B–C7B–C10B–C11B	+12.0 (9)
OHAPH-TPA			
C7–C10–C11–N12	+68.2 (9)	C10–C11–N12–C13	+174.7 (7)
C11–N12–C13–C15	–174.6 (7)	C8–C7–C10–C11	–97 (1)

The sign convention used is that of Klyne & Prelog (1960).

An antiperiplanar disposition through the N12–C13 bond with a torsion angle of $-174.6 (7)^{\circ}$ is observed for the C11–N12–C13–C15 bond.

Finally, intra- and intermolecular hydrogen bonds are observed in both compounds. The first is to be found between the imino nitrogen and the phenolic oxygen, the N...H–O distances being 2.61 (8) Å for 3'-Meo-salTPA and 2.51 (1) Å for OHAPH-TPA. A value of 2.60 (2) Å was found for salTPA (Rodríguez *et al.*, 1987). The intermolecular hydrogen bond is established between the indolic nitrogen and the phenolic oxygen of another molecule, the N–H...O distance being 2.77 (1) Å for 3'-Meo-salTPA and 2.86 (1) Å for OHAPH-TPA. These intermolecular hydrogen bonds are responsible for the different orientation of one molecule with regard to the other in the elementary cell of both compounds.

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