Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

## New Journal of Chemistry

Crystal structure and characterization of a co-product in the syntheses of a Schiff base give evidence of its zwitterionic nature in the solid state.

M.R. Rodríguez<sup>1</sup>, G.A. Espino<sup>2</sup>, O.E. Piro<sup>3</sup>, G.A. Echeverría<sup>3</sup>, B.S. Parajón-Costa<sup>1</sup>, A.C. González- Baró<sup>1</sup>

<sup>1</sup> CEQUINOR (CONICET-CCT La Plata, UNLP), Bvd. 120 N°1465, 1900 La Plata, Argentina.

<sup>2</sup> Departamento de Química, Universidad de Burgos, Pza. Misael Bañuelos s/n, E-09001 Burgos, España.

<sup>3</sup> IFLP (CONICET-CCT La Plata, UNLP), CC 67, B1900AVV, La Plata, Argentina.

## **Electronic Supplementary Information**

**Table S1**. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters ( $Å^2 x 10^3$ ) for (o-VA)<sub>2</sub>TPNH2. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

Atom	X	У	Z	U(eq)
C(1)	2513(3)	6235(3)	-2398(2)	35(1)
C(11)	2499(3)	3704(3)	-2371(2)	34(1)
C(12)	1703(3)	2099(3)	-2687(2)	39(1)
C(13)	142(4)	1331(3)	-3555(3)	50(1)
C(14)	-634(3)	2138(4)	-4080(3)	55(1)
C(15)	115(3)	3702(3)	-3742(2)	47(1)
C(16)	1703(3)	4510(3)	-2878(2)	37(1)
C(17)	1829(5)	-164(3)	-2322(3)	58(1)
O(1)	4048(2)	4408(2)	-1521(2)	37(1)
O(11)	2591(3)	1459(2)	-2066(2)	48(1)
C(2)	4870(3)	6051(2)	-1382(2)	35(1)
C(21)	4562(3)	6812(3)	-3382(2)	37(1)
C(22)	5125(3)	7212(3)	-4395(2)	44(1)
C(23)	6522(4)	7069(3)	-4526(3)	53(1)
C(24)	7343(4)	6549(4)	-3673(3)	54(1)
C(25)	6811(3)	6190(3)	-2666(3)	45(1)
C(26)	5416(3)	6339(2)	-2512(2)	37(1)
C(27)	4717(7)	8111(5)	-6195(4)	77(1)
O(2)	3166(2)	6940(2)	-3299(2)	40(1)
O(21)	4207(3)	7681(3)	-5161(2)	60(1)
C(3)	3252(3)	6557(3)	-114(2)	40(1)
C(31)	2443(3)	7548(3)	211(2)	37(1)
C(32)	641(3)	7022(2)	-68(2)	36(1)
C(33)	455(4)	8384(4)	464(3)	57(1)
C(34)	1855(5)	9665(3)	1026(3)	58(1)
S	3545(1)	9423(1)	981(1)	58(1)
Ν	3830(2)	6774(2)	-1217(2)	34(1)

 Table S2. Full bond lengths [Å] and angles [°] for (o-VA)2TPNH2.

$\begin{array}{ccccccc} C(1)-O(2) & 1.438(3) & O(11)-C(12)-C(11) & 114.5(2) \\ C(1)-N & 1.453(3) & C(13)-C(12)-C(11) & 118.9(2) \\ C(1)-C(16) & 1.516(3) & C(12)-C(13)-C(14) & 120.2(3) \\ C(11)-C(16) & 1.392(3) & C(14)-C(15)-C(16) & 120.1(3) \\ C(11)-C(12) & 1.409(3) & C(11)-C(16)-C(1) & 119.2(2) \\ C(12)-O(11) & 1.370(3) & C(11)-C(16)-C(1) & 119.2(2) \\ C(12)-C(13) & 1.384(4) & C(15)-C(16)-C(1) & 119.2(2) \\ C(13)-C(14) & 1.388(5) & C(11)-O(1)-C(2) & 112.83(16) \\ C(14)-C(15) & 1.371(4) & C(12)-O(11) & 112.16(2) \\ C(13)-C(16) & 1.402(3) & N-C(2)-O(26) & 109.10(18) \\ O(1)-C(2) & 1.468(3) & O(1)-C(2)-C(26) & 109.10(18) \\ O(1)-C(2) & 1.468(3) & O(2)-C(21)-C(26) & 110.54(18) \\ C(2)-N & 1.432(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-O(2) & 1.370(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-C(26) & 1.385(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23) & 120.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23) & 120.8(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23) & 120.8(3) \\ C(22)-C(23) & 1.382(4) & C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26) & (119.3(2) \\ C(3)-C(31) & 1.496(3) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-C(31) & 1.496(3) & C(21)-C(3) & 112.59(17) \\ C(31)-C(33) & 1.474(4) & C(32)-C(31) & 112.59(17) \\ C(31)-C(33) & 1.474(4) & C(32)-C(31) & 112.59(17) \\ C(33)-C(33) & 1.474(4) & C(32)-C(31) & 125.2(2) \\ C(3)-C(3) & 1.496(3) $				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1)-O(2)	1.438(3)	O(11)-C(12)-C(11)	114.5(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1)-N	1.453(3)	C(13)-C(12)-C(11)	118.9(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(1)-C(16)	1.516(3)	C(12)-C(13)-C(14)	120.2(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(11)-O(1)	1.369(3)	C(15)-C(14)-C(13)	121.0(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(11)-C(16)	1.392(3)	C(14)-C(15)-C(16)	120.1(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(11)-C(12)	1.409(3)	C(11)-C(16)-C(15)	119.0(2)
$\begin{array}{cccccc} C(12)-C(13) & 1.384(4) & C(15)-C(16)-C(1) & 121.6(2) \\ C(13)-C(14) & 1.388(5) & C(11)-O(1)-C(2) & 112.83(16) \\ C(14)-C(15) & 1.371(4) & C(12)-O(11)-C(17) & 117.1(2) \\ C(15)-C(16) & 1.402(3) & N-C(2)-C(26) & 109.10(18) \\ C(17)-O(11) & 1.429(3) & N-C(2)-C(26) & 109.10(18) \\ C(17)-O(11) & 1.432(3) & O(2)-C(21)-C(26) & 122.5(2) \\ C(2)-C(26) & 1.503(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-O(2) & 1.370(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(23) & 126.4(2) \\ C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(2) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(2) & 119.3(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 119.3(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-C(21) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 112.9(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 112.9(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 112.9(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 112.61(18) \\ C(32)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 126.6(2) \\ \end{array} \right$	C(12)-O(11)	1.370(3)	C(11)-C(16)-C(1)	119.2(2)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(12)-C(13)	1.384(4)	C(15)-C(16)-C(1)	121.6(2)
$\begin{array}{ccccccc} C(14)-C(15) & 1.371(4) & C(12)-O(11)-C(17) & 117.1(2) \\ C(15)-C(16) & 1.402(3) & N-C(2)-O(1) & 112.19(18) \\ C(17)-O(11) & 1.429(3) & N-C(2)-C(26) & 109.10(18) \\ O(1)-C(2) & 1.468(3) & O(1)-C(2)-C(26) & 110.54(18) \\ C(2)-N & 1.432(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(2)-C(26) & 1.503(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-O(2) & 1.370(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(23) & 126.4(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26) & 119.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-C(3) & 125.2(2) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 112.92(17) \\ C(33)-C(33) & 1.474(4) & C(32)-C(31)-C(3) & 125.2(2) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 112.61(18) \\ C(32)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(34)-C(33) & (32-6(14) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(13)-C(14)	1.388(5)	C(11)-O(1)-C(2)	112.83(16)
$\begin{array}{cccccc} C(15)-C(16) & 1.402(3) & N-C(2)-O(1) & 112.19(18) \\ C(17)-O(11) & 1.429(3) & N-C(2)-C(26) & 109.10(18) \\ O(1)-C(2) & 1.468(3) & O(1)-C(2)-C(26) & 110.54(18) \\ C(2)-N & 1.432(3) & O(2)-C(21)-C(26) & 122.5(2) \\ C(2)-C(26) & 1.503(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-O(2) & 1.370(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 119.3(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 112.92(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31) & 105.0(2) \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(33)-C(34)-S & 112.92(17) \\ C(33)-C(31) & 1.134(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(14)-C(15)	1.371(4)	C(12)-O(11)-C(17)	117.1(2)
$\begin{array}{ccccc} C(17)-O(11) & 1.429(3) & N-C(2)-C(26) & 109.10(18) \\ O(1)-C(2) & 1.468(3) & O(1)-C(2)-C(26) & 110.54(18) \\ C(2)-N & 1.432(3) & O(2)-C(21)-C(26) & 122.5(2) \\ C(2)-C(26) & 1.503(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-C(26) & 1.370(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(23) & 126.4(2) \\ C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 114.9(2) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(22) & 120.8(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 119.3(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 125.2(2) \\ C(3)-C(31) & 1.088(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-N & 108.88(18) & C(34)-S(-31) & 93.26(14) \\ O(1)-C(11)-C(16) & 111.82(18) & C(33)-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 16.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(15)-C(16)	1.402(3)	N-C(2)-O(1)	112.19(18)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(17)-O(11)	1.429(3)	N-C(2)-C(26)	109.10(18)
$\begin{array}{ccccccc} C(2)\text{-N} & 1.432(3) & O(2)\text{-}C(21)\text{-}C(26) & 122.5(2) \\ C(2)\text{-}C(26) & 1.503(3) & O(2)\text{-}C(21)\text{-}C(22) & 116.9(2) \\ C(21)\text{-}O(2) & 1.370(3) & C(26)\text{-}C(21)\text{-}C(22) & 120.6(2) \\ C(21)\text{-}C(26) & 1.385(3) & O(21)\text{-}C(22)\text{-}C(23) & 126.4(2) \\ C(21)\text{-}C(22) & 1.412(3) & O(21)\text{-}C(22)\text{-}C(21) & 114.9(2) \\ C(22)\text{-}O(21) & 1.345(4) & C(23)\text{-}C(22)\text{-}C(21) & 118.6(3) \\ C(22)\text{-}C(23) & 1.393(4) & C(24)\text{-}C(23)\text{-}C(22) & 120.5(3) \\ C(23)\text{-}C(24) & 1.387(5) & C(25)\text{-}C(24)\text{-}C(23) & 120.8(3) \\ C(24)\text{-}C(25) & 1.382(4) & C(24)\text{-}C(25)\text{-}C(26) & 119.6(3) \\ C(25)\text{-}C(26) & 1.402(3) & C(21)\text{-}C(26)\text{-}C(22) & 119.9(2) \\ C(27)\text{-}O(21) & 1.422(4) & C(21)\text{-}C(26)\text{-}C(22) & 119.3(2) \\ C(3)\text{-}N & 1.476(3) & C(25)\text{-}C(26)\text{-}C(2) & 119.3(2) \\ C(3)\text{-}C(31) & 1.496(3) & C(21)\text{-}O(2)\text{-}C(1) & 112.59(17) \\ C(31)\text{-}C(32) & 1.484(3) & C(22)\text{-}O(21) & 112.59(17) \\ C(31)\text{-}C(32) & 1.484(3) & C(22)\text{-}O(21)\text{-}C(27) & 117.6(3) \\ C(32)\text{-}C(33) & 1.474(4) & C(32)\text{-}C(31) & 112.61(18) \\ C(32)\text{-}C(33) & 1.474(4) & C(32)\text{-}C(31) & 125.2(2) \\ C(33)\text{-}C(34) & 1.340(5) & C(32)\text{-}C(31)\text{-}S & 121.92(17) \\ C(34)\text{-}S & 1.685(4) & C(33)\text{-}C(31)\text{-}S & 121.92(17) \\ C(34)\text{-}S & 1.685(4) & C(33)\text{-}C(31) & 93.26(14) \\ O(1)\text{-}C(1)\text{-}C(16) & 111.82(18) & C(33)\text{-}C(32) & 115.9(3) \\ O(2)\text{-}C(1)\text{-}C(16) & 111.34(18) & C(34)\text{-}S(31) & 93.26(14) \\ O(1)\text{-}C(11)\text{-}C(12) & 16.7(2) & C(2)\text{-}N\text{-}C(3) & 112.45(18) \\ C(16)\text{-}C(11)\text{-}C(12) & 120.7(2) & C(1)\text{-}N\text{-}C(3) & 114.02(19) \\ O(11)\text{-}C(12)\text{-}C(13) & 126.6(2) \\ \end{array}$	O(1)-C(2)	1.468(3)	O(1)-C(2)-C(26)	110.54(18)
$\begin{array}{ccccccc} C(2)-C(26) & 1.503(3) & O(2)-C(21)-C(22) & 116.9(2) \\ C(21)-O(2) & 1.37O(3) & C(26)-C(21)-C(22) & 120.6(2) \\ C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(23) & 126.4(2) \\ C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(2)-N	1.432(3)	O(2)-C(21)-C(26)	122.5(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2)-C(26)	1.503(3)	O(2)-C(21)-C(22)	116.9(2)
$\begin{array}{ccccccc} C(21)-C(26) & 1.385(3) & O(21)-C(22)-C(23) & 126.4(2) \\ C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(33)-C(32)-C(31) & 105.0(2) \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(33)-C(34)-S & 112.9(2) \\ N-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(21)-O(2)	1.370(3)	C(26)-C(21)-C(22)	120.6(2)
$\begin{array}{ccccccc} C(21)-C(22) & 1.412(3) & O(21)-C(22)-C(21) & 114.9(2) \\ C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(2) & 119.3(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 121.91(19) \\ & & & & & & & & & \\ C(33)-C(32)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 122.6(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(21)-C(26)	1.385(3)	O(21)-C(22)-C(23)	126.4(2)
$\begin{array}{ccccccc} C(22)-O(21) & 1.345(4) & C(23)-C(22)-C(21) & 118.6(3) \\ C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(21)-C(22)	1.412(3)	O(21)-C(22)-C(21)	114.9(2)
$\begin{array}{ccccccc} C(22)-C(23) & 1.393(4) & C(24)-C(23)-C(22) & 120.5(3) \\ C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 125.2(2) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & & & & & \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(34)-S(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 122.6(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(22)-O(21)	1.345(4)	C(23)-C(22)-C(21)	118.6(3)
$\begin{array}{ccccccc} C(23)-C(24) & 1.387(5) & C(25)-C(24)-C(23) & 120.8(3) \\ C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & \\ C(33)-C(34) & 1.340(5) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 122.6(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(13) & 126.6(2) \\ \end{array}$	C(22)-C(23)	1.393(4)	C(24)-C(23)-C(22)	120.5(3)
$\begin{array}{ccccccc} C(24)-C(25) & 1.382(4) & C(24)-C(25)-C(26) & 119.6(3) \\ C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-C(3) & 125.2(2) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & & \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(33)-C(34)-S & 112.9(2) \\ N-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(23)-C(24)	1.387(5)	C(25)-C(24)-C(23)	120.8(3)
$\begin{array}{ccccccc} C(25)-C(26) & 1.402(3) & C(21)-C(26)-C(25) & 119.9(2) \\ C(27)-O(21) & 1.422(4) & C(21)-C(26)-C(2) & 119.3(2) \\ C(3)-N & 1.476(3) & C(25)-C(26)-C(2) & 120.8(2) \\ C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-S & 112.92(17) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 121.91(19) \\ & & & & & & & & \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & \\ O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(33)-C(34)-S & 112.9(2) \\ N-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) \\ \end{array}$	C(24)-C(25)	1.382(4)	C(24)-C(25)-C(26)	119.6(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(25)-C(26)	1.402(3)	C(21)-C(26)-C(25)	119.9(2)
$\begin{array}{ccccccc} C(3)\text{-N} & 1.476(3) & C(25)\text{-}C(26)\text{-}C(2) & 120.8(2) \\ C(3)\text{-}C(31) & 1.496(3) & C(21)\text{-}O(2)\text{-}C(1) & 112.59(17) \\ C(31)\text{-}C(32) & 1.484(3) & C(22)\text{-}O(21)\text{-}C(27) & 117.6(3) \\ C(31)\text{-}S & 1.690(2) & \text{N-}C(3)\text{-}C(31) & 112.61(18) \\ C(32)\text{-}C(33) & 1.474(4) & C(32)\text{-}C(31)\text{-}C(3) & 125.2(2) \\ C(33)\text{-}C(34) & 1.340(5) & C(32)\text{-}C(31)\text{-}S & 112.92(17) \\ C(34)\text{-}S & 1.685(4) & C(3)\text{-}C(31)\text{-}S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(27)-O(21)	1.422(4)	C(21)-C(26)-C(2)	119.3(2)
$\begin{array}{cccccc} C(3)-C(31) & 1.496(3) & C(21)-O(2)-C(1) & 112.59(17) \\ C(31)-C(32) & 1.484(3) & C(22)-O(21)-C(27) & 117.6(3) \\ C(31)-S & 1.690(2) & N-C(3)-C(31) & 112.61(18) \\ C(32)-C(33) & 1.474(4) & C(32)-C(31)-C(3) & 125.2(2) \\ C(33)-C(34) & 1.340(5) & C(32)-C(31)-S & 112.92(17) \\ C(34)-S & 1.685(4) & C(3)-C(31)-S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(3)-N	1.476(3)	C(25)-C(26)-C(2)	120.8(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(3)-C(31)	1.496(3)	C(21)-O(2)-C(1)	112.59(17)
$\begin{array}{cccccccc} C(31)\text{-S} & 1.690(2) & \text{N-C}(3)\text{-C}(31) & 112.61(18) \\ C(32)\text{-C}(33) & 1.474(4) & C(32)\text{-C}(31)\text{-C}(3) & 125.2(2) \\ C(33)\text{-C}(34) & 1.340(5) & C(32)\text{-C}(31)\text{-S} & 112.92(17) \\ C(34)\text{-S} & 1.685(4) & C(3)\text{-C}(31)\text{-S} & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(31)-C(32)	1.484(3)	C(22)-O(21)-C(27)	117.6(3)
$\begin{array}{cccccc} C(32)\mbox{-}C(33) & 1.474(4) & C(32)\mbox{-}C(31)\mbox{-}C(3) & 125.2(2) \\ C(33)\mbox{-}C(34) & 1.340(5) & C(32)\mbox{-}C(31)\mbox{-}S & 112.92(17) \\ C(34)\mbox{-}S & 1.685(4) & C(3)\mbox{-}C(31)\mbox{-}S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(31)-S	1.690(2)	N-C(3)-C(31)	112.61(18)
$\begin{array}{cccccc} C(33)\text{-}C(34) & 1.340(5) & C(32)\text{-}C(31)\text{-}S & 112.92(17) \\ C(34)\text{-}S & 1.685(4) & C(3)\text{-}C(31)\text{-}S & 121.91(19) \\ & & & & & & & & & & & & & & & & & & $	C(32)-C(33)	1.474(4)	C(32)-C(31)-C(3)	125.2(2)
$\begin{array}{ccccccc} C(34)\text{-}S & 1.685(4) & C(3)\text{-}C(31)\text{-}S & 121.91(19) \\ & C(33)\text{-}C(32)\text{-}C(31) & 105.0(2) \\ O(2)\text{-}C(1)\text{-}N & 108.88(18) & C(34)\text{-}C(33)\text{-}C(32) & 115.9(3) \\ O(2)\text{-}C(1)\text{-}C(16) & 111.82(18) & C(33)\text{-}C(34)\text{-}S & 112.9(2) \\ N\text{-}C(1)\text{-}C(16) & 111.34(18) & C(34)\text{-}S\text{-}C(31) & 93.26(14) \\ O(1)\text{-}C(11)\text{-}C(16) & 122.6(2) & C(2)\text{-}N\text{-}C(1) & 107.56(18) \\ O(1)\text{-}C(11)\text{-}C(12) & 116.7(2) & C(2)\text{-}N\text{-}C(3) & 112.45(18) \\ C(16)\text{-}C(11)\text{-}C(12) & 120.7(2) & C(1)\text{-}N\text{-}C(3) & 114.02(19) \\ O(11)\text{-}C(12)\text{-}C(13) & 126.6(2) \end{array}$	C(33)-C(34)	1.340(5)	C(32)-C(31)-S	112.92(17)
$\begin{array}{c cccc} C(33)-C(32)-C(31) & 105.0(2) \\ \hline O(2)-C(1)-N & 108.88(18) & C(34)-C(33)-C(32) & 115.9(3) \\ O(2)-C(1)-C(16) & 111.82(18) & C(33)-C(34)-S & 112.9(2) \\ \hline N-C(1)-C(16) & 111.34(18) & C(34)-S-C(31) & 93.26(14) \\ O(1)-C(11)-C(16) & 122.6(2) & C(2)-N-C(1) & 107.56(18) \\ O(1)-C(11)-C(12) & 116.7(2) & C(2)-N-C(3) & 112.45(18) \\ C(16)-C(11)-C(12) & 120.7(2) & C(1)-N-C(3) & 114.02(19) \\ O(11)-C(12)-C(13) & 126.6(2) & & \\ \end{array}$	C(34)-S	1.685(4)	C(3)-C(31)-S	121.91(19)
$\begin{array}{ccccc} O(2)\text{-}C(1)\text{-}N & 108.88(18) & C(34)\text{-}C(33)\text{-}C(32) & 115.9(3) \\ O(2)\text{-}C(1)\text{-}C(16) & 111.82(18) & C(33)\text{-}C(34)\text{-}S & 112.9(2) \\ N\text{-}C(1)\text{-}C(16) & 111.34(18) & C(34)\text{-}S\text{-}C(31) & 93.26(14) \\ O(1)\text{-}C(11)\text{-}C(16) & 122.6(2) & C(2)\text{-}N\text{-}C(1) & 107.56(18) \\ O(1)\text{-}C(11)\text{-}C(12) & 116.7(2) & C(2)\text{-}N\text{-}C(3) & 112.45(18) \\ C(16)\text{-}C(11)\text{-}C(12) & 120.7(2) & C(1)\text{-}N\text{-}C(3) & 114.02(19) \\ O(11)\text{-}C(12)\text{-}C(13) & 126.6(2) \end{array}$			C(33)-C(32)-C(31)	105.0(2)
$\begin{array}{cccc} O(2)\text{-}C(1)\text{-}C(16) & 111.82(18) & C(33)\text{-}C(34)\text{-}S & 112.9(2) \\ \text{N-}C(1)\text{-}C(16) & 111.34(18) & C(34)\text{-}S\text{-}C(31) & 93.26(14) \\ O(1)\text{-}C(11)\text{-}C(16) & 122.6(2) & C(2)\text{-}N\text{-}C(1) & 107.56(18) \\ O(1)\text{-}C(11)\text{-}C(12) & 116.7(2) & C(2)\text{-}N\text{-}C(3) & 112.45(18) \\ C(16)\text{-}C(11)\text{-}C(12) & 120.7(2) & C(1)\text{-}N\text{-}C(3) & 114.02(19) \\ O(11)\text{-}C(12)\text{-}C(13) & 126.6(2) & & & \\ \end{array}$	O(2)-C(1)-N	108.88(18)	C(34)-C(33)-C(32)	115.9(3)
N-C(1)-C(16)111.34(18)C(34)-S-C(31)93.26(14)O(1)-C(11)-C(16)122.6(2)C(2)-N-C(1)107.56(18)O(1)-C(11)-C(12)116.7(2)C(2)-N-C(3)112.45(18)C(16)-C(11)-C(12)120.7(2)C(1)-N-C(3)114.02(19)O(11)-C(12)-C(13)126.6(2)126.6(2)114.02(19)	O(2)-C(1)-C(16)	111.82(18)	C(33)-C(34)-S	112.9(2)
O(1)-C(11)-C(16)122.6(2)C(2)-N-C(1)107.56(18)O(1)-C(11)-C(12)116.7(2)C(2)-N-C(3)112.45(18)C(16)-C(11)-C(12)120.7(2)C(1)-N-C(3)114.02(19)O(11)-C(12)-C(13)126.6(2)120.7(2)C(1)-N-C(3)	N-C(1)-C(16)	111.34(18)	C(34)-S-C(31)	93.26(14)
O(1)-C(11)-C(12)116.7(2)C(2)-N-C(3)112.45(18)C(16)-C(11)-C(12)120.7(2)C(1)-N-C(3)114.02(19)O(11)-C(12)-C(13)126.6(2)126.6(2)114.02(19)	O(1)-C(11)-C(16)	122.6(2)	C(2)-N-C(1)	107.56(18)
C(16)-C(11)-C(12)120.7(2)C(1)-N-C(3)114.02(19)O(11)-C(12)-C(13)126.6(2)	O(1)-C(11)-C(12)	116.7(2)	C(2)-N-C(3)	112.45(18)
O(11)-C(12)-C(13) 126.6(2)	C(16)-C(11)-C(12)	120.7(2)	C(1)-N-C(3)	114.02(19)
	O(11)-C(12)-C(13)	126.6(2)		

Atom	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
C(1)	34(1)	40(1)	36(1)	14(1)	13(1)	21(1)
C(11)	32(1)	36(1)	32(1)	8(1)	11(1)	13(1)
C(12)	43(1)	37(1)	39(1)	10(1)	17(1)	16(1)
C(13)	46(1)	38(1)	49(1)	3(1)	13(1)	7(1)
C(14)	36(1)	59(2)	46(1)	3(1)	1(1)	9(1)
C(15)	39(1)	59(2)	41(1)	13(1)	7(1)	22(1)
C(16)	34(1)	41(1)	35(1)	10(1)	11(1)	17(1)
C(17)	73(2)	34(1)	68(2)	15(1)	26(2)	21(1)
O(1)	32(1)	32(1)	43(1)	10(1)	5(1)	15(1)
O(11)	51(1)	35(1)	59(1)	14(1)	15(1)	19(1)
C(2)	30(1)	31(1)	38(1)	6(1)	5(1)	12(1)
C(21)	37(1)	32(1)	40(1)	7(1)	14(1)	12(1)
C(22)	46(1)	40(1)	42(1)	9(1)	19(1)	13(1)
C(23)	51(2)	48(1)	55(2)	7(1)	30(1)	12(1)
C(24)	40(1)	52(2)	65(2)	3(1)	24(1)	17(1)
C(25)	33(1)	42(1)	55(1)	5(1)	12(1)	15(1)
C(26)	32(1)	31(1)	42(1)	5(1)	10(1)	12(1)
C(27)	109(3)	78(2)	60(2)	38(2)	47(2)	37(2)
O(2)	41(1)	47(1)	41(1)	20(1)	16(1)	24(1)
O(21)	74(2)	72(1)	52(1)	34(1)	34(1)	37(1)
C(3)	50(1)	43(1)	38(1)	15(1)	18(1)	27(1)
C(31)	42(1)	38(1)	33(1)	11(1)	15(1)	19(1)
C(32)	36(1)	29(1)	50(1)	11(1)	17(1)	20(1)
C(33)	55(2)	65(2)	69(2)	21(2)	32(1)	37(1)
C(34)	76(2)	44(1)	60(2)	8(1)	28(2)	33(1)
S	58(1)	48(1)	62(1)	7(1)	17(1)	21(1)
Ν	36(1)	35(1)	35(1)	11(1)	11(1)	19(1)

**Table S3**. Anisotropic displacement parameters  $(Å^2 \times 10^3)$  for  $(o-VA)_2$ TPNH2. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2h k a^* b^* U^{12}]$ 

Atom	x	У	Z	U(eq)
H(1)	1678	6557	-2250	41
H(13)	-388	271	-3788	60
H(14)	-1677	1611	-4669	66
H(15)	-432	4226	-4088	56
H(17A)	770	-494	-2191	88
H(17B)	2509	-468	-1766	88
H(17C)	1695	-620	-3180	88
H(2)	5847	6515	-636	42
H(23)	6908	7323	-5190	64
H(24)	8262	6441	-3781	65
H(25)	7376	5852	-2095	54
H(27A)	5817	8921	-5888	116
H(27B)	3986	8452	-6649	116
H(27C)	4694	7250	-6747	116
H(3A)	4182	6782	605	48
H(3B)	2477	5497	-289	48
H(32)	-190	6046	-487	43
H(33)	-572	8356	412	68
H(34)	1891	10591	1402	69

Table S4. Hydrogen coordinates (x  $10^4$ ) and isotropic displacement parameters (Å<sup>2</sup> x  $10^3$ ) for (o-VA)<sub>2</sub>TPNH2.

 Table S5. Torsion angles [°] for (o-VA)2TPNH2.

O(1)-C(11)-C(12)-O(11)	1.5(3)	O(2)-C(21)-C(26)-C(2)	-4.2(3)
C(16)-C(11)-C(12)-O(11)	-176.4(2)	C(22)-C(21)-C(26)-C(2)	174.7(2)
O(1)-C(11)-C(12)-C(13)	-179.2(2)	C(24)-C(25)-C(26)-C(21)	1.4(4)
C(16)-C(11)-C(12)-C(13)	2.9(3)	C(24)-C(25)-C(26)-C(2)	-176.2(2)
O(11)-C(12)-C(13)-C(14)	177.7(3)	N-C(2)-C(26)-C(21)	-17.7(3)
C(11)-C(12)-C(13)-C(14)	-1.5(4)	O(1)-C(2)-C(26)-C(21)	106.1(2)
C(12)-C(13)-C(14)-C(15)	-0.7(5)	N-C(2)-C(26)-C(25)	159.9(2)
C(13)-C(14)-C(15)-C(16)	1.5(4)	O(1)-C(2)-C(26)-C(25)	-76.3(3)
O(1)-C(11)-C(16)-C(15)	-180.0(2)	C(26)-C(21)-O(2)-C(1)	-12.4(3)
C(12)-C(11)-C(16)-C(15)	-2.2(3)	C(22)-C(21)-O(2)-C(1)	168.6(2)
O(1)-C(11)-C(16)-C(1)	-5.1(3)	N-C(1)-O(2)-C(21)	50.3(2)
C(12)-C(11)-C(16)-C(1)	172.7(2)	C(16)-C(1)-O(2)-C(21)	-73.2(2)
C(14)-C(15)-C(16)-C(11)	0.0(4)	C(23)-C(22)-O(21)-C(27)	-1.6(5)
C(14)-C(15)-C(16)-C(1)	-174.8(2)	C(21)-C(22)-O(21)-C(27)	179.6(3)
O(2)-C(1)-C(16)-C(11)	106.4(2)	N-C(3)-C(31)-C(32)	103.8(3)
N-C(1)-C(16)-C(11)	-15.7(3)	N-C(3)-C(31)-S	-77.6(2)
O(2)-C(1)-C(16)-C(15)	-78.9(3)	C(3)-C(31)-C(32)-C(33)	178.2(2)
N-C(1)-C(16)-C(15)	159.1(2)	S-C(31)-C(32)-C(33)	-0.6(3)
C(16)-C(11)-O(1)-C(2)	-10.2(3)	C(31)-C(32)-C(33)-C(34)	-0.1(4)
C(12)-C(11)-O(1)-C(2)	171.95(19)	C(32)-C(33)-C(34)-S	0.7(4)
C(13)-C(12)-O(11)-C(17)	-0.9(4)	C(33)-C(34)-S-C(31)	-0.8(3)
C(11)-C(12)-O(11)-C(17)	178.3(2)	C(32)-C(31)-S-C(34)	0.8(2)
C(11)-O(1)-C(2)-N	47.8(2)	C(3)-C(31)-S-C(34)	-178.0(2)
C(11)-O(1)-C(2)-C(26)	-74.2(2)	O(1)-C(2)-N-C(1)	-68.6(2)
O(2)-C(21)-C(22)-O(21)	0.2(3)	C(26)-C(2)-N-C(1)	54.2(2)
C(26)-C(21)-C(22)-O(21)	-178.8(2)	O(1)-C(2)-N-C(3)	57.7(2)
O(2)-C(21)-C(22)-C(23)	-178.8(2)	C(26)-C(2)-N-C(3)	-179.43(18)
C(26)-C(21)-C(22)-C(23)	2.3(4)	O(2)-C(1)-N-C(2)	-73.7(2)
O(21)-C(22)-C(23)-C(24)	-179.1(3)	C(16)-C(1)-N-C(2)	50.0(2)
C(21)-C(22)-C(23)-C(24)	-0.3(4)	O(2)-C(1)-N-C(3)	160.86(18)
C(22)-C(23)-C(24)-C(25)	-1.2(4)	C(16)-C(1)-N-C(3)	-75.4(2)
C(23)-C(24)-C(25)-C(26)	0.6(4)	C(31)-C(3)-N-C(2)	169.0(2)
O(2)-C(21)-C(26)-C(25)	178.3(2)	C(31)-C(3)-N-C(1)	-68.2(3)
C(22)-C(21)-C(26)-C(25)	-2.8(3)		

**Table S6**. Hydrogen bond distances [Å] and angles [°] for (o-VA)<sub>2</sub>TPNH2.

D-HA	d(D-H)	d(HA)	d(DA)	<(DHA)
C(3)-H(3A)O(1)#1	0.97	2.51	3.321(3)	141
C(27)-H(27B)S#2	0.96	2.99	3.746(4)	136

Symmetry transformations: (#1) -x+1, -y+1, -z; (#2) x, y, z-1.

o-HVA		HVA	TPNH2				o-HVATPNH2		
FTIR	Calc.	Assignment	FTIR	Calc.	Assignment	FTIR	Raman	Calc.	Assignment
			3369 vs	3551	$v_{as} NH_2$				
			3293 s	3476	$\nu_s NH_2$				
3014 vw	3318	νOH							
						3003 vw	3005 <sup>w</sup>	3153	vN···H···O
2939 <sup>w</sup>		$\nu CH^{aldh}$				2937 vw			vCH <sup>aldh</sup>
			2919 <sup>s</sup>	3071	$v_{as} CH_2$	2923 <sup>sh</sup>	2928 <sup>m</sup>	3045	$v_{as}CH_2$
2884 <sup>w</sup>	3016	$\nu_s CH_3$				2888 <sup>vw</sup>	2892 w	2998	$v_sCH_3 + vCH^{aldh}$
			2852 <sup>vs</sup>	3036	$\nu_s CH_2$			2965	$v_s CH_2$
2839 <sup>w</sup>	2943	$\nu CH^{aldh}$				2834 <sup>w</sup>	2838 <sup>w</sup>	3000	vCH <sup>aldh</sup>
1645 vs	1704	v C=0							
					_	1631 <sup>vs</sup>	1635 vs	1685	v C=N
			1598 vs	1665	$\delta NH_2$				
1591 "	1649	ν <sup>R</sup> + δΟΗ				1583 <sup>sn</sup>	1587 <sup>m</sup>	1660	$[v^{R} + \delta N - H \cdots O]^{\circ - HVA}$
4 4 7 4 m	1622					4.4.62.1/6	4 4 7 0 m	1618	
14/1 "	1510	δ <sub>as</sub> CH <sub>3</sub>				1462 *3	1472 "	1505	$\delta_{as} CH_3$
1400 °	1489					1 1 2 2 sh	1440 m	1493	$O_{as} CH_3$
1433 5.	1480	$O_{\rm S}$ CH <sub>3</sub> + 0 OH				1433 5	1440	1497	$[O(CH_3 + N-H\cdots O) + V^n]^{O(CH_3+N-H\cdots O)}$
	1472	$O_{\rm S}$ CH <sub>3</sub> + V <sup>1</sup>	1/20 s	1/02	8 CH	1/15 m.b		1400	SCH
			1381 \$	1405		1378 w		139/	
1388 5	1/122	δΩH	1501	1377	och + prinn2	1361 m	1365 W	1370	$[\delta N_{-}HO + y^{B]0-HVA}$
1500	1422	0011	1330 W	1362	0. CH-	1333 m-w	1337 \$	1355	
1327s	1306	$[vC-O]^{ArOH} + \delta CH$	1000	1302	pwenz	1313 m	1007	1315	рwсн2 [уС-0] <sup>ArOH</sup> +[δСH] <sup>o-HVA</sup>
1270 <sup>sh</sup>	1284					1269 s		1010	
1257 s	1201	ve beng toen				1255 vs	1258 <sup>vw</sup>	1282	[νC-OCH <sub>3</sub> +δCH <sup>R</sup> ] <sup>ο-ΗVA</sup>
-			1079 <sup>w</sup>	1075	vC-N	1097 <sup>sh</sup>		1050	νC-N + [γCH] <sup>aldh</sup>
			900 <sup>sh</sup>	888	$\rho_t [NH_2 + CH_2]$	902 vw		958	$\rho_t CH_2$
895 <sup>w</sup>	958	γCH <sup>R</sup>				884 <sup>vw</sup>		920	
								882	[γCH <sup>κ</sup> ] <sup>0-ηγΑ</sup>
			849 <sup>w</sup>	840	γCH <sup>R</sup>	853 <sup>vw</sup>	856 <sup>vw</sup>	842	[γCH <sup>R</sup> ] <sup>TPNH2</sup>
			826 <sup>m</sup>	850	$\rho_w NH_2$				
838 <sup>m</sup>	822	γ ΟΗ				832 vs,b	838 <sup>w</sup>	851	γΝ-Η…Ο
			747 <sup>sh</sup>	749	$\nu$ S-CH + $\delta$ C-	750 <sup>md</sup>	757 w	762	$\nu$ S-CH + $\delta$ C-C-C(CH <sub>2</sub> )
					C-C(CH <sub>2</sub> )				
737 <sup>m</sup>	752	γCH <sup>R</sup>				736 <sup>s</sup>	735 <sup>m</sup>	740	[γCH <sup>R</sup> ] <sup>ο-ΗVA</sup>
717 <sup>s</sup>	709	$\delta^{R}$				725 <sup>s</sup>		742	[δ <sup>R</sup> ] <sup>o-HVA</sup>
			698 <sup>s,b</sup>	707	γCH <sup>R</sup>	704 <sup>sh</sup>		710	[γCH <sup>R</sup> ] <sup>TPNH2</sup>
			616 <sup>w</sup>	628	δ <sup>R</sup>	615 <sup>vw</sup>	620 <sup>m</sup>	627	$[\delta^{R}]^{TPNH2}$

**Table S7.** Assignment of the experimental FTIR and Raman spectra of o-HVATPNH2 and calculated frequencies (cm<sup>-1</sup>). Reactants are included for comparison.

**References**: R: ring; v: stretching;  $\delta$ : in-plane deformation;  $\gamma$ . out-of-plane deformation;  $\rho_w$ : wagging;  $\rho_t$ : rocking;  $\rho_t$ : twisting; as: asymmetric; s: symmetric. Bands Intensities: vs: very strong; s: strong; m: medium; w: weak; vw: very weak; b: broad; sh: shoulder.







Figure S2.<sup>13</sup>C NMR spectrum of (o-VA)<sub>2</sub>TPNH2 in DMSO-d<sub>6</sub> at room temperature



Figura S3. <sup>1</sup>H-NMR spectrum of BS in CD<sub>3</sub>OD at 25°C



Figure S4. <sup>13</sup>C{<sup>1</sup>H}-NMR spectrum of BS in CD<sub>3</sub>OD at 25°



Figure S5. COSY-NMR spectrum of BS in CD<sub>3</sub>OD at 25°C



Figure S6. NOESY-NMR spectrum of BS in CD<sub>3</sub>OD at 25°C



Figure S7. Deconvolved absorption spectra of solid SB registered by DR in 200-700 nm region.