# The Crystal and Molecular Structure of *cis*-Dichloro[(*R*)-α-methylbenzylamine]-[(*S*)-1,2,2-trimethylpropyl (*R*)-vinyl ether|platinum(II)

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The crystal and molecular structure of the title compound has been determined by single-crystal threedimensional X-ray analysis. The crystals belong to the orthorhombic system, space group  $P_{2_12_12_1}$ , with  $a=25\cdot56(3)$ ,  $b=11\cdot37(1)$ ,  $c=6\cdot84(1)$  Å, Z=4. The structure, solved by standard methods, has been refined by full-matrix least-squares methods to a final conventional R index of 0.069, by use of 1764 independent reflexions collected by the Weissenberg method with Cu K $\alpha$  radiation. Chemical knowledge of the absolute configuration of the amine and vinyl ether indicated the absolute configuration of the whole molecule. The platinum atom has a square-planar configuration, but its principal coordination plane does not bisect the olefinic double bond, the midpoint of such a bond lying 0.38 Å above this plane. Furthermore the double bond is slightly displaced from the perpendicular to the coordination plane. While the molecules are held together only by van der Waals interactions, a hydrogen bond, which could play an important role in determining the conformation of the coordinated vinyl ether, links the nitrogen of the amine group and the oxygen atom.

### Introduction

The current interest in olefin-platinum complexes with optically active ligands stems largely from their utility in the study of stereospecific coordination phenomena.

After the solution, in our laboratory, of the structure of the trans-dichloro(benzylamine)[(2R, 3S)3-methyl-1pentene]platinum(II) complex (Merlino, Lazzaroni & Montagnoli, 1971), we undertook the investigation of the crystal and molecular structure of cis-dichloro- $[(R)-\alpha$ -methylbenzylamine] [(S)-1,2,2-trimethylpropylvinyl ether]platinum(II), for which also two diastereoisomers are possible. The n.m.r. spectra however gave evidence of the formation in the crystallization of only one of them, which probably represents the more stable one at least in the solid state. The purpose of this research was to establish its absolute configuration; the chemical knowledge of the configuration of two asymmetric groupings present in the molecule, besides the olefin asymmetric centre, made this determination possible (Mathieson, 1956).

Information about the conformation of the molecule in the solid state was briefly reported in a preliminary communication (Sartori, Leoni, Lazzaroni & Salvadori, 1974); the results of the full crystal structure investigation and refinement of the compound are reported here.

#### Experimental

As previously reported (Sartori *et al.*, 1974), the compound was prepared by displacement of ethylene with (S)-1,2,2-trimethylpropyl vinyl ether from the corresponding ethylene–Pt(II) complex. Beautiful air-stable yellow crystals were grown from solution in a mixture of acetone, diethyl ether and pentane (1:1:2). Most of them were blade-shaped, platy normal to **a**. From Weissenberg and precession photographs the space

group was determined as  $P2_12_12_1$ . The lattice constants were derived from least-squares refinement of powder diffraction data:  $a = 25.56 \pm 0.03$ ,  $b = 11.37 \pm 0.01$ , c = $6.84 \pm 0.01$  Å; V = 1988 Å<sup>3</sup>. The formula weight is 515.4 ( $C_{16}H_{27}NOCl_2Pt$ ); the density, measured at 20°C by flotation in a concentrated aqueous solution of ferric sulphate, is  $D_m = 1.70$  g cm<sup>-3</sup>; the calculated density is  $D_c = 1.72$  g cm<sup>-3</sup> for Z = 4. The linear absorption coefficient for Cu K $\alpha$  radiation ( $\lambda = 1.5418$  Å) is  $\mu = 159.4$  cm<sup>-1</sup>. The intensity data were recorded with nickel-filtered Cu Ka radiation by means of Weissenberg photographs, with the multiple-film technique and integration process. Seven layers with c as rotation axis (l=0 to 6) were recorded and 2294 independent reflexions (1764 observed) were collected. The intensities, measured with a Nonius microdensitometer, have been corrected for Lorentz and polarization factors and for incipient but incomplete  $\alpha_1 - \alpha_2$  spot doubling. The absorption correction was performed by computing the transmission factors by means of a program (Alberti, 1968) based on the Monte Carlo method proposed by Alberti & Gottardi (1966) for crystals of any shape and absorption; for this purpose the dimensions of the crystal used for intensity data collection (a small parallelepiped  $0.09 \times 0.16 \times 0.44$  mm in size, cleaved from a larger plate) were carefully measured under a microscope with a micrometer evepiece and its faces were identified. For this crystal and for the linear absorption coefficient of the compound the transmission coefficients were found to range from 0.11 to 0.35.

#### Determination and refinement of the structure

The position of the platinum atom was readily located from a three-dimensional Patterson synthesis. After a cycle of least-squares refinement of the Pt coordinates

# Table 1. Observed and calculated structure factors

Columns within each group contain the values h, 10  $F_o$ , 10 $|F_c|$  and  $\alpha$  (expressed in millicycles). Six reflexions, which are probably strongly affected by secondary extinction, are marked with an asterisk.

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3 688 628 250 6 1702 1767 500 5 602 518 230 8 1868 1950 500	1 672 667 750 3 331 321 750 4.0.1	1 1451 1067 767 2 402 363 224 3 1148 1217 752 4 195 250 789	10 444 603 0 14 322 306 500 21 348 426 500 23 234 202 500	13 424 403 769 14 424 452 402 15 256 256 884 16 683 701 474	• 1 dee 1111 424 • 2 1040 1314 781 3 1341 1482 836 • 1240 1367 882	17 457 476 234 18 412 416 775 20 407 435 775 22 304 334 411	24 146 234 0 25 144 176 0 26 198 254 0 20 234 245 0	23 228 275 73 28 184 180 4 25 182 184 82	2 640 326 123 3 626 608 66 6 337 336 101 3 1044 1064 20	• 220 242 700 ? 252 251 4 • 235 247 263 * 239 267 22	15 Jul Jan 25 16 176 188 241 17 203 241 36
7 J43 351 250 8 1858 1574 500 4 514 681 250 10 1014 1050 500	2 150 3 1544 750 3 1607 1743 250 4 171 134 250	5 717 646 141 6 676 636 747 7 336 376 941 8 322 303 778	24 200 201 500 20 372 375 500 20 213 353 500 300 141 220 500	17 100 240 477 10 304 307 443 14 349 300 477 21 314 341 445	5 1647 1822 809 6 1038 484 433 7 1447 1287 768 8 734 868 944	24 216 255 557 25 266 275 550 27 221 267 333	H=1+4 0 323 377 250	0 577 524 250 1 705 673 0	0 001 300 225 7 075 1000 11 0 724 003 011 7 737 728 070	10 163 235 146 11 173 207 66 14 136 150 122	 
11 525 474 150 12 405 Jun 500 14 859 012 0 18 852 786 0	5 10 Je 1042 250 9 444 504 750 10 J53 203 750 11 1407 2003 750	0 201 200 011 10 201 200 011 11 1111 1030 750 13 1300 1177 755	***** 0 50 550 750	24 274 143 464 24 306 307 475 26 350 375 467 26 230 306 476	4 1000 1005 200 13 859 621 126 13 863 105 202 14 768 728 198	4.7.3 0 4.4 444 750	2 405 700 47 3 746 424 34 4 451 411 43	2 807 527 100 3 702 253 37 4 500 510 132 5 404 405 134	11 416 300 411 12 365 333 460 16 403 410 24	0 520 524 750 - 347 431 232	5 205 107 002 6 616 675 760 7 214 411 616 7 200 636 766
20 244 473 0 21 424 375 750 22 644 640 0 23 344 314 750	15 1572 1873 755 17 402 834 750 14 204 185 750 22 130 332 250	17 711 661 215 10 604 356 166 20 203 160 166 21 270 274 205	2 422 1034 47 3 1115 1114 115 4 1845 1041 36 5 1631 1307 140	H.7.2 0 208 320 750 1 470 465 84	13 516 644 621 16 546 537 643 17 636 576 747 18 636 680 941	2 406 417 741 3 716 622 630 4 340 .30 642 5 760 726 640	546 334 800 7 546 334 800 8 1001 305 561 9 673 663 600	7 305 304 224 * 445 446 424 * 286 246 257 10 550 440 867	16 427 422 46 17 426 431 53 16 367 355 154 19 475 567 17	5 187 144 220 7 171 214 755 9 128 173 808 10 147 210 792	
24 405 343 0 30 206 194 500 H.0.0	23 444 442 253 24 149 222 250 25 541 113 210 27 461 456 253	25 368 393 241 27 378 364 240 29 251 473 229	• 1801 1738 33 7 1075 1047 234 • 1549 1041 445 • 403 874 860	2 643 615 31 3 661 612 134 4 767 777 26 3 779 766 223	14 742 ct1 767 20 345 356 55 21 551 126 216 22 240 301 142	6 514 446 33 7 451 44, 761 8 499 473 47 9 480 567 167 10 667 400 17	10 005 72 003 11 041 005 033 12 430 467 024 13 666 374 005 14 69 454	14 471 505 410 13 457 466 464 14 466 433 754 15 323 354 4	20 .00 274 225 21 343 620 402 22 362 141 741 23 237 246 406		- 410 4/2 750 - 410 4/2 759 - 231 /62 776 - 144 186 225
0 1764 1400 0 2 1261 1330 3 3 354 328 230 4 444 722 0	31 186 198 250 31 186 198 250	444 474 474 474 474 474 474 474 474 474	10 1002 1370 407 11 1070 1015 421 12 100 734 412 13 775 704 457 14 363 137 204	• 455 434 5 7 731 641 237 • 411 657 484 4 620 600 803	13 423 404 154 24 87 301 181 25 24 242 111 26 274 275 205	11 342 304 140 12 636 347 184 13 361 286 62 14 472 404 432	13 347 220 20 16 300 356 155 17 571 536 75 18 510 400 51	17 242 264 24 18 256 267 62 19 203 221 173 20 215 208 667	HIJID HIJID 1 403 460 31	- 135 172 500 J 565 675 0 5 883 406 0 6 173 151 0 7 846 836 3	12 230 217 234 12 217 378 247 14 217 378 247
5 364 338 250 6 341 416 0 7 485 400 230 8 400 424 200	0 446 766 253 1 418 864 772 2 401 854 857 3 1187 1284 257	3 072 016 240 6 1122 1066 052 5 1061 1021 7.7 6 1067 1022 567	15 644 653 62 16 643 644 63 17 546 546 134 14 636 676 26	11 524 531 003 14 624 363 966 13 393 377 969 15 376 317 40		15 240 207 424 16 300 340 405 17 5,7 334 633 16 367 432 673	10 415 415 110 20 416 420 5 22 265 310 417 24 128 186 400	21 170 170 700 22 102 2.1 901 13 140 107 000 24 175 200 057	J 704 647 17 6 663 J40 480 5 274 621 21 6 674 366 466	• 333 301 0 • 7e5 7e6 0 10 337 333 0 11 574 515 0	2 134 184 122 3 166 114 67 4 226 252 136 5 248 255 55
4 353 242 250 10 1001 1047 300 11 335 230 250 12 1044 1222 300 14 1174 1247 300	4 1001 1866 () 5 1600 1633 .C. 6 666 668 63 7 1605 1717 223 6 1286 1313 105	0 1044 1034 744 0 741 743 464 4 962 736 733 10 674 612 982 11 669 348 224	10 546 510 75. 20 723 736 976 21 651 667 616 22 560 566 963 23 756 368 900	10 330 205 03 17 330 207 105 18 630 607 56 19 257 273 108 20 606 616 67	3 1/48 2051 300 8 447 638 200 6 1448 201 143	20 306 225 915 21 306 275 915 21 76 310 236 22 140 210 1	27 146 246 185	 2 433 574 744	- 545 517 433 4 602 326 488 10 673 611 667 11 734 742 493	12 370 350 0 10 203 735 0 15 331 220 500 16 206 231 0	• 44.5 200 225 7 221 249 26 • 100 -53 235

by means of the full-matrix least-squares program of Busing, Martin & Levy, adapted for the X-RAY 70 System (Stewart, 1970), a difference Fourier synthesis revealed all the nonhydrogen atoms.

The knowledge of the absolute configuration of the amine and the vinyl ether used (R and S respectively), allowed us to choose, between the two possible enantiomorphous arrangements of the atoms, the solution corresponding to the correct absolute configuration of the whole molecule.

Three subsequent least-squares refinement cycles of positional coordinates and isotropic thermal parameters of all the non-hydrogen atoms yielded an agreement index  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.091$ . Two more refinement cycles, in which anisotropic temperature factors in the form  $\exp \{-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})\}$  were introduced for platinum and chlorine atoms, reduced the  $R_1$  value to 0.074.

During the later stages of refinements six reflexions (marked with an asterisk in Table 1) were excluded from further refinement because they are probably affected by secondary extinction.



Fig. 1. The molecular structure of *cis*-dichloro[(R)- $\alpha$ -methylbenzylamine] [(S)-1,2,2-trimethylpropyl (R)-vinyl ether]-platinum(II).

Moreover, while initially unit weights were assigned to all observed reflexions, at this point the following weighting scheme was introduced:  $1/w = 1.0/(A + F_o + BF_o^2)$ ; following the suggestions of Cruickshank (Stewart, 1970) that the coefficients A and B can be conveniently chosen as  $A = 2F_{\min}$  and  $B = 2/F_{\max}$ , we found most suitable for them the values A = 32.0, B = 0.005. A final analysis of the average  $w|\Delta F|^2$  as a function of  $|F_o|$  and  $\sin \theta$  showed in fact a smooth distribution indicating the validity of the weighting scheme.

The final R values obtained were  $R_1 = 0.069$  and  $R_2 = [\sum w ||F_o| - |F_c||^2 / \sum w ||F_o|^2]^{1/2} = 0.089$ . The shifts of the parameters in the last cycle were less than one tenth of the corresponding standard deviations.

The whole least-squares refinement process was performed without introduction of the hydrogen atoms. In a three-dimensional Fourier difference synthesis calculated at the end of the refinement only a few hydrogen atoms were in fact unequivocally located (among them the proton involved in an intramolecular hydrogen bond and some of those bonded to the carbons of the benzene ring), but for most of them the most reasonable positions were occupied by very smeared peaks or obscured by residual electron density from the heavier atoms.

The atomic scattering factors used in the structurefactor calculations were taken from *International Tables for X-ray Crystallography* (1962).

The observed and calculated structure factors are compared in Table 1. The final positional and thermal parameters are given in Table 2.

### Description and discussion of the structure

The molecular structure of the examined diastereoisomer is illustrated in Fig. 1, which shows a projection of the molecule onto the ab plane. The chiral centre of the coordinated vinyl group appears to have an absolute configuration R, and then the diastereoisomer is defined as RRS.

Table 2. Positional and thermal parameters for the nonhydrogen atoms

Standard deviations are given in parentheses. Values of the anisotropic thermal parameters for platinum and chlorine atoms are respectively multiplied by 10<sup>5</sup> and by 10<sup>4</sup>.

	x		у		Ζ	$\beta_{11}$	$\beta_{22}$	β	33	$\beta_{12}$		B13	1	$\beta_{23}$
Pt	0.0364	7 (4) 0.8	3667 (8)	0.2	8517 (14)	166 (1)	627 (5)	1823	(19)	23 (3)	1	5 (5)	1	1 (11)
CI(1)	0.0007	(3) 0.8	888 (6)	- 0·0	134 (10)	22 (1)	88 (5)	162	(15)	18 (2)		4 (3)	12	2 (8)
Cl(2)	-0.0455	(3) 0.7	832 (7)	<b>0</b> ∙4	061 (11)	17 (1)	104 (6)	214	(18)	-5 (2)		3 (3)	1:	5 (8)
	x	y	Z		B (Å <sup>2</sup> )		x		у		Z		<b>B</b> (Å	Ų)
C(1)	0.0729 (9)	0.6509 (24)	0.5770	(38)	3.82 (45)	C(10)	0.1009	(10)	0.9614	(23)	0.2399	(44)	<b>4·3</b> 7	(49)
$\tilde{C}(\tilde{2})$	0.0772(12)	0.6180 (29)	0.7955	(58)	5.68 (62)	C(11)	0.1147	(11)	1.1112	(25)	0.4995	(44)	4.42	(52)
Č(3)	0.1225(10)	0.6212(21)	0.4665	(40)	3.47 (43)	C(12)	0.0747	(17)	1.0847	(40)	0.6665	(73)	7.79	(95)
C(4)	0.1722(12)	0.6645 (31)	0.5230	(47)	5.31 (56)	C(13)	0.1631	(13)	1.1638	(35)	0.5637	(53)	6.08	(67)
$\hat{C}(5)$	0.2166 (14)	0.6300 (29)	0.4158	(55)	5.78 (72)	C(14)	0.1488	(14)	1.2889	(33)	0.6631	(58)	6.51	(80)
Č(6)	0.2115(14)	0.5586 (30)	0.2589	(57)	6.32 (72)	C(15)	0.1990	(22)	1.1727	(55)	0.3822	(95)	11.61	(1.58)
$\tilde{C}(\tilde{7})$	0.1624(13)	0.5148 (31)	0.2035	(59)	6.19 (67)	C(16)	0.1937	(22)	1.0898	3 (51)	0.7073	(100)	11.36	(1.53)
$\overline{C(8)}$	0.1178(11)	0.5466(24)	0.3010	(51)	4.79 (51)	N	0.0679	(9)	0.7809	) (20)	0.5615	(36)	4.20	(43)
C(9)	0.1122(11)	0.8563(23)	0.1644	(40)	4.40 (52)	0	0.1258	(7)	0.9921	(16)	0.4099	(28)	3.98	(33)

Table 3. Bond distances (Å) with their standard deviations

Pt - Cl(1)	2.315 (7)	C(6)—C(7)	1.40 (5)
Pt - Cl(2)	2.332 (7)	C(7) - C(8)	1.37 (5)
PtC(9)	2.12 (3)	C(8) - C(3)	1.42 (4)
PtC(10)	2.20(3)	C(9) - C(10)	1.33 (4)
Pt—X*	2.05 (3)	C(10)-O	1.37 (3)
Pt—N	2.15 (2)	0 C(11)	1.51 (3)
N - C(1)	1.49 (4)	C(11) - C(12)	1.56 (5)
C(1) - C(2)	1.54 (5)	C(11) - C(13)	1.44 (5)
C(1) - C(3)	1.52 (4)	C(13) - C(14)	1.62 (6)
C(3) - C(4)	1.42 (4)	C(13) - C(15)	1.55 (7)
C(4) - C(5)	1.41 (5)	C(13) - C(16)	1.51 (7)
C(5) - C(6)	1.35 (5)		

\* X defines the midpoint of the olefinic double bond.

Table 4. Bond angles with their standard deviations

Cl(1) - Pt Cl(2)	91°25 (16)'
Cl(1) - Pt - C(9)	89 26 (46)
Cl(1) - Pt - C(10)	90 23 (47)
$Cl(1) - Pt - X^*$	89 55 (49)
Cl(1) - Pt - N	177 26 (32)
Cl(2) - Pt - N	86 58 (38)
Cl(2) - Pt - C(9)	170 49 (44)
C(2) - Pt - C(10)	153 6 (43)
Cl(2) –Pt—X*	170 44 (48)
C(9) - Pt - C(10)	35 59 (60)
C(9)—Pt—N	91 50 (58)
C(10)-PtN	91 58 (58)
NX*	92 0 (59)
Pt - C(9) - C(10)	75 (1·ô°
Pt - C(10) - C(9)	69 (1.6)
C(9) - C(10) - O	117 (2.4)
C(10) - O - C(11)	119 (2)
$O_{}C(11) - C(12)$	104(2)
$O_{}C(11) - C(13)$	109 (2)
C(12) - C(11) - C(13)	115(3)
C(11) - C(13) - C(14)	107 (3)
$\mathbf{C}(11) - \mathbf{C}(13) - \mathbf{C}(15)$	107 (3)
C(1) - C(13) - C(16)	114 (3)
C(14) - C(13) - C(15)	114 (4)
C(15) - C(13) - C(16)	105 (4)
C(14) - C(13) - C(16)	109 (4)
N - C(1) - C(2)	108 (2)
N - C(1) - C(3)	105 (2)
C(2) - C(1) - C(3)	112 (2)
C(1) - C(3) - C(4)	122 (2)
$\vec{C}(1) - \vec{C}(3) - \vec{C}(8)$	117 (2)
C(3) - C(4) - C(5)	119 (3)
C(4) - C(5) - C(6)	120 (3)
C(5) - C(6) - C(7)	121 (3)
C(6) - C(7) - C(8)	121 (3)
C(7) - C(8) - C(3)	118 (3)
C(8) - C(3) - C(4)	120 (2)

\* X defines the midpoint of the olefinic double bond.

The bond distances are reported both in Fig. 1 and in Table 3, while the bond angles are listed in Table 4; finally some selected least-squares planes and the angles between pairs of them are given in Table 5. These structural parameters were calculated respectively by means of the programs *BONDLA* and *LSQPL*; both of them are incorporated in the 'Crystal Structure Calculations System X-RAY 70' (Stewart, 1970).

The bond distances concerning the platinum atom agree well with similar data available in the literature (Alderman, Owston & Rowe; 1960, Benedetti, Corradini & Pedone, 1969; Spagna & Zambonelli, 1971; Merlino et al., 1971; Cotton, Francis, Frenz & Tsutsui, 1973); among such distances it is interesting to observe that our platinum-chlorine bond lengths are, within the error limits, nearly equal, unlike other Pt-olefin complexes in which the bonds *trans* to the olefin appear significantly longer than the *cis* ones. Such equality is well explained by observing that in our compound one Pt-Cl bond is *trans* to the olefin while the other is *trans* to a N-bonded amine; in fact, the influence of modest  $\sigma$ -donor ligands such as N-bonded amines is comparable with that of modest  $\sigma$ -donors which are also  $\pi$ -acceptors such as olefins, both of them giving rise to trans Pt-Cl bond lengths up to 2.33 Å (Hartley, 1973).

The various ligand-Pt-ligand angles are typical of an almost undistorted square-planar configuration of the platinum atom; the second least-squares plane listed in Table 5 confirms that the atoms Pt, Cl(1), Cl(2) and N really lie in the same plane, since their



Fig. 2. Projection of the crystal structure of *cis*-dichloro[(R)- $\alpha$ -methylbenzylamine] [(S)-1,2,2-trimethylpropyl (R)-vinyl ether]platinum(II) along [001].

### Table 5. Parameters of some selected least-squares planes

The equation of the plane is in the form Ax + By + Cz = D, where x, y and z are fractional coordinates, calculated after Schomaker, Waser, Marsh & Bergman (1959).

Plane						
1	Atoms defining the plane C(3), C(4), C(5), C(6), C(7), C(8) Deviations: C(3), -0.007; C(4) 0	$ \begin{array}{r}     A \\     -3.0185 \\     .003; C(5) -0. \end{array} $	<i>B</i> 9·0180 004; C(6) 0·0	C -4.0868 008; C(7) - 0	D 3·3323 0·012; C(8) 0·0	011; C(1) −0·041 Å
2	Atoms defining the plane Pt, Cl(1), Cl(2), N Deviations: Pt 0.026; Cl(1) $-0.0$ The acute angle between plane 2 :	A - 3.1270 13; Cl(2) 0.000 and plane 1 is 2	<i>B</i> 10·5863 ; N - 0·014; 56·80°.	C 2·3510 X* 0·376; C	$     \begin{array}{r}       D \\       9.3876 \\       (9) - 0.287;       (9)       (9)      $	C(10) 1·039 Å
3	Atoms defining the plane Pt, N, C(1) The acute angles between plane 3	A 23.6463 and planes 1 a	<i>B</i> 0.5964 and 2 are 80.9	C - 2·5719 97 and 78·84	D 0.6279 ° respectively.	
4	Atoms defining the plane Pt, C(9), C(10) The acute angle between plane 4 a	A 10·3232 and plane 2 is 8	<i>B</i> - 3·1652 39·48°.	С 5·9605	D 0·5720	

\* X defines the midpoint of the olefinic double bond.

mean deviation from the plane is only 0.013 Å. On the other hand the mid-point of the olefin C(9)-C(10)double bond deviates by as much as 0.38 Å from the plane. Such a value, apart from the dramatically greater deviation of 0.59 Å reported for PtCl(acac) ( $H_2C=CHOH$ ) (where acac<sup>-</sup> is the acetylacetonate anion), is the highest of a series of deviations reported by Cotton et al. (1973) for platinum(II)  $\pi$ -complexes. The plane defined by the C(9)-C(10) double bond and by the Pt atom lies practically perpendicular to the plane of the square of coordination (dihedral angle  $89^{\circ}29'$ ); however, within the Pt, C(9), C(10) plane, the double bond appears slightly displaced ( $6^{\circ}20'$ ) from the perpendicular to the coordination plane. Furthermore, Table 5 shows that the Pt, N, C(1) plane deviates from perpendicularity to the Pt, Cl(1), Cl(2), N plane (dihedral angle 78° 50').

All the other distances and angles, not involving the Pt atom, are acceptable within the limits of the large standard deviations in the positional parameters of the lighter atoms. The atoms of the benzene ring lie in a plane (mean deviation from the best plane 0.017 Å), which appears to be inclined toward the Pt atom  $[C(3)\cdots Pt \text{ distance}=3.52 \text{ Å}]$  and contains also the C(1)-H bond. Finally the methyl group C(2) is in a quasi-*anti* position with respect to Pt.

Noteworthy is the presence of an intramolecular hydrogen bond between the nitrogen of the amine group and the oxygen atom, which can be inferred from the N···O distance as low as 3.00 Å. Such a bond is confirmed also by inspection of the  $\Delta F$  map in which the proton involved in this bond is one of the few hydrogen atoms clearly visible; from its coordinates (x=0.0961, y=0.8321, z=0.5476) we calculated distances N-H=0.93 Å and H···O=2.18 Å and an angle N-H-O=146°29', which are in a good agreement with the values reported for the N-H···O bond by Hamilton & Ibers (1968).

There are no hydrogen bonds between different molecules. Since all the intermolecular contacts cor-

respond to distances greater than 3.50 Å (the shortest intermolecular distance, 3.55 Å, being that of the contact between C(1) and the symmetry-equivalent  $[-x, y-\frac{1}{2}, \frac{1}{2}-z]$  of Cl(1)), we can conclude that the molecules of *cis*-dichloro[(*R*)- $\alpha$ -methylbenzylamine]-[(*S*)-1,2,2-trimethylpropyl (*R*)-vinyl ether]platinum(II) are held together only by van der Waals interactions.

A drawing of the molecular packing, as viewed along c, is given in Fig. 2.

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