

$$\sum_{hkl} w(kI_o - I_c)^2,$$

where $w = I_o^{-2}$. The formula

$$I = \text{const.}(Z-f)^2(\Sigma h_i^2)^{-3}\Sigma pF^2$$

was used to compute the values of the I_c . A plot of I_o/I_c versus Σh_i^2 showed no indication of any trend, consequently no temperature factor was used. The values of $(Z-f)$ were deduced by comparison of the values of I_c listed by Hörl & Marton and those calculated with the above formula at $x=0.0558$ omitting the factor $(Z-f)^2$.

The results are: $x=0.0530$, $\sigma=0.0020$. The corresponding N-N distance is 1.04 Å, $\sigma=0.04$ Å, a result which does not differ significantly from the spectroscopic value. Thermal anisotropy, which cannot be determined with the data at hand, may account for part or all of the discrepancy, or, it may be that stacking faults, mentioned as a possibility by Hörl & Marton, give rise to intensity differences which lead to an error in the positional parameter. The observed and calculated intensities, for $x=0.0530$, are presented in Table 1. These data yield $R_1=100\Sigma|I_o-I_c|/\Sigma I_o=34\%$. The value of R_1 for $x=0.0558$ is 39%. Fifteen of the reflections listed in Table 1 allow the calculation of $|F_o|$; for these

$$R = 100\Sigma||F_o - F_c|/|\Sigma|F_o|| = 17.6\%.$$

It is interesting that the minimum value of R , 17.4%, occurs at $x=0.0545$.

In this structure each nitrogen atom has, in addition to the one intramolecular neighbor at 1.04 Å, six neighbors at 3.60 Å and six at 3.65 Å in adjacent molecules. The intermolecular distances (at 20 °K.) are much larger than the value 3.0 Å implied by the usual van der Waals radius (Pauling, 1960).

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Unit cell and space group of cembrene. By JAMES A. IBERS, *Shell Development Company, Emeryville, California, U.S.A.*

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Cembrene, $C_{20}H_{32}$, is a diterpene found in the sap of the pine tree *Pinus albicaulis*. The crystals for this study were kindly supplied by Prof. W. G. Dauben of the University of California, Berkeley, and were used without further purification. The white crystals display a columnar habit. With precession photographs taken with copper K radiation filtered through nickel foil we have found the crystals to be orthorhombic with

$$a = 13.8 \pm 0.1, \quad b = 21.4 \pm 0.2, \quad c = 6.24 \pm 0.05 \text{ \AA}.$$

On these photographs the even orders from the respective pinacoids were observed up to $h=8$, $k=14$, and $l=4$, but no odd orders were observed. Reflections of all other types were present on the precession photographs of the

Table 1. *Diffraction data for α -nitrogen*

$(hkl)^*$	I_o^\dagger	I_c	(hkl)	I_o	I_c
111	18,000	14,178	420	75	37
200	2,250	5,553	421}	75	{ 2
210	375	482	412}	75	{ 60
211	525	606	332	75	68
220	3,000	1,702	422	<i>a</i>	14
221	225	177	430	300	204
311	1,050	1,043	431}	525	{ 16
222	225	283	413}	<i>a</i>	{ 328
230	600	407	333}	<i>a</i>	{ 4
321}	900	{ 610	511}	<i>a</i>	{ 4
312}		{ 31	250}		{ 76
400	<i>a</i>	26	432}	300	{ 166
322	375	264	423}		{ 5
411	75	125	521}	75	{ 125
331	75	92	512}		{ 0

* Space group extinctions, to which Hörl & Martin assigned the value zero for both I_o and I_c , are omitted.

† Values of Hörl & Martin modified by a scale factor of 1.50.

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$h0l$ and $0kl$ zones and on $hk0$ and hkl Weissenberg photographs. Hence the space group is probably $D_2^4-P2_12_12_1$. No test for a piezoelectric effect was made. The density measured by suspension of the crystals in a methanol-water gradient density column is 0.98 ± 0.01 g.cm.⁻³, in excellent agreement with a density of 0.98 g.cm.⁻³ calculated for four molecules in the unit cell.

This unit cell and space group determination was undertaken on the chance that such information might favor one of the several structures for cembrene proposed on the basis of chemical and physical evidence. This did not prove to be the case. Because of the size and complexity of the unit cell, no further work is contemplated on this structure.