

laboratory in order to clarify the stability and selectivity factors related to such complexes.

We thank the Bat-Sheva Foundation of Israel for financial support.

References

- ARTE, E., FENEAU-DUPONT, J., DECLERCQ, J.-P., GERMAIN, G. & VAN MEERSSCHE, M. (1979). *Acta Cryst.* B35, 1215–1217.
- BRÜGGE, H. J., FÖLSING, R., KNÖCHEL, A. & DREISSIG, W. (1985). *Polyhedron*, 4, 1493–1498.
- CAMBILLAU, C., BRAM, G., CORSET, J. & RICHE, C. (1982). *Can. J. Chem.* 60, 2554–2563.
- CRUICKSHANK, D. W. J. (1970). In *Crystallographic Computing*, edited by F. R. AHMED, pp. 187–197. Copenhagen: Munksgaard.
- DALLY, M. D. (1978). In *Synthetic Multidentate Macrocyclic Compounds*, edited by R. M. IZATT & J. J. CHRISTENSEN, pp. 207–243. New York: Academic Press.
- DEJEHET, F., DEBUYST, R., MULLIE, F., ARIETTA, J. M., GERMAIN, G. & VAN MEERSSCHE, M. (1983). *J. Chim. Phys.* 80, 355–362.
- DEJEHET, F., DEBUYST, R., SPIRLET, M., DECLERCQ, J.-P. & VAN MEERSSCHE, M. (1983). *J. Chim. Phys.* 80, 819–825.
- GROTH, P. (1981). *Acta Chem. Scand. Ser. A*, 35, 721–724.
- HARRISON, D., GIORGETTI, A. & BÜNZLI, J.-C. G. (1985). *J. Chem. Soc. Dalton Trans.* pp. 885–890.
- HILGENFELD, R. & SAENGER, W. (1982). In *Host Guest Complex Chemistry. II. Topics in Current Chemistry*, edited by F. L. BOSCHKE, Vol. 101, pp. 1–82. New York: Springer-Verlag.

- HOLT, E. M., ALCOCK, N. W., HENDRIXSON, R. R., MALPASS, G. D., GHIRARDELLI, R. G. & PALMER, R. A. (1981). *Acta Cryst.* B37, 1080–1085.
- JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- LEE, T.-J., HSIEH, J.-C., LEE, T.-Y., CHIU, C.-Y. & CHANG, C.-T. (1985). *Proc. Natl. Sci. Counc. Repub. Chin.(A)*, 9, 99–106.
- MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). *MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univ. of York, England, and Louvain, Belgium.
- MAVERICK, E., SEILER, P., SCHWEIZER, W. B. & DUNITZ, J. D. (1980). *Acta Cryst.* B36, 615–620.
- OWEN, J. D. (1980). *J. Chem. Soc. Dalton Trans.* pp. 1066–1075.
- PEDERSEN, C. J. (1967). *J. Am. Chem. Soc.* 89, 2495–2496, 7017–7036.
- POONIA, N. S. & BAJAV, A. V. (1979). *Chem. Rev.* 79, 389–445.
- RATH, P. & HOLT, E. M. (1985). *J. Chem. Soc. Chem. Commun.* pp. 665–667.
- SHANNON, R. D. (1976). *Acta Cryst.* A32, 751–767.
- SHELDRIK, G. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
- SHOHAM, G., CHRISTIANSON, D. W., BARTCH, R. A., HEO, G. S., OLSHER, U. & LIPSCOMB, W. N. (1984). *J. Am. Chem. Soc.* 106, 1280–1285.
- SHOHAM, G., LIPSCOMB, W. N. & OLSHER, U. (1983). *J. Am. Chem. Soc.* 105, 1247–1252.
- WEBER, E. & VÖGTLE, F. (1981). In *Host Guest Complex Chemistry. I. Topics in Current Chemistry*, edited by F. L. BOSCHKE, Vol. 98, pp. 1–41. New York: Springer Verlag.

Acta Cryst. (1989). C45, 1158–1161

The Structure of Tricarbonyl(styrene)chromium, a Crystal Active in Second-Harmonic Generation*

BY GEORGE M. BROWN

Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

AND CLAUDE C. FRAZIER

Martin Marietta Laboratories, Baltimore, Maryland 20742, USA

(Received 19 September 1988; accepted 11 January 1989)

Abstract. [Cr(CO)₃(C₆H₅CH=CH₂)], $M_r = 240.178$, orthorhombic, $P2_12_12_1$, $a = 11.5456(6)$, $b = 12.3227(9)$, $c = 7.3741(5)$ Å, $V = 1049.14(12)$ Å³, at 291 K. $\lambda(\text{Mo } K\alpha_1) = 0.70930$ Å; $Z = 4$, $D_x = 1.520$ g cm⁻³, $\mu = 10.44$ cm⁻¹, $F(000) = 488$. The absolute structure was determined. $R(F) = 0.029$ for 1306 data having $|F|_o^2 > \sigma(|F|_o^2)$; $\sigma_1 = 1.31$. The styrene ligand is disordered, with two orientations

relative to the Cr(CO)₃ group about equally populated. The Cr–CO linkages are nearly eclipsed with respect to Cr–C_{ring} bonds, in contrast to the staggered arrangement in tricarbonyl(benzene)chromium. The molecular orientation is far from optimal for second-harmonic generation, suggesting the possibility of successful crystal ‘engineering’ to produce an acentric crystal of a slightly modified compound with a much enhanced generating property.

*Research sponsored in part by the Division of Materials Sciences, Office of Basic Energy Sciences, US Department of Energy, under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

Introduction. Because of the important technical applications of second-harmonic generations (s.h.g.), there has been recent interest in the s.h.g. properties of

organometallic complexes of transition metals (Frazier, Harvey, Cockerham, Hand, Chauchard & Lee, 1986) and of their inclusion compounds in host crystals (Eaton, Anderson, Tam & Wang, 1987). Organic crystals efficient in second-harmonic generation are known to be acentric crystals of conjugated molecules having low-lying charge-transfer states. Because many transition-metal organic complexes involve conjugated ligands and show charge transfers, Frazier *et al.* (1986) surveyed the s.h.g. properties of about 60 such compounds, calling attention to the need for knowledge of their crystal structures in interpreting the results. Understanding of the structural basis of second-harmonic generation in such compounds may lead to the design of new crystalline and polymeric generators. This report describes the X-ray crystal-structure analysis of tricarbonyl(styrene)chromium, the compound included in the survey of Frazier *et al.* that showed the strongest s.h.g. signal strength, about 1.8 times that of ammonium dihydrogen phosphate.

Experimental. A specimen of the yellow crystals was selected that displayed all 12 faces of the forms $\{100\}$, $\{010\}$, $\{101\}$, and $\{110\}$ and had minimum and maximum diameters of 0.20 and 0.38 mm. All diffraction data were obtained with a Huber 5042 diffractometer with graphite monochromator. Cell parameters were from least-squares refinement based on 2θ , χ , and φ data for 40 resolved $\text{Mo } K\alpha_1$ peaks ($39.95 \leq 2\theta \leq 44.22^\circ$; hkl and $\bar{h}\bar{k}l$ on both sides of the 2θ zero for each of 10 different hkl triplets). The θ - 2θ scan method was used to collect 1580 intensity data to $2\theta = 55^\circ$, including 1403 independent reflections and some duplicates and equivalents. The index ranges were 0-14, 0-15 and 0-9 for h , k and l respectively. The intensity data were corrected for absorption by the Busing & Levy (1957) method using Gaussian integration, the extreme correction factors being 1.200 and 1.297.

The basic phase problem was solved immediately by the heavy-atom method, but refinement was complicated by disorder of orientation of the styrene ligand with respect to the $\text{Cr}(\text{CO})_3$ group. The nature of the disorder is shown in Fig. 1, which represents the final structure. To a first approximation, one of the 'fractional' ligands can be thought of as rotated with respect to the other by $\sim 25^\circ$ about the perpendicular to the ring through its center and then altered by rotation of the $\text{CH}=\text{CH}$ group by $\sim 180^\circ$ about the bond linking it to the ring. Corresponding atoms from the two fractional ligands, except $\text{C}(10A)$ and $\text{C}(10B)$, are formally too close together for successful least-squares refining of all the fractional-atom parameters independently; consequently, it was necessary to represent each of the fractional styrene ligands as a semi-rigid body, while treating the seven atoms of the $\text{Cr}(\text{CO})_3$ group in the usual way. The semi-rigid treatment of

each fractional styrene ligand was effected by application of constraints in the refinement as described by Busing (1971) and by defining extra parameters for direct least-squares refinement of some angles and interatomic distances characterizing the two ligands. The Oak Ridge least-squares program (Busing, Martin & Levy, 1962, 1980) was used. Each fractional styrene unit was constrained to have the following geometrical characteristics: $6/mmm$ symmetry for the C_6 ring; phenyl H atoms on bisectors of the C_6 ring exterior angles; vinyl group planar, with $\text{C}(4)-\text{C}(10)-\text{H}$ angle 125° , $\text{C}(10)-\text{C}(11)-\text{H}$ angles 125° ; $\text{C}(5)-\text{C}(4)-\text{C}(10)$ and $\text{C}(9)-\text{C}(4)-\text{C}(10)$ angles equal. The styrene molecular parameters directly adjusted were the following: for each C_6 ring, three coordinates for the centroid and three rotation angles; an out-of-ring-plane bending angle for each $\text{C}(4)-\text{C}(10)$ bond; the two angles $\text{C}(4)-\text{C}(10)-\text{C}(11)$; the two torsion angles $\text{C}(5)-\text{C}(4)-\text{C}(10)-\text{C}(11)$; the two bond lengths $\text{C}(4)-\text{C}(10)$; and, in common for both of the fractional styrene units, one ring $\text{C}-\text{C}$ bond length, one $\text{C}-\text{H}$ length, and one vinyl $\text{C}=\text{C}$ length. The sum of the occupancy factors of the two styrenes was constrained to the value unity. Each whole or fractional non-hydrogen atom was given the usual six anisotropic thermal parameters, and each H atom was given the same anisotropic thermal parameters as the atom bearing it.

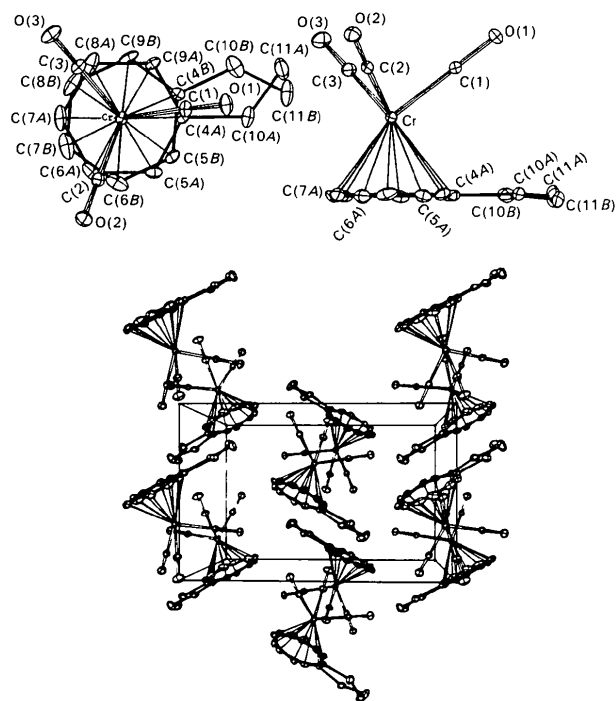


Fig. 1. (Top) Two views at right angles showing the disordered molecule of tricarbonyl(styrene)chromium. (Bottom) View of the crystal structure approximately in the $-b$ direction.

The scattering factors, including f' and f'' for Cr, were from *International Tables for X-ray Crystallography* (1974). The function minimized in refinement was $\sum w[|F|_o^2 - k^2|F|_c^2]$, where k is the scale factor on $|F|_c$ and w is the weight given by $w = 1/[\sigma^2(|F|_o^2) + 0.03|F|_o^2]$ and $\sigma^2(|F|_o^2)$ is the variance of $|F|_o^2$ from counting statistics. No extinction corrections were necessary. For damping of the parameter shifts, which was necessitated by the partial overlap of the styrene units, the diagonal elements of the least-squares matrix were multiplied by the factor 1.4 (see Rae, 1973; Levenberg, 1944). This alteration of the matrix causes the standard errors derived to be underestimated, perhaps by a factor as much as two.

No final parameter shift exceeded two-thirds of its apparent standard error. The final values of the usual measures of goodness of fit are as follows: $R(F)$, 0.029; $R(F^2)$, 0.035; $wR(F^2)$, 0.065; σ_1 , 1.297. The fact that the corresponding values (0.033, 0.042, 0.076, and 1.505) attained in refinement of the enantiomeric structure are all significantly higher shows that the structure reported is the correct absolute structure.

Table 1 contains the coordinates of the atoms and of the centroids of the two C_6 rings, along with the equivalent isotropic thermal parameters U_{eq} of the non-hydrogen atoms. Note that the coordinate e.s.d.'s given for atoms C(4A) through C(11B) are not values directly determined but values derived from the e.s.d.'s of the parameters refined for the semi-rigid ligands. Bond lengths and angles, including those directly adjusted in the refinement, are given in Table 2.* The two styrene orientations, *A* and *B*, are almost equally populated, having occupancy factors 0.491 (4) and 0.509 respectively.

Discussion. The normals to the two plane C_6 rings are at an angle of $1.6(2)^\circ$ to each other, and the angle between the two vectors $CG(A) \rightarrow C(4A)$ and $CG(B) \rightarrow C(4B)$ is $24.6(1)^\circ$. The distance $CG(A) - CG(B)$ is $0.057(6) \text{ \AA}$. Given the extent of overlapping of the two fractional ligands, the description of the disorder seems reasonably satisfactory. The geometry of the $Cr(CO)_3$ group and the relation of the group to each of the fractional styrene ligands is generally consistent with the structure of tricarbonyl(benzene)chromium as found by Bailey & Dahl (1965) at room temperature and by Rees & Coppens (1973) at 78 K, except that for each of the two fractional styrene C_6 rings three of the $Cr-C_{ring}$ bonds almost eclipse the three $Cr-C_{CO}$ bonds. In contrast, the two kinds of

Table 1. *Coordinates and equivalent isotropic thermal parameters U_{eq}*

Warning: parameter e.s.d.'s are underestimates (see text).

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

	x	y	z	$U_{eq}(\text{\AA}^2)$
Cr	0.46582 (3)	0.56530 (3)	0.31521 (5)	0.0491 (1)
O(1)	0.69702 (20)	0.67018 (23)	0.26410 (32)	0.102 (1)
O(2)	0.38166 (21)	0.71274 (18)	0.02205 (31)	0.086 (1)
O(3)	0.51795 (27)	0.40397 (17)	0.02464 (35)	0.109 (1)
C(1)	0.60866 (26)	0.62809 (25)	0.28414 (36)	0.066 (1)
C(2)	0.41313 (24)	0.65507 (22)	0.13655 (36)	0.059 (1)
C(3)	0.49870 (28)	0.46637 (23)	0.13708 (37)	0.069 (1)
C(4A)	0.48863 (25)	0.59049 (24)	0.61247 (37)	0.048 (1)
C(5A)	0.39002 (29)	0.64520 (25)	0.55697 (53)	0.065 (2)
C(6A)	0.30320 (28)	0.59012 (32)	0.46574 (54)	0.089 (3)
C(7A)	0.31498 (29)	0.48034 (32)	0.43001 (42)	0.104 (2)
C(8A)	0.41359 (34)	0.42563 (24)	0.48551 (51)	0.103 (3)
C(9A)	0.50041 (29)	0.48071 (25)	0.57674 (49)	0.059 (2)
C(10A)	0.58283 (55)	0.64996 (42)	0.70462 (77)	0.087 (2)
C(11A)	0.67675 (74)	0.60629 (95)	0.7691 (13)	0.137 (4)
C(4B)	0.50555 (27)	0.54975 (28)	0.60785 (37)	0.055 (1)
C(5B)	0.43547 (32)	0.63978 (24)	0.58343 (43)	0.063 (2)
C(6B)	0.33059 (32)	0.62957 (31)	0.49388 (53)	0.099 (3)
C(7B)	0.29580 (29)	0.52932 (36)	0.42874 (42)	0.116 (3)
C(8B)	0.36589 (35)	0.43929 (28)	0.45315 (46)	0.115 (3)
C(9B)	0.47076 (33)	0.44950 (24)	0.54271 (51)	0.079 (2)
C(10B)	0.61477 (55)	0.56059 (45)	0.69840 (71)	0.114 (3)
C(11B)	0.65758 (79)	0.64337 (82)	0.7849 (10)	0.129 (4)
CG(A)*	0.40180 (22)	0.53541 (22)	0.52124 (29)	
CG(B)*	0.40068 (24)	0.53954 (23)	0.51829 (29)	

* Centroids of the C_6 rings.

Table 2. *Bond lengths (\AA) and angles ($^\circ$)*

Cr—C(1)	1.836 (3)	Cr—C(8B)	2.186 (4)
Cr—C(2)	1.825 (3)	Cr—C(9B)	2.203 (4)
Cr—C(3)	1.832 (3)	C(1)—O(1)	1.154 (4)
Cr—C(4A)	2.230 (3)	C(2)—O(2)	1.162 (3)
Cr—C(5A)	2.217 (4)	C(3)—O(3)	1.153 (3)
Cr—C(6A)	2.203 (4)	Cr—CG(A)	1.729 (2)
Cr—C(7A)	2.201 (3)	Cr—CG(B)	1.705 (2)
Cr—C(8A)	2.214 (4)	C—C (ring)*	1.385 (1)
Cr—C(9A)	2.228 (3)	C=C (vinyl)*	1.30 (6)
Cr—C(4B)	2.215 (3)	C—H (all)*	0.83 (1)
Cr—C(5B)	2.209 (3)	C(4A)—C(10A)*	1.477 (6)
Cr—C(6B)	2.191 (4)	C(4B)—C(10B)*	1.433 (7)
Cr—C(7B)	2.180 (4)		
C(3)—Cr—C(1)	90.3 (1)	CG(B)—Cr—C(3)	126.7 (1)
C(1)—Cr—C(2)	87.4 (1)	C(4A)—C(10A)—C(11A)*	125.2 (5)
C(2)—Cr—C(3)	87.4 (1)	C(4B)—C(10B)—C(11B)*	129.5 (5)
CG(A)—Cr—C(1)	125.7 (1)	C(5A)—C(4A)—C(10A)* and	
CG(A)—Cr—C(2)	128.4 (1)	C(9A)—C(4A)—C(10A)*	120.0 (0)
CG(A)—Cr—C(3)	125.2 (1)	C(5B)—C(4B)—C(10B)* and	
CG(B)—Cr—C(1)	125.7 (1)	C(9B)—C(4B)—C(10B)*	120.0 (0)
CG(B)—Cr—C(2)	126.9 (1)		

Torsion angles

C(5A)—C(4A)—C(10A)—C(11A)*	177.0 (6)	Out-of-plane bends	
C(5B)—C(4B)—C(10B)—C(11B)*	8.9 (5)	C(4A)—C(10A) bond*	1.67 (7)
		C(4B)—C(10B) bond*	0.71 (5)

* These parameters were adjusted in the semi-rigid treatment of the 'fractional' styrene ligands in least-squares refinement.

bonds are almost exactly staggered in the benzene complex.

The principal purpose of this study was to relate the molecular properties and the crystal structure to the s.h.g. property. For tricarbonyl(benzene)chromium the outstanding spectral feature is a sharp intense band at

* Lists of F values, anisotropic thermal parameters, and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51816 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

31 220 cm⁻¹, attributed to metal-to-benzene charge transfer with some metal-to-CO charge transfer (Geoffroy & Wrighton, 1979). The net charge transfer in that molecule should be along the direction from the centroid of the (CO)₃ group through the chromium atom to the centroid of the six-membered ring, and there should be a similarly directed transfer in the styrene analog. It seems reasonable to assume that the tricarbonyl(styrene)chromium molecule is a 'one-dimensional' charge-transfer system with a single significant second-order molecular hyperpolarizability, β_{uuu} , in the direction indicated.

For a crystal of class 222 of such a molecule, symmetry and the Kleinman (1962) relations allow only a single macroscopic second-order hypolarizability coefficient, d_{xyz} . That coefficient has been shown by Zyss & Oudar (1982) to be proportional to the unique molecular hyperpolarizability coefficient and to the product $\sin\varphi\cos\varphi\cos\theta\sin^2\theta$, where φ and θ are spherical polar coordinates defining the orientation of the transfer vector with respect to Cartesian base vectors parallel to the unit-cell axes. The trigonometric function of φ and θ is equivalent to the product of the three direction cosines of the vector. For the disordered molecule of tricarbonyl(styrene)chromium in the crystal we take the transfer direction to be along the best least-squares line through the 12 atoms of the two fractional C rings and the seven atoms of the Cr(CO)₃ group. The direction cosines $\cos\theta_x$, $\cos\theta_y$, and $\cos\theta_z$ are -0.4121 (16), -0.2158 (18), and 0.8852 (7); and their product is 0.0787 (1), to be compared with the extreme or optimal values $\pm 1/3\sqrt{3} = \pm 0.1925$ of the cosine product, which correspond to values of $\arccos(\pm 1/\sqrt{3})$ for each of θ_x , θ_y , and θ_z (either 54.74 or 125.26° for each). The orientation of the tricarbonyl(styrene)chromium molecule clearly is not optimal for second-harmonic generation.

A more favorable orientation could have increased the magnitude of d_{xyz} by a factor as large as

$0.1925/0.0787 = 2.44$ and the efficiency of harmonic generation by as much as that factor squared, ~ 6 . It is therefore possible that so-called 'molecular and crystal engineering' can be used to produce a similar molecule with as good or better molecular polarizability properties in an acentric crystal in which the molecule has an orientation more favorable for efficient harmonic generation. The preference, of course, is for a crystal of one of the classes 2, *m* and *mm2*, for which with the same molecular polarizability there can in principle be one or more macroscopic polarizability coefficients with maximum magnitude twice that of the single coefficient allowed for class 222 (Zyss & Oudar, 1982) and therefore an increase in s.h.g. efficiency over that of the crystal used in this study by a factor of ~ 24 .

References

- BAILEY, M. & DAHL, L. F. (1965). *Inorg. Chem.* **4**, 1314–1319.
 BUSING, W. R. (1971). *Acta Cryst.* **A27**, 683–684.
 BUSING, W. R. & LEVY, H. A. (1957). *Acta Cryst.* **10**, 180–182.
 BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). *ORFLS. A Fortran Crystallographic Least-Squares Program*. Report TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
 BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1980). Program *XFLS4*. Revision of program *ORFLS*. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
 EATON, D. F., ANDERSON, A. G., TAM, W. & WANG, Y. (1987). *J. Am. Chem. Soc.* **109**, 1886–1888.
 FRAZIER, C. C., HARVEY, M. A., COCKERHAM, M. P., HAND, H. M., CHAUCHARD, E. A. & LEE, C. H. (1986). *J. Phys. Chem.* **90**, 5703–5706.
 GEOFFROY, G. L. & WRIGHTON, M. S. (1979). *Organometallic Photochemistry*, p. 59. New York: Academic Press.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
 KLEINMAN, D. A. (1962). *Phys. Rev.* **126**, 1977–1979.
 LEVENBERG, K. (1944). *Quart. App. Math.* **2**, 164–168.
 RAE, A. D. (1973). *Acta Cryst.* **A29**, 74–77.
 REES, B. & COPPENS, P. (1973). *Acta Cryst.* **B29**, 2515–2528.
 ZYSS, J. & OUDAR, J. L. (1982). *Phys. Rev. A*, **26**, 2028–2048.

Acta Cryst. (1989). **C45**, 1161–1164

Structure of 4-Methoxy-1-(*N*-phenyl)iminonaphthalene

BY ANTHONY LINDEN, T. STANLEY CAMERON AND JAMES W. HILBORN

Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, B3H 4J3, Canada

(Received 14 December 1988; accepted 4 January 1989)

Abstract. C₁₈H₁₅NO, $M_r = 261.32$, monoclinic, $P2_1/c$, $a = 10.280$ (2), $b = 16.731$ (3), $c = 8.027$ (1) Å, $\beta = 90.33$ (2)°, $V = 1380.4$ Å³, $Z = 4$, $D_x = 1.257$ g cm⁻³,

Mo $K\alpha$ radiation (graphite-monochromated), $\lambda = 0.70926$ Å, $\mu = 0.84$ cm⁻¹, $F(000) = 552$, $T = 293$ K, 2426 unique reflections, 915 with $I > 2\sigma(I)$, final

0108-2701/89/081161-04\$03.00

© 1989 International Union of Crystallography