mainly to the negative charge localized on the metal atom through coordination with the CO ligands. Of course, some delocalization of charge may be obtained by utilization of the *d*-orbital electrons of the metal in π-bonding with the empty antibonding MO's of the ligands. The strength of the Mn–Mn bond has been estimated as 34 ± 13 kcal.mol^{-1} (Cotton & Monchamp, 1960).

$Tc_2(CO)_{10}$ (Hileman *et al.*, 1961) has been shown (Trueblood & Wallach, 1961) to be isomorphous with $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$. A three-dimensional X-ray examination of $Tc_2(CO)_{10}$ is in progress (Fisher & Dahl, to be published) for the purpose of comparing its molecular features with those of the manganese and rhenium compounds. Other recently prepared isoelectronic dimeric species with presumably similar molecular configurations include

$[Cr_2(CO)_{10}]^{2-}$, $[Mo_2(CO)_{10}]^{2-}$, $[W_2(CO)_{10}]^{2-}$, $[Co_2(CN)_{10}]^{6-}$, and $[Co_2(CNCH_3)_{10}]^{4+}$.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

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A refinement of the crystal structure of sanidinized orthoclase. By P. H. Ribbe, *Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England*

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Introduction

The structure of sanidine, a monoclinic potash felspar, was first examined by Taylor (1933). In 1949 Cole, Sörum & Kennard published a full three-dimensional refinement of this structure, calling it 'sanidinized orthoclase' because the crystal they examined was orthoclase (Spencer's (1937) specimen 'C') irreversibly inverted to the form of natural sanidine by extended heat-treatment at 1000°C. Their paper contains details of the physical and chemical properties of this material. Because the hand-calculated atomic coordinates which they report for sanidine gave an R-factor $\Sigma||F_o|-|F_c||/\Sigma|F_o| = 0{\cdot}14$, it was thought worth while to press the refinement somewhat further, using their photometrically measured structure factors (Cole, 1949) and an automatic three-dimensional refinement program.

The need to know this structure with the maximum attainable accuracy arises from recent rapid advances in the knowledge of other felspar structures, notably those of celsian, microcline, maximum microcline, low albite, high albite, bytownite, primitive anorthite and transitional anorthite—all of which have been refined in three dimensions. In order that meaningful comparisons may be made amongst this extensive and petrogenetically important series of minerals, it is desirable to have the best possible structure data. This note presents an improved set of atomic coordinates, interatomic distances, and interbond angles for sanidinized orthoclase.

Experimental details and results

The calculations were carried out on EDSAC II computer at the University of Cambridge. An automatic refinement program employing difference-Fourier techniques (Wells, 1961) was used, and after a number of cycles the R-factor dropped from 0·119 to 0·099.*

Table 1. *Refined coordinates of atoms in the unit cell of sanidinized orthoclase*

Atom	No. in cell	Coordinates in decimal fractions of the unit cell x	y	z
$O_A(1)$	4	0	0·1472	0
$O_A(2)$	4	0·6343	0	0·2858
O_B	8	0·8273	0·1469	0·2253
O_C	8	0·0347	0·3100	0·2579
O_D	8	0·1793	0·1269	0·4024
Si_1	8	0·0097	0·1850	0·2233
Si_2	8	0·7089	0·1178	0·3444
K	4	0·2840	0	0·1352

Table 2. *Interatomic distances for sanidinized orthoclase*

	$Si_1(O_A(1))$	$Si_2(O_A(2))$
Si–O_A	1·643 Å	1·645 Å
Si–O_B	1·645	1·631
Si–O_C	1·647	1·645
Si–O_D	1·643	1·638
Mean	1·645 Å	1·640 Å
O_A–O_B	2·626 Å	2·686 Å
O_A–O_C	2·744	2·598
O_A–O_D	2·623	2·675
O_B–O_C	2·713	2·676
O_B–O_D	2·723	2·709
O_C–O_D	2·679	2·717
Mean	2·685 Å	2·675 Å

K–$O_A(1)$	2·910 Å
K–$O_A(2)$	2·707
K–O_B	3·017
K–O_C	3·140
K–O_D	2·953

* The discrepancy between the R-factor of 0·14 of Cole *et al.* (1949) and that of 0·119 is assumed to be due to the new approximation to the atomic scattering factor curves (Forsyth & Wells, 1959) used in these calculations.

Table 3. *Interbond angles for sanidinized orthoclase*

	$Si_1(O_A(1))$	$Si_2(O_A(2))$
O_A–Si–O_B	106° 01′	110° 07′
O_A–Si–O_C	113° 03′	104° 35′
O_A–Si–O_D	105° 54′	108° 47′
O_B–Si–O_C	111° 01′	109° 53′
O_B–Si–O_D	111° 47′	111° 31′
O_C–Si–O_D	109° 01′	111° 41′
Mean	109° 28′	109° 26′
Si_1–$O_A(1)$–Si_1	145° 07′	
Si_2–$O_A(2)$–Si_2		137° 52′
Si_1–O_B–Si_2	152° 17′	
Si_1–O_C–Si_2	131° 25′	
Si_1–O_D–Si_2	141° 40′	

The only significant changes in atomic parameters and, therefore, interatomic distances (Tables 1–3) were those effected by a shift of 0·057 Å in the z coordinate of the potassium ion. However, it is interesting to note that the tetrahedral group Si_1 (in which the larger Al atoms tend to be concentrated in the ordered potassium felspar, microcline) is in fact found to be slightly larger than the group Si_2, although according to the statistical tests for significance they must be considered to be the same size (as in Cole *et al.*, 1949).

A further refinement of the structure to $R=0{\cdot}095$ was achieved by increasing B in the temperature-factor expression $\exp[-B(\sin\theta/\lambda)^2]$ from the initial 1·9 $Å^2$ to 2·0 $Å^2$. This change is not considered to be significant.

The standard deviations of coordinates of all atoms were improved by $\sim 7\%$ compared with those reported by Cole, Sörum & Kennard (1949); the new values are not listed here.

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