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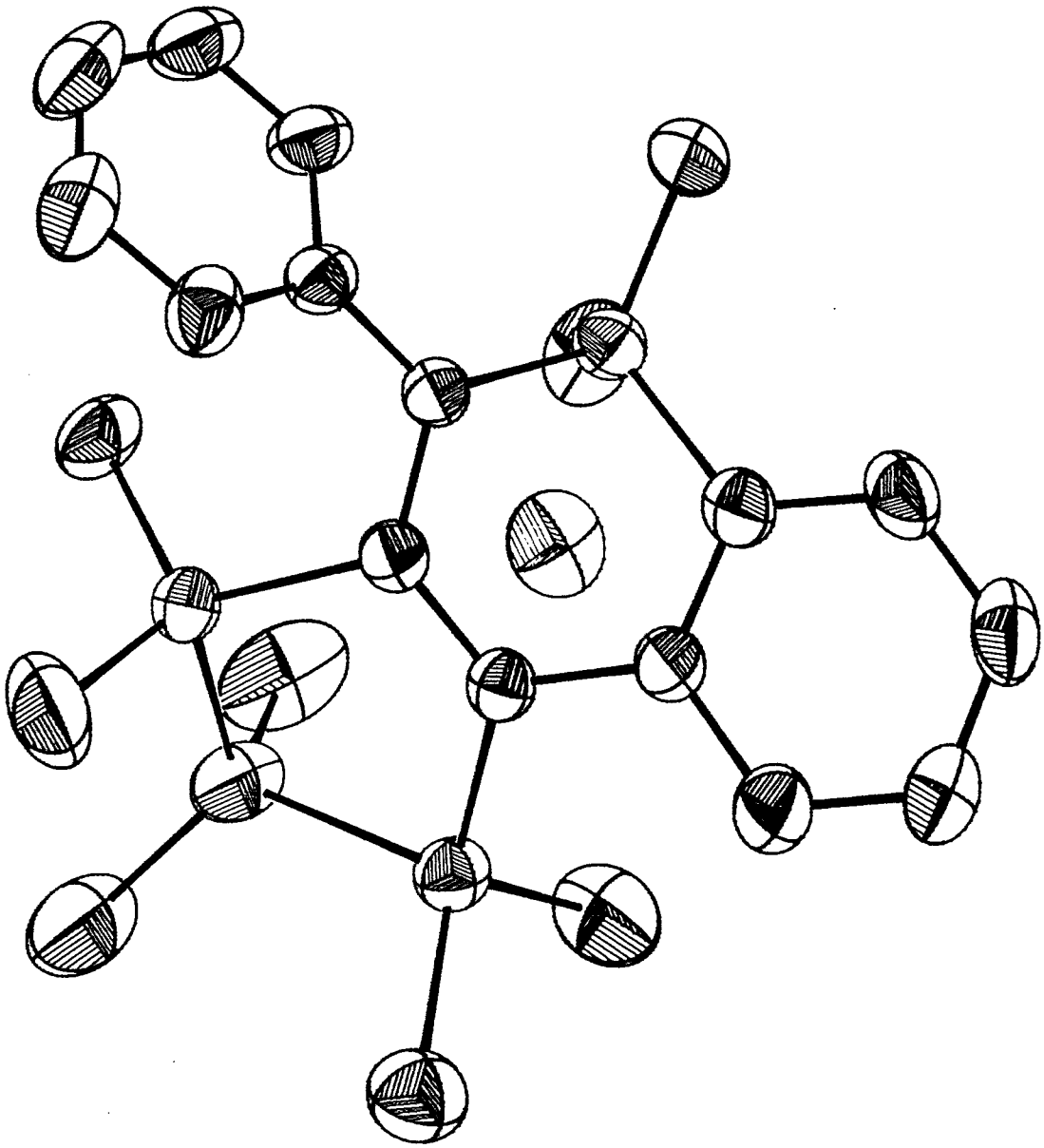

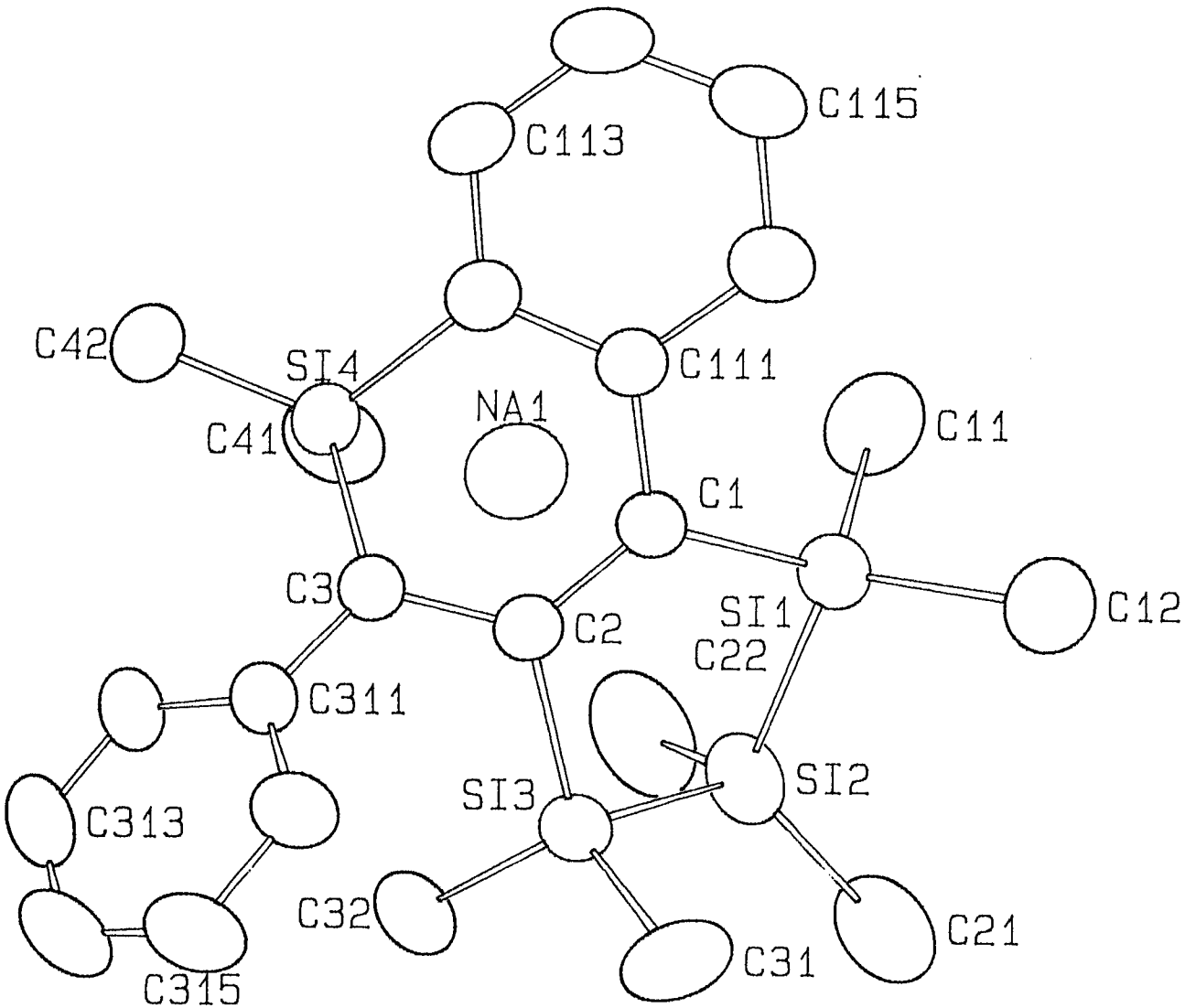
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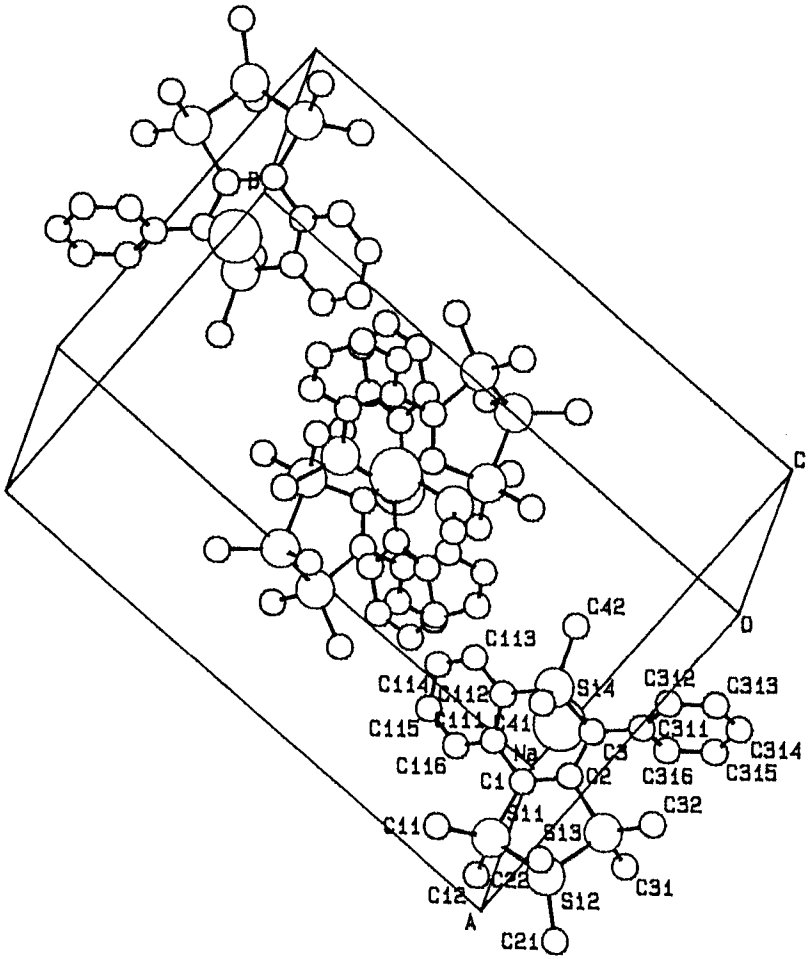
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C3
C316
C315
C1
C2
C32
C11
S11
S13
C22
C31
C12
S12
A
C21

HOJ02

Experimental

Data Collection

A colorless rod crystal of $C_{23}H_{33}Si_4Na$ having approximate dimensions of 0.20 x 0.30 x 0.30 mm was mounted in a glass capillary in a random orientation. Preliminary examination and data collection were performed with Mo Kα radiation (λ = 0.70930 Å) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal, incident beam monochromator.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 25 reflections in the range $10 < \theta < 13°$, measured by the computer controlled diagonal slit method of centering. The cubic cell parameters and calculated volume are: a = 11.491(1), b = 18.486(2), c = 12.723(1) Å, α = 90.00(1)°, β = 100.47(1), γ = 90.00(1) V = 2657.7 Å^3. For Z = 4 and F.W. = 444.85 the calculated density is 1.11g/cm^3. As a check on crystal quality, omega scans of several intense reflections were measured; the width at half-height was 0.00° with a take-off angle of 2.8°, indicating good crystal quality.From the systemtic absences of :

h01 : 1=2n

0k0 : k=2n

and from subsequent least-squares refinement, the space group was determeined to be $P2_1/c$ (#14).

The data were collected at a temperature of 23 ± 1 °C using the ω–θ scan technique. The scan rate varied from 1 to 20 °/min (in omega). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections where a slow scan rate is used. Data were collected to a maximum 2θ of 50.0°. The scan range (in deg.) was determined as a function of θ to correct for the separation of the kα doublet (ref 1); the scan width was calculated as follows:

$$\omega \text{ scan width} = 0.4 + 0.580 \tan\theta$$

Moving-crystal moving-counter background counts were made by scanning an additional 25% above and below this range. Thus the ratio of peak counting time to background counting time was 2:1. The counter aperture was also adjusted as a function of θ. The horizontal aperture width ranged from 1.3 to 1.6 mm; the vertical aperture was set at 4.0 mm. The diameter of the incident beam collimator was 0.7 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector; the attenuator factor was 13.4.

Data Reduction

A total of 9632 reflections were collected. of which 4828 were unique and not systematically absent. As a check on crystal and electronic stability 3 representative reflections were measured every 120 min. The slope of the least-squares line through a plot of intensity versus time was -1 ± 1 counts/hour which corresponds to a total loss in intensity of 12.7%. A linear decay correction was applied. The correction factors on I ranged from 1.000 to 1.071 with an average value of 1.032.

Lorentz and polarization corrections were applied to the data. The linear absorption coefficient is 2.4 cm^{-1} for Mo kα radiation. No absorption correction was made. An extinction correction was not necessary. Intensities of eqivalent reflections were averaged. The agreement factors for the averaging of the 6075 observed and accepted reflections was 2.4% based on intensity and 2.2% based on Fo.

Structure Solution and Refinement

The structure was solved by direct methods. Using 288 reflections (minimum E of 1.90) and 2672 relationships, a total 30 phase sets were produced. A total of 19 atoms were located from an E-map prepared from the phase set with probability statistics: absolutefigure of merit = 1.27, residual = 0.08, and psi zero = 1.406. The remaining atoms were located in succeeding difference Fourire syntheses and refined anisotropically. Hydrogen atoms were not included in the calculations. The structure was refined in full-matrix least-squares where the function minimized was $\Sigma w(|Fo|-|Fc|)^2$ and the weight w is defined as 1.0 for all observed reflections.

Scattering factors were taken from Cromer and Waber (ref 2). Anomalous dispersion effects were included in Fc (ref 3.); the values for $\Delta f'$ and $\Delta f''$ were those of Cromer (ref 4.). Only the 2888 reflections having intensities greater than 3.0 times their standard deviation were used in the refinements. The final cycle of refinement included 688 variable parameters and converged (largest parameter shift was 1.34 times is esd) with unweighted and weighted agreement factors of :

$$R_1 = \Sigma|Fo-Fc|/\Sigma|Fo| = 0.050$$

$$R_2 = SQRT(\Sigma w(Fo-Fc)^2/\Sigma wFo^2) = 0.063$$

The standard deviation of an observation of unit weight was 1.08. The highest peak in the final difference Fourier had a height of 0.31 e/Å^3 with an estimated error bsed on ΔF (ref5) of 0.06; the minimum negative peak had a height of 0.00 e/Å^3 with an estimated error bsed on ΔF of 0.06. Plots of $\Sigma w(|Fo|-|Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ, and various classes of indices showed no unusual trends.

All calculations were performed on a VAX computer using SDP/VAX (ref 6.).

References

(1) "CAD4 Operations Manual", Enraf-Nonius, Delft, 1977.

(2) D. T. Cromer and J. T. Waber, "International Tables for X-Ray Crystallography", vol. IV, The Kynoch Press, Birmingham, England, 1974, Table 2.2B.

(3) J. A. Ibers and W. C. Hamilton, Acta Crystallogr., 17, 781 (1964).

(4) D. T. Cromer, "International Tables for X-Ray Crystallography," Vol. IV, The Knoch Press, Birmingham, England, 1974, Table 2.3.1.

(5) D. W. J. Cruickshank, Acta Crystallogr., 2, 154 (1949).

(6) B. A. Frenz, "The Enraf-Nonius CAD 4 SDP-A Real-time System for Concurent X-Ray Data Colletion and Crystal Structure Determination," in Computing in Crystallography, H. Schenk, R. Olthof-Hazekamp, H. van Konoingsveld, and G. C. Bassi, Eds, Delft University Press. Delft, Holland, 1978, pp64-71.

Tables of Experimental Details

A. Crystal Data

$C_{23}H_{33}Si_4Na$

F.W. 444.844 F(000) = 952

crystal dimensions: 0.20 x 0.30 x 0.30 mm

Mo Kα radiation (λ = 0.70930 Å)

temperature = 23 ± 1 °C

monoclinic space group $P2_1/c$

a = 11.491 (1) Å b = 18.486 (1) Å c = 12.723 (1) Å

α = 90.00 (1) β = 100.47 (1) γ = 90.00 (1)°

v = 2657.7 $Å^3$

Z = 4 ρ = 1.11 g/cm^3

μ= 2.4 cm^{-1}

B. Intensity Measurements

Instruments:	Enraf-Nonius CAD4 diffractometer
Monochromator:	Graphite crystal, incident beam
Attenuator:	Zr foil, factor 13.4
Take-off angle:	2.8°
Detector aperture:	1.3 to 1.6 mm horizontal 4.0 mm vertical
Crystal-detector dist.:	21 cm
Scan type:	ω-θ
Scan rate:	1-20°/min (in omega)
Scan width, deg:	$0.4 + 0.580 \tan \theta$
Maximum 2θ	50.0°
No. of refl. measured:	9632 total, 4828 unique
Corrections:	Lorentz-polarization Linear decay (from 1.000 to 1.071 on I) Reflection averaging (agreement on I = 2.4%)

C. Structure Solution and Refinement

Solution:	Direct methods
Hydrogen atoms:	Located and refined isotropically
Refinement:	Block-diagonal least-squares
Minimization function:	$\Sigma w(\lvert Fo\rvert-\lvert Fc\rvert)^2$
Least-squares weights:	$4Fo^2/\sigma^2(Fo^2)$
Anomalous dispersion:	All non-hydrogen atoms
Reflections included:	2888 with $Fo^2>3.0\sigma(Fo^2)$
Parameters refined:	352
Unweighted agreement factor:	0.050
Weighted agreement factor:	0.063
Esd of Obs. of unit weight:	1.90
Convergence, largest shift:	1.34σ
High peak in final diff. map:	0.31 (6) e/Å^3
Low peak in final diff. map:	0.00 (0) e/Å^3
Computer hardware:	VAX
Computer software:	SDP/VAX (Enraf-Nonius & B. A. Frenz & Associates, Inc.)

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A2)
Si1	0.9425(1)	0.03842(9)	0.2738(1)	3.23(3)
Si2	0.8800(2)	-0.0555(1)	0.1561(1)	4.75(4)
Si3	0.7372(1)	-0.08799(9)	0.2545(1)	3.29(3)
Si4	0.5487(1)	0.11706(9)	0.2729(1)	3.51(3)
Na	0.6942(2)	0.0530(1)	0.5124(2)	4.37(5)
C1	0.8011(4)	0.0550(3)	0.3242(4)	2.7(1)
C2	0.7055(4)	0.0054(3)	0.3086(4)	2.5(1)
C3	0.5856(4)	0.0239(3)	0.3142(4)	2.7(1)
C11	0.9895(6)	0.1216(4)	0.2091(5)	5.6(2)
C12	1.0747(5)	0.0096(4)	0.3749(5)	4.5(1)
C21	0.9825(7)	-0.1318(5)	0.1381(7)	8.5(2)
C22	0.8089(8)	-0.0196(6)	0.0170(6)	8.5(3)
C31	0.8028(6)	-0.1572(4)	0.3585(6)	5.8(2)
C32	0.6083(5)	-0.1302(4)	0.1662(5)	4.7(1)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(A2)
C41	0.5463(7)	0.1293(4)	0.1262(5)	6.6(2)
C42	0.4047(6)	0.1537(4)	0.3019(6)	6.2(2)
C111	0.7873(4)	0.1278(3)	0.3684(4)	2.8(1)
C112	0.6771(4)	0.1650(3)	0.3531(4)	3.0(1)
C113	0.6724(5)	0.2330(3)	0.4015(5)	3.8(1)
C114	0.7693(5)	0.2644(3)	0.4630(5)	4.2(1)
C115	0.8753(5)	0.2284(3)	0.4786(5)	4.1(1)
C116	0.8841(5)	0.1620(3)	0.4330(4)	3.4(1)
C311	0.4990(4)	-0.0324(3)	0.3242(4)	2.9(1)
C312	0.3849(5)	-0.0333(3)	0.2619(5)	4.1(1)
C313	0.3103(5)	-0.0911(4)	0.2641(5)	5.2(2)
C314	0.3409(6)	-0.1493(4)	0.3279(5)	5.6(2)
C315	0.4497(6)	-0.1494(3)	0.3951(5)	5.0(1)
C316	0.5258(5)	-0.0911(3)	0.3944(4)	3.7(1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)]

Table of General Displacement Parameter Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
Si1	2.72(5)	3.68(6)	3.36(6)	-0.22(5)	0.71(4)	-0.28(6)	3.23(3)
Si2	3.76(7)	6.07(9)	4.62(7)	-0.48(7)	1.29(5)	-1.91(7)	4.75(4)
Si3	3.12(6)	3.04(6)	3.59(6)	-0.02(5)	0.31(5)	-0.73(6)	3.29(3)
Si4	3.13(6)	3.44(6)	3.74(6)	0.34(6)	0.06(5)	0.45(6)	3.51(3)
Na	5.0(1)	4.8(1)	3.26(9)	0.09(9)	0.76(8)	-0.14(9)	4.37(5)
C1	2.6(2)	2.7(2)	2.6(2)	-0.2(2)	0.3(2)	-0.4(2)	2.7(1)
C2	2.7(2)	2.7(2)	2.1(2)	0.1(2)	0.1(2)	-0.1(2)	2.5(1)
C3	2.6(2)	2.4(2)	2.9(2)	-0.1(2)	0.3(2)	-0.2(2)	2.7(1)
C11	6.0(3)	6.2(4)	4.9(3)	-1.2(3)	1.9(2)	0.6(3)	5.6(2)
C12	3.4(2)	5.1(3)	5.0(3)	0.3(2)	1.1(2)	-0.6(3)	4.5(1)
C21	5.6(3)	9.4(5)	11.5(5)	0.3(3)	4.0(3)	-4.4(4)	8.5(2)
C22	8.2(5)	12.1(7)	5.1(4)	0.8(5)	1.1(3)	-0.7(4)	8.5(3)
C31	5.7(3)	5.1(3)	6.2(4)	1.5(3)	-0.1(3)	1.5(3)	5.8(2)
C32	4.7(3)	5.4(3)	4.0(2)	-1.1(3)	1.0(2)	-1.8(2)	4.7(1)

Table of General Anisotropic Displacment Parameter Expressions - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C41	8.6(4)	6.7(4)	4.2(3)	0.4(4)	0.2(3)	2.4(3)	6.6(2)
C42	3.7(3)	6.9(4)	7.6(4)	1.8(3)	-0.1(3)	0.1(3)	6.2(2)
C111	2.8(2)	2.5(2)	3.1(2)	-0.2(2)	0.7(2)	0.1(2)	2.8(1)
C112	3.3(2)	2.5(2)	3.4(2)	-0.1(2)	0.7(2)	0.5(2)	3.0(1)
C113	4.0(2)	2.7(2)	4.8(3)	0.4(2)	1.2(2)	0.5(2)	3.8(1)
C114	5.3(3)	2.4(2)	5.2(3)	-0.5(2)	1.5(2)	-0.6(2)	4.2(1)
C115	4.0(2)	3.3(2)	4.9(3)	-1.2(2)	0.5(2)	-0.6(2)	4.1(1)
C116	3.2(2)	3.3(2)	3.9(2)	-0.4(2)	0.7(2)	-0.2(2)	3.4(1)
C311	3.0(2)	2.8(2)	3.2(2)	-0.2(2)	0.9(2)	-0.5(2)	2.9(1)
C312	3.1(2)	4.7(3)	4.4(3)	-0.5(2)	0.6(2)	-0.7(2)	4.1(1)
C313	3.4(2)	6.9(4)	5.6(3)	-1.3(3)	1.2(2)	-2.2(3)	5.2(2)
C314	5.6(3)	5.1(3)	7.0(3)	-2.9(2)	3.3(2)	-2.4(3)	5.6(2)
C315	7.2(3)	3.5(3)	5.0(3)	-1.1(2)	3.2(2)	-0.4(2)	5.0(1)
C316	4.1(2)	3.4(2)	3.9(2)	-0.5(2)	1.2(2)	-0.5(2)	3.7(1)

The form of the anisotropic displacement parameter is:
exp[-0.25{h2a2B(1,1) + k2b2B(2,2) + l2c2B(3,3) + 2hkabB(1,2) + 2hlacB(1,3) + 2klbcB(2,3)}] where a,b, and c are reciprocal lattice constants.

Table of Refined Displacement Parameter Expressions - Beta's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
Si1	0.0053(1)	0.00269(5)	0.00536(9)	-0.0005(1)	0.0025(2)	-0.0006(1)
Si2	0.0074(1)	0.00443(7)	0.0074(1)	-0.0012(2)	0.0046(2)	-0.0041(2)
Si3	0.0061(1)	0.00222(4)	0.0057(1)	-0.0001(1)	0.0011(2)	-0.0016(1)
Si4	0.0061(1)	0.00251(5)	0.0060(1)	0.0008(1)	0.0002(2)	0.0010(1)
Na	0.0098(2)	0.00354(8)	0.0052(1)	0.0002(2)	0.0027(3)	-0.0003(2)
C1	0.0051(4)	0.0020(2)	0.0041(3)	-0.0005(4)	0.0010(5)	-0.0008(4)
C2	0.0053(4)	0.0020(2)	0.0033(3)	0.0003(4)	0.0004(5)	-0.0002(4)
C3	0.0052(4)	0.0018(2)	0.0046(3)	-0.0003(4)	0.0009(6)	-0.0005(4)
C11	0.0118(6)	0.0046(3)	0.0078(5)	-0.0028(7)	0.0069(9)	0.0013(6)
C12	0.0067(5)	0.0038(2)	0.0079(4)	0.0006(6)	0.0038(7)	-0.0014(6)
C21	0.0109(6)	0.0069(4)	0.0185(7)	0.0006(8)	0.014(1)	-0.0096(8)
C22	0.0161(9)	0.0089(5)	0.0081(6)	0.002(1)	0.004(1)	-0.0014(9)
C31	0.0112(7)	0.0038(2)	0.0099(6)	0.0037(7)	-0.000(1)	0.0032(6)
C32	0.0092(5)	0.0040(2)	0.0065(4)	-0.0027(6)	0.0037(8)	-0.0038(5)

Table of Refined Displacement Parameter Expressions - Beta's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)
C41	0.0168(8)	0.0049(3)	0.0067(5)	0.0009(9)	0.001(1)	0.0053(6)
C42	0.0072(5)	0.0050(3)	0.0122(6)	0.0042(7)	-0.000(1)	0.0003(8)
C111	0.0055(4)	0.0019(2)	0.0049(3)	-0.0005(4)	0.0026(6)	0.0003(4)
C112	0.0064(4)	0.0019(2)	0.0054(3)	-0.0003(4)	0.0026(6)	0.0010(4)
C113	0.0079(5)	0.0020(2)	0.0077(4)	0.0009(5)	0.0043(7)	0.0012(5)
C114	0.0104(5)	0.0017(2)	0.0083(4)	-0.0013(5)	0.0052(8)	-0.0013(5)
C115	0.0079(5)	0.0024(2)	0.0078(4)	-0.0029(5)	0.0019(8)	-0.0014(5)
C116	0.0063(4)	0.0024(2)	0.0062(4)	-0.0009(5)	0.0025(6)	-0.0005(4)
C311	0.0058(4)	0.0021(2)	0.0051(3)	-0.0004(4)	0.0033(6)	-0.0011(4)
C312	0.0061(4)	0.0034(2)	0.0071(4)	-0.0013(5)	0.0022(7)	-0.0016(5)
C313	0.0067(5)	0.0051(3)	0.0089(5)	-0.0032(6)	0.0042(8)	-0.0047(6)
C314	0.0110(5)	0.0037(2)	0.0111(5)	-0.0070(6)	0.0117(8)	-0.0051(6)
C315	0.0141(6)	0.0025(2)	0.0081(4)	-0.0027(6)	0.0112(8)	-0.0008(5)
C316	0.0080(5)	0.0025(2)	0.0062(4)	-0.0011(5)	0.0042(7)	-0.0012(5)

The form of the anisotropic displacement parameter is:
exp[-(B(1,1)*h2 + B(2,2)*k2 + B(3,3)*l2 + B(1,2)*hk + B(1,3)*hl
+ B(2,3)*kl)].

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Si1	0.0345(7)	0.0466(8)	0.0425(7)	-0.0028(7)	0.0089(6)	-0.0036(7)
Si2	0.0476(8)	0.077(1)	0.0585(9)	-0.0061(9)	0.0163(7)	-0.0242(9)
Si3	0.0395(7)	0.0384(7)	0.0455(8)	-0.0003(7)	0.0040(6)	-0.0093(7)
Si4	0.0396(7)	0.0435(8)	0.0474(8)	0.0043(7)	0.0007(7)	0.0057(7)
Na	0.063(1)	0.061(1)	0.041(1)	0.001(1)	0.010(1)	-0.002(1)
C1	0.033(2)	0.034(3)	0.033(2)	-0.003(2)	0.003(2)	-0.004(2)
C2	0.034(2)	0.035(3)	0.026(2)	0.002(2)	0.001(2)	-0.001(2)
C3	0.033(2)	0.031(3)	0.036(2)	-0.001(2)	0.003(2)	-0.003(2)
C11	0.076(4)	0.079(5)	0.062(4)	-0.015(4)	0.025(3)	0.008(4)
C12	0.043(3)	0.065(4)	0.063(3)	0.003(3)	0.014(3)	-0.008(3)
C21	0.070(4)	0.120(6)	0.146(6)	0.003(4)	0.051(4)	-0.056(5)
C22	0.104(6)	0.154(8)	0.064(5)	0.010(6)	0.014(4)	-0.008(5)
C31	0.073(4)	0.065(4)	0.079(4)	0.019(4)	-0.001(4)	0.019(4)
C32	0.059(3)	0.069(4)	0.051(3)	-0.014(3)	0.013(3)	-0.023(3)

Table of General Anisotropic Displacement Parameter Expressions - U's (Continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C41	0.109(5)	0.084(5)	0.053(4)	0.005(5)	0.002(4)	0.031(4)
C42	0.046(3)	0.087(5)	0.096(5)	0.022(4)	-0.001(4)	0.002(4)
C111	0.035(2)	0.032(3)	0.039(2)	-0.003(2)	0.009(2)	0.002(2)
C112	0.042(3)	0.032(3)	0.042(3)	-0.002(2)	0.009(2)	0.006(2)
C113	0.051(3)	0.034(3)	0.061(3)	0.005(3)	0.015(3)	0.007(3)
C114	0.067(3)	0.030(3)	0.066(3)	-0.007(3)	0.019(3)	-0.008(3)
C115	0.051(3)	0.041(3)	0.061(3)	-0.015(3)	0.007(3)	-0.008(3)
C116	0.040(3)	0.042(3)	0.049(3)	-0.005(2)	0.009(2)	-0.003(3)
C311	0.037(2)	0.036(3)	0.040(2)	-0.002(2)	0.012(2)	-0.006(2)
C312	0.039(3)	0.059(4)	0.056(3)	-0.007(3)	0.008(2)	-0.009(3)
C313	0.043(3)	0.088(5)	0.070(4)	-0.017(3)	0.015(3)	-0.027(4)
C314	0.071(3)	0.064(4)	0.088(4)	-0.037(3)	0.042(3)	-0.030(3)
C315	0.091(4)	0.044(3)	0.064(3)	-0.014(3)	0.040(3)	-0.005(3)
C316	0.052(3)	0.043(3)	0.049(3)	-0.006(3)	0.015(2)	-0.007(3)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Table of Root-Mean-Square Amplitudes of Anisotropic Displacement in Angstroms

Atom	Min.	Int'med.	Max.
Si1	0.183	0.201	0.221
Si2	0.198	0.217	0.307
Si3	0.178	0.199	0.231
Si4	0.181	0.215	0.233
Na	0.202	0.247	0.253
C1	0.166	0.189	0.195
C2	0.159	0.183	0.195
C3	0.169	0.183	0.198
C11	0.211	0.275	0.304
C12	0.200	0.239	0.269
C21	0.198	0.306	0.437
C22	0.251	0.320	0.396
C31	0.198	0.297	0.308
C32	0.188	0.233	0.297
C41	0.183	0.319	0.340
C42	0.188	0.306	0.327
C111	0.171	0.191	0.200
C112	0.168	0.204	0.213
C113	0.179	0.219	0.254
C114	0.167	0.242	0.272
C115	0.171	0.248	0.254
C116	0.191	0.210	0.225
C311	0.174	0.187	0.216
C312	0.193	0.226	0.259
C313	0.193	0.229	0.331
C314	0.174	0.227	0.362
C315	0.194	0.214	0.325
C316	0.196	0.209	0.244

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
Si2	Si1	C1	99.1(2)	C41	Si4	C112	110.9(3)
Si2	Si1	C11	114.3(2)	C42	Si4	C112	110.9(3)
Si2	Si1	C12	110.2(2)	C2	Na	C3	30.6(1)
C1	Si1	C11	110.6(3)	C2	Na	C111	55.2(2)
C1	Si1	C12	117.0(3)	C3	Na	C111	68.4(2)
C11	Si1	C12	105.8(3)	Si1	C1	C2	122.9(4)
Si1	Si2	Si3	90.65(9)	Si1	C1	C111	116.0(3)
Si1	Si2	C21	120.9(3)	C2	C1	C111	120.6(4)
Si1	Si2	C22	111.4(3)	Si3	C2	Na	131.9(2)
Si3	Si2	C21	113.1(3)	Si3	C2	C1	116.2(4)
Si3	Si2	C22	111.3(3)	Si3	C2	C3	118.7(3)
C21	Si2	C22	108.5(4)	Na	C2	C1	80.2(3)
Si2	Si3	C2	99.2(2)	Na	C2	C3	70.6(3)
Si2	Si3	C31	108.8(2)	C1	C2	C3	124.4(4)
Si2	Si3	C32	110.2(2)	Si4	C3	Na	97.3(2)
C2	Si3	C31	115.8(3)	Si4	C3	C2	112.7(4)
C2	Si3	C32	114.4(2)	Si4	C3	C311	124.8(3)
C31	Si3	C32	108.1(3)	Na	C3	C2	78.8(3)
C3	Si4	C41	111.2(3)	Na	C3	C311	105.8(3)
C3	Si4	C42	116.6(3)	C2	C3	C311	120.6(4)
C3	Si4	C112	99.9(2)	Na	C111	C1	82.7(3)
C41	Si4	C42	107.3(3)	Na	C111	C112	83.5(3)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
Na	C111	C116	101.8(3)	C111	C116	C115	122.6(5)
C1	C111	C112	122.9(4)	C3	C311	C312	122.7(5)

C1	C111	C116	120.2(4)	C3	C311	C316	122.1(4)
C112	C111	C116	116.9(5)	C312	C311	C316	115.1(5)
Si4	C112	C111	116.2(4)	C311	C312	C313	121.3(5)
Si4	C112	C113	125.3(4)	C312	C313	C314	122.3(5)
C111	C112	C113	118.4(4)	C313	C314	C315	118.7(6)
C112	C113	C114	122.6(5)	C314	C315	C316	119.7(6)
C113	C114	C115	119.0(5)	C311	C316	C315	122.6(5)
C114	C115	C116	120.4(5)				

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Si1	Si2	2.320(2)	C1	C2	1.417(7)
Si1	C1	1.875(5)	C1	C111	1.479(7)
Si1	C11	1.871(8)	C2	C3	1.433(7)
Si1	C12	1.879(6)	C3	C311	1.460(7)
Si2	Si3	2.316(3)	C111	C112	1.421(7)
Si2	C21	1.877(9)	C111	C116	1.406(7)
Si2	C22	1.926(8)	C112	C113	1.405(8)
Si3	C2	1.917(5)	C113	C114	1.367(8)
Si3	C31	1.895(7)	C114	C115	1.369(8)
Si3	C32	1.859(6)	C115	C116	1.370(8)
Si4	C3	1.828(5)	C311	C312	1.402(7)
Si4	C41	1.874(7)	C311	C316	1.404(7)
Si4	C42	1.884(7)	C312	C313	1.373(9)
Si4	C112	1.858(5)	C313	C314	1.35(1)
Na	C2	2.763(5)	C314	C315	1.379(8)
Na	C3	2.656(5)	C315	C316	1.388(9)
Na	C111	2.669(6)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Torsion Angles in Degrees

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C1	Si1	Si2	Si3	-26.23 (0.17)
C1	Si1	Si2	C21	-143.85 (0.36)
C1	Si1	Si2	C22	86.96 (0.34)
C11	Si1	Si2	Si3	-143.88 (0.25)
C11	Si1	Si2	C21	98.49 (0.41)
C11	Si1	Si2	C22	-30.69 (0.39)
C12	Si1	Si2	Si3	97.08 (0.21)
C12	Si1	Si2	C21	-20.54 (0.39)
C12	Si1	Si2	C22	-149.72 (0.35)
Si2	Si1	C1	C2	14.89 (0.41)
Si2	Si1	C1	C111	-156.83 (0.33)
C11	Si1	C1	C2	135.27 (0.42)
C11	Si1	C1	C111	-36.44 (0.44)
C12	Si1	C1	C2	-103.44 (0.44)
C12	Si1	C1	C111	84.84 (0.43)
Si1	Si2	Si3	C2	30.47 (0.16)
Si1	Si2	Si3	C31	-90.86 (0.24)
Si1	Si2	Si3	C32	150.80 (0.23)
C21	Si2	Si3	C2	154.78 (0.33)
C21	Si2	Si3	C31	33.45 (0.38)
C21	Si2	Si3	C32	-84.89 (0.37)
C22	Si2	Si3	C2	-82.84 (0.37)
C22	Si2	Si3	C31	155.83 (0.40)
C22	Si2	Si3	C32	37.49 (0.41)
Si2	Si3	C2	Na	-130.46 (0.26)
Si2	Si3	C2	C1	-29.73 (0.36)
Si2	Si3	C2	C3	140.61 (0.35)
C31	Si3	C2	Na	-14.34 (0.42)
C31	Si3	C2	C1	86.38 (0.43)
C31	Si3	C2	C3	-103.28 (0.43)
C32	Si3	C2	Na	112.30 (0.33)
C32	Si3	C2	C1	-146.97 (0.37)
C32	Si3	C2	C3	23.36 (0.46)
C41	Si4	C3	Na	149.11 (0.30)
C41	Si4	C3	C2	68.21 (0.45)
C41	Si4	C3	C311	-95.93 (0.49)
C42	Si4	C3	Na	-87.54 (0.32)
C42	Si4	C3	C2	-168.43 (0.39)
C42	Si4	C3	C311	27.43 (0.54)
C112	Si4	C3	Na	32.02 (0.23)
C112	Si4	C3	C2	-48.88 (0.39)
C112	Si4	C3	C311	146.99 (0.42)
C3	Si4	C112	C111	34.94 (0.43)
C3	Si4	C112	C113	-143.12 (0.47)
C41	Si4	C112	C111	-82.37 (0.47)
C41	Si4	C112	C113	99.57 (0.53)
C42	Si4	C112	C111	158.55 (0.42)

Table of Torsion Angles in Degrees (continued)

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C42	Si4	C112	C113	-19.52	(0.58)
C3	Na	C2	Si3	-111.54	(0.43)
C3	Na	C2	C1	131.95	(0.43)
C111	Na	C2	Si3	141.31	(0.36)
C111	Na	C2	C1	24.80	(0.27)
C111	Na	C2	C3	-107.15	(0.32)
C2	Na	C3	Si4	-111.75	(0.35)
C2	Na	C3	C311	118.90	(0.45)
C111	Na	C3	Si4	-54.23	(0.19)
C111	Na	C3	C2	57.53	(0.28)
C111	Na	C3	C311	176.43	(0.35)
C2	Na	C111	C1	-23.54	(0.25)
C2	Na	C111	C112	100.86	(0.32)
C2	Na	C111	C116	-142.96	(0.38)
C3	Na	C111	C1	-55.09	(0.27)
C3	Na	C111	C112	69.31	(0.29)
C3	Na	C111	C116	-174.51	(0.37)
Si1	C1	C2	Si3	10.36	(0.53)
Si1	C1	C2	Na	142.46	(0.34)
Si1	C1	C2	C3	-159.36	(0.38)
C111	C1	C2	Si3	-178.29	(0.35)
C111	C1	C2	Na	-46.19	(0.41)
C111	C1	C2	C3	11.99	(0.70)
Si1	C1	C111	Na	-140.17	(0.28)
Si1	C1	C111	C112	142.44	(0.41)
Si1	C1	C111	C116	-40.73	(0.59)
C2	C1	C111	Na	47.92	(0.42)
C2	C1	C111	C112	-29.48	(0.70)
C2	C1	C111	C116	147.35	(0.48)
Si3	C2	C3	Si4	-138.80	(0.28)
Si3	C2	C3	Na	127.91	(0.30)
Si3	C2	C3	C311	26.09	(0.59)
Na	C2	C3	Si4	93.29	(0.28)
Na	C2	C3	C311	-101.82	(0.43)
C1	C2	C3	Si4	30.68	(0.59)
C1	C2	C3	Na	-62.61	(0.43)
C1	C2	C3	C311	-164.43	(0.45)
Si4	C3	C311	C312	29.25	(0.70)
Si4	C3	C311	C316	-153.20	(0.43)
Na	C3	C311	C312	140.13	(0.45)
Na	C3	C311	C316	-42.33	(0.55)
C2	C3	C311	C312	-133.71	(0.53)
C2	C3	C311	C316	43.84	(0.70)
Na	C111	C112	Si4	-77.25	(0.31)
Na	C111	C112	C113	100.95	(0.46)
C1	C111	C112	Si4	-0.28	(0.64)
C1	C111	C112	C113	177.93	(0.47)
C116	C111	C112	Si4	-177.21	(0.38)

Table of Torsion Angles in Degrees (continued)

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C116	C111	C112	C113	1.00	(0.72)
Na	C111	C116	C115	-89.63	(0.55)
C1	C111	C116	C115	-178.00	(0.50)
C112	C111	C116	C115	-0.98	(0.78)
Si4	C112	C113	C114	177.56	(0.45)
C111	C112	C113	C114	-0.47	(0.82)
C112	C113	C114	C115	-0.16	(0.89)
C113	C114	C115	C116	0.21	(0.90)
C114	C115	C116	C111	0.38	(0.89)
C3	C311	C312	C313	172.37	(0.53)
C316	C311	C312	C313	-5.33	(0.80)
C3	C311	C316	C315	-171.80	(0.52)
C312	C311	C316	C315	5.92	(0.80)
C311	C312	C313	C314	1.65	(0.97)
C312	C313	C314	C315	1.86	(1.00)
C313	C314	C315	C316	-1.31	(0.95)
C314	C315	C316	C311	-2.76	(0.91)