THE EFFECT OF CATION SUBSTITUTIONS

ON THE PHYSICAL PROPERTIES

OF TRIOCTAHEDRAL MICAS

by

Robert Miller Hazen

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Unit cell dimensions and refractive indices have been determined for synthetic hydrous trioctahedral micas in which each of $Co^{+2}$, $Cu^{+2}$, $Fe^{+2}$ and $Ni^{+2}$ completely occupies the octahedral sites. Zn and Mn micas with excess aluminum have also been synthesized, but syntheses of pure $Zn^{+2}$, $Mn^{+2}$, $Cd^{+2}$ and $Pb^{+2}$ micas were not successful. Tetrahedral substitutions of $B^{+3}$, $Fe^{+3}$ and $Ga^{+3}$ for $Al^{+3}$ and $Ge^{+4}$ for $Si^{+4}$; and interlayer cation substitutions of $Rb^{+}$, $Cs^{+}$, $NH_4^{+}$ and $Na^{+}$ for $K^{+}$ provide additional data on linear relationships that exist between ionic radii (Shannon and Prewitt) and unit cell edges, and between ionic radii cubed and unit cell volumes of these micas. The influence of substitutions on the unit cell are such that octahedral substitutions predominantly affect the a-dimension, interlayer substitutions the c-dimension, and tetrahedral substitutions affect both dimensions.

Tetrahedral and interlayer cation substitutions of a wide range of ionic radii were found to form stable micas. However, octahedral cations of greater than 0.78 A° average ionic radius do not form stable trioctahedral micas of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$. The instability of such micas is shown to be due to the misfit of smaller tetrahedral layers onto a larger octahedral layer. The composition of natural biotites are explained on the basis of this model. In addition, quantitative predictions of the amount of $Fe^{+3}$ in octahedral and tetrahedral positions in synthetic annite were made, and have been confirmed by Mössbauer and analytical chemistry techniques. A nomogram is constructed in which, for any given composition of a hydrous trioctahedral mica, the relative stability of the mica may be determined.

Thesis Supervisor: David R. Wones
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## Introduction

Trioctahedral micas are subject to a wide variety of cation substitutions. Several authors have demonstrated that such substitutions have a profound effect on both the physical properties and the stabilities of these layer silicates (Hatch et al., 1957; Wones, 1963b; Klingsberg and Roy, 1957). A list of several recent studies on synthetic hydrous trioctahedral micas is given in Table One. While data is now available for a dozen such mica end-members, there has been little attempt to systematically examine changes in mica properties with composition. The present study is an attempt to quantitatively define the effects of a wide range of cation substitutions on the physical properties of hydrous triocta-hedral micas.

TABLE 1. Previous Studies of Synthetic Hydrous Trioctahedral Micas

| Composition | Emphases of Study | References |
|---|---|---|
| $KMg_3AlSi_3O_{10}(OH)_2$ | Physical Properties & Stability<br>Stability<br>Structure | Yoder & Eugster (1954)<br>Wones (1967)<br>Steinfink (1962) |
| $KFe_3AlSi_3O_{10}(OH)_2$ | Stability & Physical Properties<br>Stability & Physical Properties | Eugster & Wones (1962)<br>Wones, Burns & Carroll (1971) |
| $K(Mg,Fe)_3AlSi_3O_{10}(OH)_2$ | Physical Properties<br>Stability | Wones (1963)<br>Wones & Eugster (1965) |
| $KMg_3FeSi_3O_{10}(OH)_2$ | Physical Properties | Wise & Eugster (1964) |
| $KFe_3FeSi_3O_{10}(OH)_2$ | Physical Properties | Wones (1963a) |
| $KMg_3BSi_3O_{10}(OH)_2$ | Physical Properties<br>Physical Properties | Eugster & Wright (1960)<br>Stubicon & Roy (1962) |
| $KMg_3GaSi_3O_{10}(OH)_2$<br>$KNi_3AlSi_3O_{10}(OH)_2$ | Stabilities only | Klingsberg & Roy (1957)<br>DeVries & Roy (1958) |
| $KZn_3AlSi_3O_{10}(OH)_2$<br>$KMn_3AlSi_3O_{10}(OH)_2$ | Unit Cell Parameters | Frondel & Ito (1966) |
| $NaMg_3AlSi_3O_{10}(OH)_2$ | Physical Properties | Carman (1969) |
| $NH_4Mg_3AlSi_3O_{10}(OH)_2$ | Physical Properties | Eugster & Munoz (1966) |

## Mica Compositions Studied

The hydrous magnesian trioctahedral mica, phlogopite,
$KMg_3AlSi_3O_{10}(OH)_2$, was used as the reference composition in
this study. Attempted 100% octahedral substitutions for $Mg^{+2}$
included $Mn^{+2}$, $Co^{+2}$, $Ni^{+2}$, $Cu^{+2}$, $Zn^{+2}$, $Cd^{+2}$, and $Pb^{+2}$. Data
of Wones (1963b) on the $Fe^{+2}$ mica  annite, and synthetic bio-
tites on the join phlogopite-annite, have also been employed.
Tetrahedral cation substitutions were $Ga^{+3}$, $Fe^{+3}$, and $B^{+3}$ for
$Al^{+3}$, and $Ge^{+4}$ for $Si^{+4}$; while substitutions into the inter-
layer cation $K^+$ position include $Rb^+$, $Cs^+$, $Cu^+$, and $Ag^+$. In
addition, $Na^+$ phlogopite data of Carman (1969) and $NH_4^+$ phlo-
gopite data of Eugster and Munoz (1966) have been used in
this study. Finally, a number of double 100% cation substi-
tutions into the phlogopite structure were studied, including
ferriannite-$KFe_3^{+2}Fe^{+3}Si_3O_{10}(OH)_2$ (data of Wones, 1963a),
nickelous ferriphlogopite-$KNi_3FeSi_3O_{20}(OH)_2$, cobaltous ferri-
phlogopite-$KCo_3FeSi_3O_{10}(OH)_2$ and sodium-zinc phlogopite-
$NaZn_3AlSi_3O_{10}(OH)_2$.

## Experimental Technique

A complete list of chemicals and their lot numbers used in starting material preparation will be found in Table Two. Cobaltous hydroxide was prepared by the T.A. Edison precipitation method (U.S. Patent # 1,167,484) in which ammonium hydroxide is added to a cobaltous sulfate solution. The precipitate of $Co(OH)_2$ is washed five times in deionized and distilled water, and then dried at 100°C for 4h. $\gamma$-alumina was prepared by heating $AlCl_3 \cdot 6H_2O$ for 1h. at 750°C. The silicaʈ glass was cleaned both magnetically and in acid, and fired at 800°C for 2h. before using. $K_2O \cdot 2SiO_2$ was prepared by D.R. Wones from cleaned $SiO_2$ glass and $KHCO_3$ after the method of Schairer and Bowen (1955). Starting materials of five types were used:

1) Oxide Mix

2) $K_2Si_2O_5$ plus oxides

3) $KAlSi_3O_8$ gel plus $R^{+2}$ oxide or hydroxide

4) $KFeSi_3O_8$ gel plus $R^{+2}$ oxide or hydroxide

5) Mica gel

All gels were prepared by titration of standardized nitrate solutions. The solution mixes were dried and fired as described by Shaw (1963). Oxide mixes were prepared by weighing and mixing dried oxides or hydroxides, and then grinding in an agate mortar until homogeneous.

Charges were sealed with excess deionized and distilled water, or 30% $H_2O_2$ solution in Au or $Ag_{80}Pd_{20}$ 1/8" x 1/2"

capsules. In several runs oxygen fugacities were controlled by the solid buffer technique of Eugster (1957). Standard cold seal hydrothermal pressure apparatus was used in all runs (Tuttle, 1949). Pressure measurements are believed accurate within 1%, and the error in temperature is within $\pm 3°C$. All runs were rapidly quenched (2 minutes) in a cool water bath.

X-ray powder diffraction examination of all runs was performed on a Picker diffractometer using Cu $K_\alpha$ radiation, and data was collected on a servoriter strip chart recorder. Both $CaF_2$ (Baker's Analytical Reagent lot #91548; annealed 3X at 800°C for 1h.; a = 5.4620 $\pm$.0005) and $BaF_2$ (Baker's lot #308; annealed 2X at 800°C for 1h.; a = 6.1971 $\pm$ .0002) were employed as internal standards. Least squares unit cell refinements were performed on the Appleman, Handworker and Evans program. Optical data was obtained using a Zeiss binocular polarizing microscope with a white light source. Determination of mica indices of refraction were accomplished with Cargille's Index of Refraction Liquids, which are accurate to within $\pm$.0005. All x-ray diffraction and optical work was performed at room temperature (24° $\pm$ 1°C).

TABLE 2. Chemicals used in starting material preparation

Chemicals used in oxide mix preparation

| Formulae | Manufacturer (& Grade)* | Lot Number |
|---|---|---|
| $SiO_2$ glass | Corning (lump cullet) | 7940 |
| $GeO_2$ (trigonal) | Fisher | 786604 |
| $AlCl_3 \cdot 6H_2O$ | Mallinkrodt | 15961X |
| $Fe_2O_3$ | Fisher | 762942 |
| $B_2O_3$ | J.T. Baker | 39315 |
| MgO | Fisher | 787699 |
| MnO | K & K | 10868 |
| $CoSO_4 \cdot 7H_2O$ | Mallinkrodt | n.d. |
| NiO | Matheson, Coleman & Bell | CB918 NX345 |
| CuO | Mallinkrodt | X40588 |
| ZnO | Baker & Adamson | B354 |
| CdO | Baker & Adamson | A244X364J |
| $Ni(OH)_2$ | K & K | 16214 |
| $NH_4(OH)$ | J.T. Baker | 24037 |
| $KHCO_3$ | J.T. Baker | 21537 |

TABLE 2. Continued

| Formulae | Manufacturer (& Grade)* | Lot Number |
|---|---|---|
| K(OH) | J.T. Baker | 14890 |
| $Ag_2O$ | K & K | 17692 |
| $Cu_2O$ | Fisher | n.d. |

Additional chemicals used in gel preparations

| | | |
|---|---|---|
| "Ludox"** | Dupont (High Silica) | n.d. |
| Ag Metal | Fisher | 71096 |
| Cu Metal | Baker & Adamson | N-023 |
| Zn Metal | Merck | 40678 |
| Pb Metal | Fisher (8/1000" foil) | n.d. |
| Ga Metal | J.T. Baker (99.999%) | n.d. |
| $KNO_3$ | J.T. Baker | 30158 |
| $NaNO_3$ | J.T. Baker | 33275 |
| $RbNO_3$ | K & K | 18088 |
| $CsNO_3$ | K & K | 7824 |

TABLE 2. Continued

| Formulae | Manufacturer (& Grade)* | Lot Number |
|---|---|---|
| $Mg(NO_3)_2 \cdot 6H_2O$ | Mallinkrodt | 37012 |
| $Mn(NO_3)_2$ | Mallinkrodt (50% solution) | 27357 |
| $Al(NO_3)_3 \cdot 9H_2O$ | Mallinkrodt | 26829 |
| $Cr(NO_3)_3 \cdot 9H_2O$ | Mallinkrodt | 795204 |

*All chemicals reagent grade unless noted.

**Dupont Ludox was analyzed by F. Frey. Solids after drying and firing at 300°C

include by weight $SiO_2 = 99.0\%$ and $Na_2O = 1.0\%$.

TABLE 3. Mica Synthesis Experiments

Micas of the form $R^+Mg_3AlSiO_{10}(OH)_2$

| $R^+$ cation | $R^+$ ionic radius (A°) | Run # | $P_T = P_{H_2O}$ (in kbars) | T(°C) (±3°) | Duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| $K^+$ | 1.38 | M#1 | 2.0 | 800 | 70 | gel | Au | 100% phlogopite |
| $Rb^+$ | 1.49 | M#105 | 2.0 | 700 | 140 | gel | Au | Rb-phlogopite, Forsterite, & $RbAlSi_2O_6$ |
| | | M#98 | 2.0 | 300 | 340 | gel | Au | do. plus glass |
| $Cs^+$ | 1.70 | M#106 | 2.0 | 700 | 140 | gel | Au | Cs-Phlogopite, Forsterite, & $CsAlSi_2O_6$ |
| | | M#99 | 2.0 | 300 | 340 | gel | Au | Forsterite, $CsAlSi_2O_6$ & glass |
| $Ag^+$ | 1.15 | M#46 | 2.0 | 310 | 48 | gel | Au | Silver Metal & glass |
| | | M#67 | 2.0 | 540 | 48 | gel | Pt | do. |
| | | M#90 | 2.0 | 600 | 72 | $Mg_3AlSi_3$ gel plus $AgO$ | Au | Silver Metal, Chlorite & glass |
| $Cu^+$ | 0.96 | M#122 | 2.0 | 630 | 96 | Oxide Mix | Au | $Cu_2O$, Talc & unknown |

TABLE 3. Continued

Micas of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$

| $R^+$ cation | $R^+$ ionic radius (A ). | Run # | $P_T = P_{H_2O}$ (in kbars) | $T(°C)$ ( 3°) | Duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| $Mg^{+2}$ | 0.720 | M#1 | 2.0 | 800 | 70 | gel | Au | 100% Phlogopite |
| $Mn^{+2}$ | 0.83 | M#13 | 2.0 | 450 | 96 | Oxide Mix & $K_2Si_2O_5$ gel | Au | $\alpha$-$Mn_2O_3$; $\gamma$-$Mn_2O_3$ & sanidine |
| | | M#18 | 2.0 | 280 | 216 | Reduced Oxide Mix | Au | MnO; $Mn(OH)_2$ & glass |
| | | M#19 | 2.0 | 362 | 120 | Reduced Oxide Mix | Au | Tephroite, Kalsitite & Leucite |
| | | M#32 | 2.0 | 603 | 120 | Gel | Au | $Mn(OH)_2$ & Manganophyllite |
| | | M#62 | 2.0 | 725 | 72 | Gel | Au | $\gamma$-$Mn_2O_3$ & Sanidine |
| | | M#86 | 2.0 | 540 | 96 | Reduced Gel | Au | Braunite, Tephroite Sanidine & <10% Mica |
| | | M#84 | 2.0 | 580 | 670 | Reduced Gel | Au | Braunite & Sanidine |
| | | M#91 | 1.0 kb $CH_4$ | 500 | 336 | M#32 | Ag-Pd | $Mn(OH)_2$ & Manganophyllite |
| | | M#92 | 1.0 kb $CH_4$ | 500 | 336 | Gel | Ag-Pd | Tephroite, Kalsilite & Leucite |
| | | M#117 | 1.0 kb $CH_4$ | 600 | 96 | MnO plus Kfs gel | Ag-Pd | Tephroite, Kalsilite & Leucite |

TABLE 3. Continued

| $R^{+2}$ cation | $R^{+2}$ ionic radius ($A°$) | Run # | $P_T = P_{H_2O}$ (in kbars) | $T(°C)$ ($\pm 3°$) | duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| $Co^{+2}$ | 0.745 | M#114 | 2.0 | 750 | 48 | $Co(OH)_2$ plus gel | Au | 100% Cobaltous Phlogopite |
| | | SR#12 | 1.0 | 710 | 48 | $Co(OH)_2$ plus gel | Au | 100% Cobaltous Phlogopite |
| | | SR#34 | 0.2 | 880 | 48 | SR#12 | Au | CoO, Co Olivine & Leucite |
| $Ni^{+2}$ | 0.69 | M#7*b* | 2.0 | 600 | 145 | Oxide mix plus $K_2Si_2O_5$ gel | Au | 100% Nickelous Phlogopite |
| | | M#115 | 2.0 | 750 | 48 | $Ni(OH)_2$ plus gel | Au | 100% Nickelous Phlogopite |
| $Cu^{+2}$ | 0.73 | M#29 | 2.0 | 600 | 120 | Gel | Au | 80% Cupric Phlogopite, glass and minor unidentified $\phi$ |
| | | M#49 | 2.0 | 703 | 96 | Gel | Au | 50% Cupric Phlogopite, glass and unidentified phase |
| | | M#77 | 2.0 | 260 | 215 | Gel | Au | Cupric Phlogopite, Cu-Pyroxene & Muscovite |

TABLE 3. Continued

| $R^{+2}$ cation | $R^{+2}$ ionic radius (A°) | Run # | $P_T = P_{H_2O}$ (in kbars) | T(°C) (±3°) | Duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| $Zn^{+2}$ | 0.75 | M#8 | 2.0 | 600 | 145 | Oxide mix & $K_2Si_2O_5$ | Au | Willemite, Kalsilite & Leucite |
| | | M#17 | 2.0 | 280 | 215 | Oxide mix & $K_2Si_2O_5$ | Au | Willemite, Mica & minor Leucite |
| | | M#61 | 2.0 | 725 | 72 | Gel | Au | Willemite, Kalsilite & Leucite |
| | | M#94 | 2.0 | 530 | 50 | Gel | Au | Willemite, Mica & Leucite |
| | | M#101 | 2.0 | 500 | 290 | Gel | Au | Willemite, Mica & Leucite |
| $Cd^{+2}$ | 0.95 | M#9 | 2.0 | 600 | 145 | Oxide mix & $K_2Si_2O_5$ | Au | Cd-Olivine & Leucite |
| | | M#22 | 2.0 | 385 | 360 | Reduced Oxide mix | Au | Cd-Olivine & Sanidine |
| $Pb^{+2}$ | 1.18 | M#57 | 2.0 | 650 | 290 | Gel | Au | $Pb_4SiO_6$ & unknown |
| | | M#66 | 2.0 | 410 | 170 | Gel | Au | $K_2Pb_4Si_8O_{21}$, Sanidine & $Pb_3O_4$ |

Table 3. Continued

| $R^{+3}$ cation | $R^{+3}$ ionic radius ($A°$) | Run # | $P_T = P_{H_2O}$ (in kbars) | $T(°C)$ ($\pm 3°$) | Duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| | | | Micas of the form $KMg_3R^{+3}Si_3O_{10}(OH)_2$ | | | | | |
| $Al^{+3}$ | 0.39 | M#1 | 2.0 | 800 | 70 | Gel | Au | 100% Phlogopite |
| $B^{+3}$ | 0.12 | M#30 | 2.0 | 603 | 120 | Oxide Mix & $K_2Si_2O_5$ | Au | 50% Boron Phlogopite, Glass |
| | | M#108 | 2.0 | 720 | 120 | Oxide Mix & $K_2Si_2O_5$ | Au | 95% Boron Phlogopite |
| $Ga^{+3}$ | 0.47 | M#46 | 2.0 | 310 | 45 | Gel | Au | 40% Gallium, Phlogopite, $Ga_2O_3$, unknown ∅, & glass |
| | | M#109 | 2.0 | 720 | 120 | Gel | Au | 100% Gallium Phlogopite |
| $Fe^{+3}$ | 0.49 | M#100 | 2.0 | 500 | 265 | Oxide Mix & $K_2SiO_5$ | Au | 100% Ferri-Phlogopite |
| | | M#107 | 2.0 | 720 | 120 | Oxide Mix & $K_2Si_2O_5$ | Au | 100% Ferri-Phlogopite |
| | | M#111 | 2.0 | 690 | 215 | Oxide Mix & $K_2Si_2O_5$ | Au | 100% Ferri-Phlogopite |
| $Cr^{+3}$ (IV) | n.d. | M#44 | 2.0 | 700 | 96 | Gel | Au | $Cr_2O_3$, Forsterite & unknown ∅ |
| | | M#72 | 2.0 | 410 | 31 | Gel | Au | $Cr_2O_3$, Forsterite & glass |

TABLE 3. Continued

| $R^{+4}$ cation | $R^{+4}$ ionic radius (A°) | Run # | $P_T = P_{H_2O}$ (in kbars) | $T(°C)$ ($\pm 3°$) | Duration (hours) | Starting Materials | Capsule Buffer | Products |
|---|---|---|---|---|---|---|---|---|
| | | | Micas of the form $KMg_3AlR_3^{+4}O_{10}(OH)_2$ | | | | | |
| $Si^{+4}$ | 0.26 | M#1 | 2.0 | 800 | 70 | Gel | Au | 100% Phlogopite |
| $Ge^{+4}$ | 0.40 | M#63 | 2.0 | 725 | 75 | Oxide Mix | Au | 100% Ge-Phlogopite |
| | | | Micas of the form $KR_3^{+2}FeSi_3O_{10}(OH)_2$ | | | | | |
| $Mg^{+2}$ | 0.72 | M#100 | 2.0 | 500 | 265 | Oxide Mix & $K_2Si_2O_5$ | Au | 100% Ferri-phlogopite |
| | | M#107 | 2.0 | 720 | 120 | Oxide Mix & $K_2Si_2O_5$ | Au | 100% Ferri-phlogopite |
| | | M#111 | 2.0 | 690 | 215 | Oxide Mix & $K_2Si_2O_5$ | Au | 100% Ferri-phlogopite |
| $Ni^{+2}$ | 0.69 | M#123 | 2.0 | 700 | 24 | $Ni(OH)_2$ & $KFeSi_3O_8$ Gel | Au | 100% Nickelous Ferri-phlogopite |
| $Co^{+2}$ | 0.745 | M#127 | 2.0 | 700 | 24 | $Co(OH)_2$ & $KFeSi_3O_8$ Gel | Au | 100% Cobaltous Ferri-phlogopite |

## Unit Cell Parameters

1M unit cell dimensions and volumes, as well as molecular weights and calculated densities, for synthetic hydrous trioctahedral micas of this and other studies are listed in Table Four. Smith and Yoder (1956) have shown that trioctahedral micas often possess an ideal pseudo-trigonal unit cell, defined by $a_m = b_m/\sqrt{3}$ and $\beta_m = 99°54'$. The conversion from the monoclinic 1M to trigonal 3T cell is accomplished by $a_t = a_m$ and $c_t = 3c_m \cdot \sin\beta_m$. Of the micas examined, only sodium and boron phlogopites depart appreciably from these ideal relations.

Crowley and Roy (1960) have demonstrated that pressure of formation does not significantly affect unit cell parameters of phlogopite. Similarly, synthetic micas examined in this study showed no systematic variations of cell parameters with temperature or pressure. However, Eugster and Wright (1966) have noted that the physical properties of boron phlogopite appear to vary with temperature and pressure of formation. Also, Carman (1969) has clearly documented the tendency of sodium phlogopite to hydrate below 80°C. Thus, sodium and boron phlogopite, once again depart from the ideal case. It should be noted that sodium and boron phlogopites have the smallest cell dimensions of all micas studied.

TABLE 4. Unit Cell Parameters of Synthetic Hydrous Trioctahedral Micas

Micas of Known Composition

| Composition | $a_m$ (A°) | $b_m$ (A°) | $c_m$ (A°) | $\beta_m$ | Vol (A°)³ | GFW | $\rho_{calc}$ gm/cm³ | Run# or Reference |
|---|---|---|---|---|---|---|---|---|
| $KMg_3AlSi_3O_{10}(OH)_2$ | 5.315±.001 | 9.204±.002 | 10.311±.003 | 99°54'±4' | 497.0±0.6 | 417.3 | 2.79 | M#1 |
| | 5.314±.001 | 9.208±.002 | 10.314±.005 | 99°54'±2' | 497.0±1.0 | | | Wones (1966) |
| | 5.314±.01 | 9.204±.02 | 10.314±.005 | 99°54'±5' | 497.0±1.0 | | | Yoder & Eugster (1954) |
| $Na^+Mg_3AlSi_3O_{10}(OH)_2$ | 5.265±.008 | 9.203±.006 | 9.994±.001 | 97°45'±8 | 479.8±0.8 | 401.2 | 2.78 | Carman (1969) 1 |
| $NH_4^+$ | 5.311±.008 | 9.224±.004 | 10.443±.007 | 99°42' | 504.2 | 396.2 | 2.61 | Eugster & Munoz (1966) |
| $Rb^+$ | 5.34±.01 | 9.24±.02 | 10.48±.05 | 99°54' | 510.0 | 463.6 | 3.02 | M#105   2 |
| $Cs^+$ | 5.37±.01 | 9.30±.02 | 10.83±.05 | 99°54' | 516.8 | 510.8 | 3.18 | M#106   2 |
| $KCo_3^{+2}AlSi_3O_{10}(OH)_2$ | 5.340±.001 | 9.240±.005 | 10.345±.002 | 99°58'±2 | 502.8±0.3 | 521.1 | 3.44 | M#114 |
| | 5.341±.001 | 9.240±.002 | 10.347±.002 | 99°54' | 503.3 | | | SR#12   2 |
| $Ni_3^{+2}$ | 5.303±.005 | 9.172±.001 | 10.286±.002 | 99°56'±3' | 493.1±.5 | | | M#7b |
| | 5.297±.003 | 9.175±.003 | 10.281±.004 | 99°50'±3' | 492.3±.3 | 520.5 | 3.51 | M#115 |
| | n.d. | n.d. | 10.17 | n.d. | n.d. | | | Klingsberg & Roy (1957) |
| $Cu_3^{+2}$ | 5.334±.001 | 9.238±.002 | 10.314±.004 | 99°54' | 498.8±.4 | 535.0 | 3.56 | M#29   2 |
| | 5.330±.001 | 9.234±.002 | 10.316±.003 | 99°56'±2' | 497.8±.2 | | | M#49 |
| $Fe_3^{+2}$ | 5.401±.01 | 9.347±.005 | 10.297±.01 | 100°10'±12' | 511.7 | 511.9 | 3.32 | Wones (1963b) |
| | 5.397±.001 | 9.348±.002 | 10.316±.005 | 99°54'± | 512.0 | | | Wones, Burns & Carrol (1971)   2 |
| $(FeMg)_3$-Mole % Fe 0.169 | 5.339±.006 | 9.230±.001 | 10.311±.002 | 99°50'±4' | 500.6 | | | Wones (1963b) |
| 0.250 | 5.333±.002 | 9.242±.001 | 10.312±.001 | 99°56'±1' | 500.6 | | | |
| 0.352 | 5.349±.005 | 9.260±.002 | 10.293±.006 | 99°38'±6' | 502.6 | | | |
| 0.450 | 5.343±.007 | 9.276±.001 | 10.312±.003 | 99°57'±4' | 503.4 | | | |
| 0.550 | 5.358±.003 | 9.285±.003 | 10.297±.002 | 100°0'±1' | 504.5 | | | |
| 0.765 | 5.373±.01 | 9.312±.003 | 10.297±.009 | 100°3'±6' | 507.3 | | | |
| 0.880 | 5.389±.003 | 9.335±.002 | 10.322±.004 | 99°58'±4' | 511.4 | | | |

TABLE 4. Continued

| Composition | $a_m$ (A°) | $b_m$ (A°) | $c_m$ (A°) | $\beta_m$ | Vol (A°)³ | GFW | $\rho_{calc}$ gm/cm³ | Run # or Reference [1] |
|---|---|---|---|---|---|---|---|---|
| $KMg_3\underline{B}^{+3}Si_3O_{10}(OH)_2$ | 5.29±.002 | 9.177±.001 | 10.246±.002 | 98°34'±4' | 491.9±.2 | 401.1 | 2.77 | M#108 |
| | 5.32±.01 | 9.165±.02 | 10.29±.01 | 100°10'±10' | 496.5 | | | Eugster & Wright (1960) |
| | 5.310 | 9.150 | 10.234 | 100° 8' | 489.5 | | | Stubican & Roy (1962) |
| $\underline{Ga}^{+3}$ | 5.327±.002 | 9.218±.005 | 10.359±.002 | 99°49'±2' | 501.2±.3 | 460.0 | 3.05 | M#109 |
| | n.d. | n.d. | 10.26 | n.d. | n.d. | | | Klingsberg & Roy (1957) |
| $\underline{Fe}^{+3}$ | 5.354±.001 | 9.273±.002 | 10.316±.004 | 99°54' | 505.0±.2 | 446.1 | 2.93 | M#107   [2] |
| | 5.358±.003 | 9.276±.003 | 10.321±.004 | 99°58'±4' | 505.2±.3 | | | M#111   [3] |
| | 5.34±.01 | 9.28±.005 | 10.35±.01 | 99°55'±10' | 505.6 | | | Wise & Eugster (1964) |
| $KMg_3Al\underline{Ge}^{+4}O_{10}(OH)_2$ | 5.393±.002 | 9.341±.004 | 10.600±.002 | 99°54' | 526.1±1.0 | 550.8 | 3.48 | M#63   [2] |
| | 5.387±.002 | 9.378±.02 | 10.593±.003 | 99°43'±2' | 525.5±1.0 | 550.8 | | M#68 |
| $KFe_3^{+2}Fe^{+3}Si_3O_{10}(OH)_2$ | 5.430±.002 | 9.404±.005 | 10.341±.006 | 100°4'±10' | 519.9 | 540.76 | 3.45 | Wones (1963a) |
| $KNi_3Fe^{+3}i_3O_{10}(OH)_2$ | 5.335±.005 | 9.237±.005 | 10.332±.006 | 99°55'±10' | 501.5±.08 | 549.34 | 3.63 | M#123 |
| $KCo_3Fe^{+3}Si_3O_{10}(OH)_2$ | 5.368±.001 | 9.329±.002 | 10.346±.002 | 99°50'±5' | 510.1±.04 | 550.00 | 3.58 | M#127 |

Synthetic Micas of Unknown Composition

$R^{+2}$ Cation & Extra Phases

| | $a_m$ | $b_m$ | $c_m$ | $\beta_m$ | Vol | GFW | $\rho$ | Run # |
|---|---|---|---|---|---|---|---|---|
| $\underline{Zn}^{+2}$ | 5.31±.02 | 9.205±.01 | 10.25±.05 | 99°50'±10' | 492.5±1.0 | | | M#17 |
| Willemite 25% in all runs | 5.303±.004 | 9.214±.005 | 10.285±.003 | 99°41'±3' | 495.4±.4 | | | M#94 |
| | 5.328±.002 | 9.226±.002 | 10.312±.004 | 99°59'±1' | 498.9±.2 | | | M#101 |
| Willemite reported from all runs | 5.325±.005 | 9.210±.005 | 10.210 | 99°50'±10' | 493.0±1.0 | | | Frondel & Ito (1966) [4] |
| $\underline{Mn}^{+2}$ | 5.27±.01 | 9.20±.02 | 10.17±.03 | 99°50'±10' | | | | M#32 |
| MN(OH)₂ 25% in all runs | 5.31±.01 | 9.21±.01 | 10.31±.01 | 99°45'±6' | 503±3 | | | M#91 |
| Tephroite reported in all runs | 5.32±.01 | 9.394±.01 | 10.32±.01 | 99°50'±10' | | | | Frondel & Ito (1966) [4] |

1. X-ray diffraction performed at 130°C.
2. 1M unit cell calculated from ideal 3T cell data.
   $a_m = a_t$, $b_m = \sqrt{3} \cdot a_t$, $c_m = c_t/3 \cdot \sin 99°54'$, $\beta_m = 99°54'$
3. Mössbauer analyses of ferriphlogopites by R. Burns reveals 5 to 15% $Fe^{+2}$ in all runs.
4. Unit cell parameters calculated on the Appleman, Handworker & Evans Program by this author from Frondel & Ito (1966), Table 7, p. 1421.

## Optical Data

Indices of refraction for synthetic hydrous trioctahedral micas of this and other studies are found in Table Five. Due to the psuedo-trigonal habit of these micas, $\gamma \simeq \beta$ , and thus two refractive indices are definitive. Other optical parameters considered include birefringence $B = \gamma - \alpha$ and the observed mean refractive index $\bar{n} = \sqrt[3]{\alpha \cdot \gamma^2} \simeq \frac{2\gamma + \alpha}{3}$ . While synthetic crystallites seldom exceeded $20\mu$ in size, thus making 2V determination difficult, all observed $2V \simeq 0°$. Micas are colorless except for those containing cations of the transition metal series. Intense pleochroism was observed only in iron-bearing trioctahedral micas, whereas faint pleochroism was noted in cobalt and copper phlogopites.

A useful, but seldom used optical property is the specific refractive energy K, defined by $K = \bar{n}-1/\rho$ where $\bar{n}$ is the mean refractive index and $\rho$ the density. Gladstone and Dale (1864) demonstrated that K for liquids may be calculated from the formula: $K = k_1 (P_1/100) + k_2 (P_2/100) +$ etc., where $k_1$ , $k_2$ , etc. are the specific refractive energies of the components of the liquids and $P_1$ , $P_2$ , etc. are the weight percentages of these components. H.W. Jaffe (1956) applied the rule of Gladstone and Dale to minerals, treating oxides as the components of the minerals. Jaffe obtained reasonable agreement between observed and calculated $\bar{n}$ in this manner. However, it is interesting to note that the calculated $\bar{n}$ for hydrous silicates displayed consistent positive deviations from considered in Jaffe's study

observed $\bar{n}$. Deviations ranged from a low of $-.001$ to as high as $+0.064$ for the twenty-five hydrous-silicates discussed.

Similarly, synthetic hydrous micas of this study display consistently positive deviations of $\bar{n}_{calc.}$ from $\bar{n}_{obs.}$. Only annites display a negative deviation, and positive deviations as high as $+0.087$ are noted. It would thus appear that the value cited for $k(H_2O)$ by Larsen and Berman (1934) of 0.034 cannot be applied directly to water in the silicate minerals. A significantly smaller value for $k(H_2O)$ is implied by the above data. Another source of error in the calculated K for silicates may result from erroneous k values for transition metals. Jaffee (1956) notes that $k(Fe_2O_3)$ varies from 0.290 in silicates to 0.404 in oxides. It thus appears that k for transition metals may be lowered considerably in a silicate environment. However, k values for copper, cobalt, nickel, etc. are known only for the oxide environment. This may, in part, explain the anomalously high values for $\bar{n}$ calculated. It seems that further refinement of k values are needed before the rule of Gladstone and Dale may be effectively applied to silicate minerals.

TABLE 5.  Optical Properties of Synthetic Hydrous Trioctahedral Micas

| Composition | $\alpha$ | $\gamma$ | $B_{obs}$ [1] | $\bar{n}_{obs}$ [2] | $\bar{n}_{calc}$ [3] | Deviation $\Delta\bar{n}$ | Color, Pleochroism & other remarks | Run# or Reference |
|---|---|---|---|---|---|---|---|---|
| $\underline{KMg_3}\underline{Al}Si_3O_{10}(OH)_2$ | 1.550 .002 | 1.587 .002 | 0.037 | 1.575 | 1.586 | +0.011 | Colorless, 2V≈0° | M#1 |
| | 1.550 .002 | 1.581 .001 | 0.031 | 1.571 | | +0.016 | "      — | Wones (1966) |
| | 1.548 .003 | 1.588 .003 | 0.040 | 1.575 | | +0.011 | "      2V≈0° | Yoder & Eugster (1954) |
| $Na^+$ | 1.545 .003 | 1.569 .004 | 0.024 | 1.561 | 1.581 | +0.020 | Colorless | Carman (1969)[4] |
| $Rb^+$ | 1.540 .01 | 1.575 .01 | 0.035 | 1.560 | 1.647 | +0.087 | Colorless | M#105 |
| $Cs^+$ | 1.570 .01 | 1.605 .01 | 0.035 | 1.590 | 1.601 | +0.011 | Colorless | M#106 |
| $\underline{Fe}_3^{+2}$ | 1.633 .002 | 1.700 .002 | 0.067 | 1.678 | 1.667 | -0.011 | Pleochroic: | Wones (1963b) |
| | 1.636 .002 | 1.690 .002 | 0.055 | 1.672 | | -0.005 | X = Red or yellow-brown  Z = light green | Wones & Carroll (1971)[5] |
| $\underline{Co}_3^{+2}$ | 1.607 .002 | 1.668 .002 | 0.061 | 1.648 | 1.688 | +0.040 | Pale Purple to Lavendar | M#114 |
| $\underline{Ni}_3^{+2}$ | 1.614 .002 | 1.675 .002 | 0.061 | 1.654 | 1.702 | +0.048 | Medium green      2V=0° | M#115 |
| | n.d. | 1.652 | | | | | | Klingsberg & Roy (1957) |
| $\underline{Cu}_3^{+2}$ | 1.588 .004 | 1.630 .004 | 0.042 | 1.616 | 1.690 | +0.074 | Medium blue | M#29 |
| $\underline{B}^{+3}$ | 1.549 .002 | 1.580 .002 | 0.031 | 1.570 | 1.581 | +0.011 | Colorless | M#108 |
| | 1.546 .002 | 1.568 .002 | 0.022 | 1.560 | | +0.021 | " | Eugster & Wright (1960) |
| $\underline{Ga}^{+3}$ | 1.558 .003 | 1.598 .003 | 0.040 | 1.585 | n.d. | n.d. | Colorless | M#109 |
| | n.d. | 1.598 | - | - | - | - | - | Klingsberg & Roy (1957) |
| $\underline{Fe}^{+3}$ | 1.601 .002 | 1.642 .002 | 0.041 | 1.628 | 1.656 | +0.028 | Pleochroic: | M#111 |
| | 1.600 .001 | 1.642 .001 | 0.040 | 1.629 | | +0.027 | X = reddish-brown  Z = pale orange | Wise & Eugster (1964) |
| $\underline{Ge}_3^{+4}$ | 1.596 .003 | 1.646 .003 | 0.050 | 1.623 | n.d. | n.d. | Colorless | M#63 |
| $\underline{Fe}_3^{+2}\underline{Fe}^{+3}$ | 1.705 .005 | 1.748 .003 | 0.043 | 1.734 | 1.711 | -0.023 | n.d. | Wones (1963a) |
| $\underline{Co}_3^{+2}\underline{Fe}^{+3}$ | 1.715 .005 | 1.760 .005 | 0.0 | 1.745 | 1.787 | +.042 | x=red-brown  z= pale purple | M#127 |
| $\underline{Ni}_3^{+2}\underline{Fe}^{+3}$ | 1.730 .005 | 1.770 .005 | 0.040 | 1.757 | 1.799 | +.042 | x=red-brown  z=pale green | M#123 |

1.  $B = \gamma - \alpha$

2.  $\bar{n} = \sqrt{\alpha \gamma^2} \simeq \dfrac{\alpha + 2\gamma}{3}$

3.  $\bar{n}_{calc.} = \rho \cdot k + 1$, where $\rho$ = density in $gm/cm^3$ and $k$ = specific refractive energy after the rule of Gladstone and Dale (1864).

4.  Indices of refraction determined on mica heated to 80°C and immediately placed into oil.

5.  Recent Mossbauer work reveals appreciable $Fe^{+3}$ in all synthetic annites.

## Sources of Error

The majority of trioctahedral micas synthesized represent 100% reaction from starting materials, and are thus assumed to be of ideal composition. However, rubidium and cesium phlogopites represented only $\approx$20-25% of the reactants in those runs. These micas are thought to approximate ideal composition on the basis of the observed trioctahedral x-ray patterns and the predicted unit cell parameters. Due to difficulties in standardizing gallium in nitrate solution, the gallium phlogopite gel may be slightly difficient in $Ga^{+3}$, explaining why a maximum reaction of only 95% was obtained. Another possible source of error in the assumed compositions was revealed through Mössbauer studies of iron-bearing phlogopites. Roger Burns has shown a minimum of 10% $Fe^{+3}$ in all annites, and from 5 to 15% $Fe^{+2}$ in ferriphlogopites. Thus, one might also expect multiple valence states in Ni, Co and Cu-bearing micas. Seifert and Schreyer (1971) have demonstrated the presence of $Mg^{+2}$ in tetrahedral coordination in Mg-rich synthetic trioctahedral micas. However, the assumption is made that all $R^{+2}$-cations in this study are in octahedral coordination unless noted otherwise.

In the investigation by Frondel and Ito (1966), and in this study, end-member zinc phlogopite $KZn_3AlSi_3O_{10}(OH)_2$ was not achieved. In all experiments in which mica was produced, $\geq$25% willemite-$Zn_2SiO_4$ with minor leucite and/or glass were also present. While the mica is clearly zinc-bearing, having cell parameters and indices of refraction

higher than phlogopite, the excess willemite is evidence of less than three $Zn^{+2}$ atoms per mica formula unit. Neumann (1949) has well documented the great preference of zinc for tetrahedral coordination. Thus, one possible explanation for such a zinc-poor mica is that the zinc enters the tetrahedral layer, while aluminum fills the three octahedral sites; i.e., $KAl_3^{+3}(Zn_2^{+2},Si_2^{+4})_3O_{10}(OH)_2$. A structural study of the natural zinc mica hendricksite from Franklin, New Jersey, would aid in an understanding of zinc's role in the layer silicates.

Synthesis of end-member manganese phlogopite-$KMn_3AlSi_3O_{10}$-$(OH)_2$ was also unsuccessful. Frondel and Ito (1966) report that tephroite-$Mn_2SiO_4$ is present as a major phase in all mica-bearing runs, while in the present study pyrochroite-$Mn(OH)_2$ accompanies the mica phase. Thus, while the unit cell parameters of the mica are greater than those of phlogopite, there are fewer than three manganese atoms per mica formula unit. Burns (1970, p. 43) has demonstrated from absorption spectra evidence that the distorted octahedral site of the phlogopite structure may stabilize manganese in the plus-three valence state. Furthermore, natural manganophyllites invariably contain aluminum in more than 10% of the octahedral sites. Therefore, the manganese-poor mica synthesized in this study may represent a solid solution between the components $KMn_3^{+2}AlSi_3O_{10}(OH)_2$ + $KMn_2^{+3}AlSi_3O_{10}(OH)_2$ + $KAl_2AlSi_3O_{10}(OH)_2$. Further study on natural manganophyllites is needed to define the extent of $Mn^{+3}/Mn^{+2}$ substitution

in the mica's distorted octahedral sites.

## Relations between Cell Parameters and Ionic Radii

There exist several systematic relations between unit cell parameters and ionic radii of substituting cations. For example, the cell dimensions $a_m$, $b_m$ and $c_m$ are each proportional to the Shannon and Prewitt (revised 1970) ionic radii of cations substituting into the tetrahedral, octahedral or interlayer positions. This relation is clearly demonstrated by Figure One of $b_m$ vs. octahedral cation ionic radii. The single exception to this rule is that of $c_m$ vs. interlayer cation ionic radii (Fig. #2). The distinct negative curvature has been explained by Prewitt as the result of increasing coordination number of the interlayer cation with increasing ionic radii of this cation. For a given cation, an increase in coordination number is accompanied by a decrease in effective ionic radii. As expected, unit cell volumes are linearly related to the cube of the substituting cations' ionic radii for octahedral and tetrahedral substitutions, and display a slight negative curvature in the interlayer case (Figs. #3 and #4).

It is of interest to consider how $b_m$ (the cell dimension within the mica layers) varies with respect to $d_{001}$ (the dimension perpendicular to the layers) for each type of cation substitution. A plot of $b_m$ vs. $d_{001}$ (Fig. #5) demonstrates that octahedral, tetrahedral and interlayer cation substitutions have differing effects on the size and shape of the unit cell. For example, octahedral substitutions have a profound influence on $b_m$, while $d_{001}$ remains virtually constant. The

near-vertical slope of the $R^{+2}$ line is a result of this fact. On the other hand, interlayer cation substitutions alter the thickness $d_{001}$ of the layers, while having a much smaller effect on $b_m$. $R^{+3}$ and $R^{+4}$ tetrahedral substitutions influence both $b_m$ and $d_{001}$. It should be noted that these observations agree with the theoretical predictions of Takeda and Morimoto (1970).

Figure #1--Monoclinic $b_m$ unit cell dimension vs. ionic

radius of the octahedral cation for micas of

the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$.  Black dots

represent biotites on the join phlogopite--

annite synthesized by Wones (1963b).

$b_m \propto$ Ionic Radius $R^{+2}$

• Wones (1963)
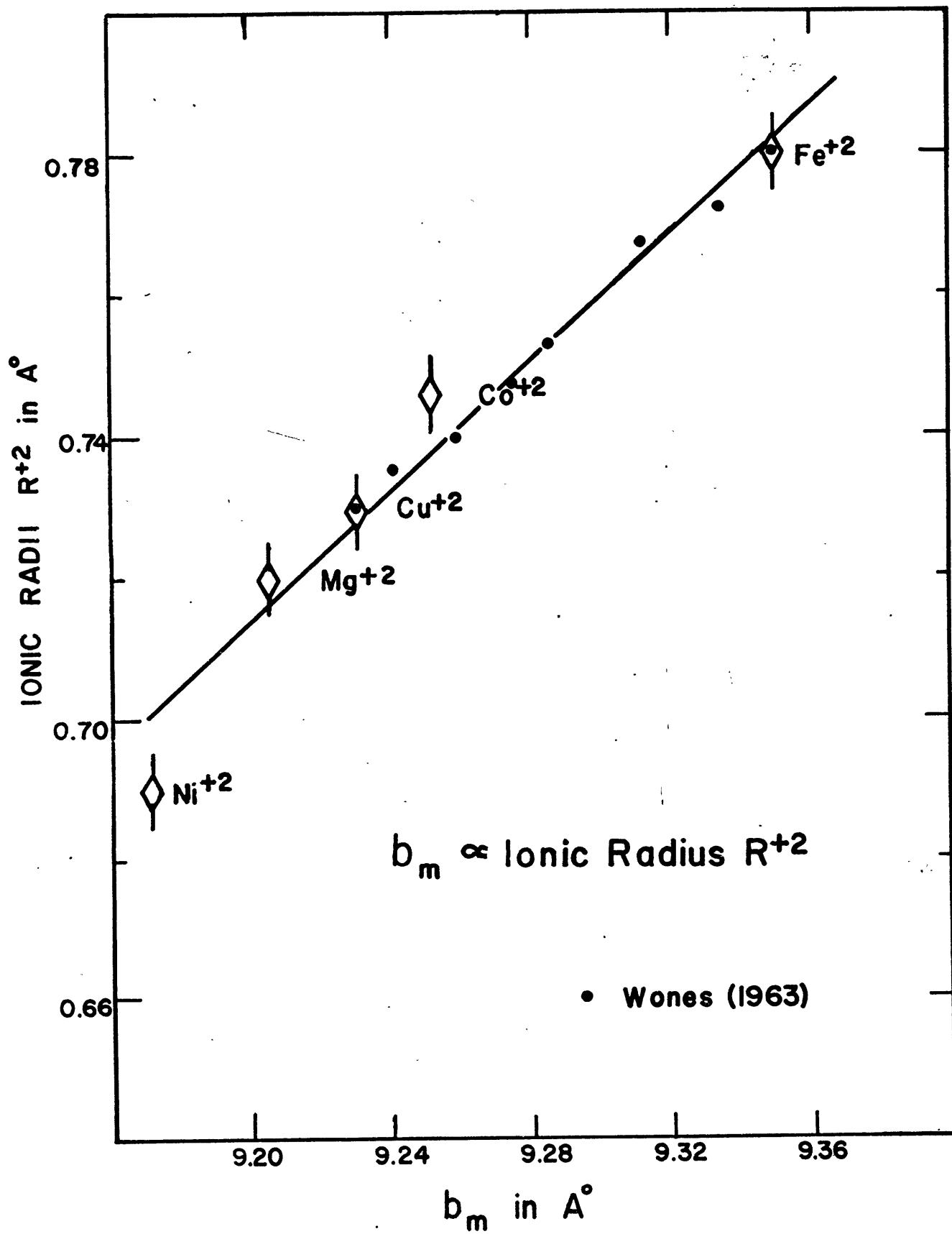
Figure #2--Monoclinic $c_m$ unit cell dimension vs. ionic

radius of the interlayer cation for micas of

the form $R^+Mg_3AlSi_3O_{10}(OH)_2$.
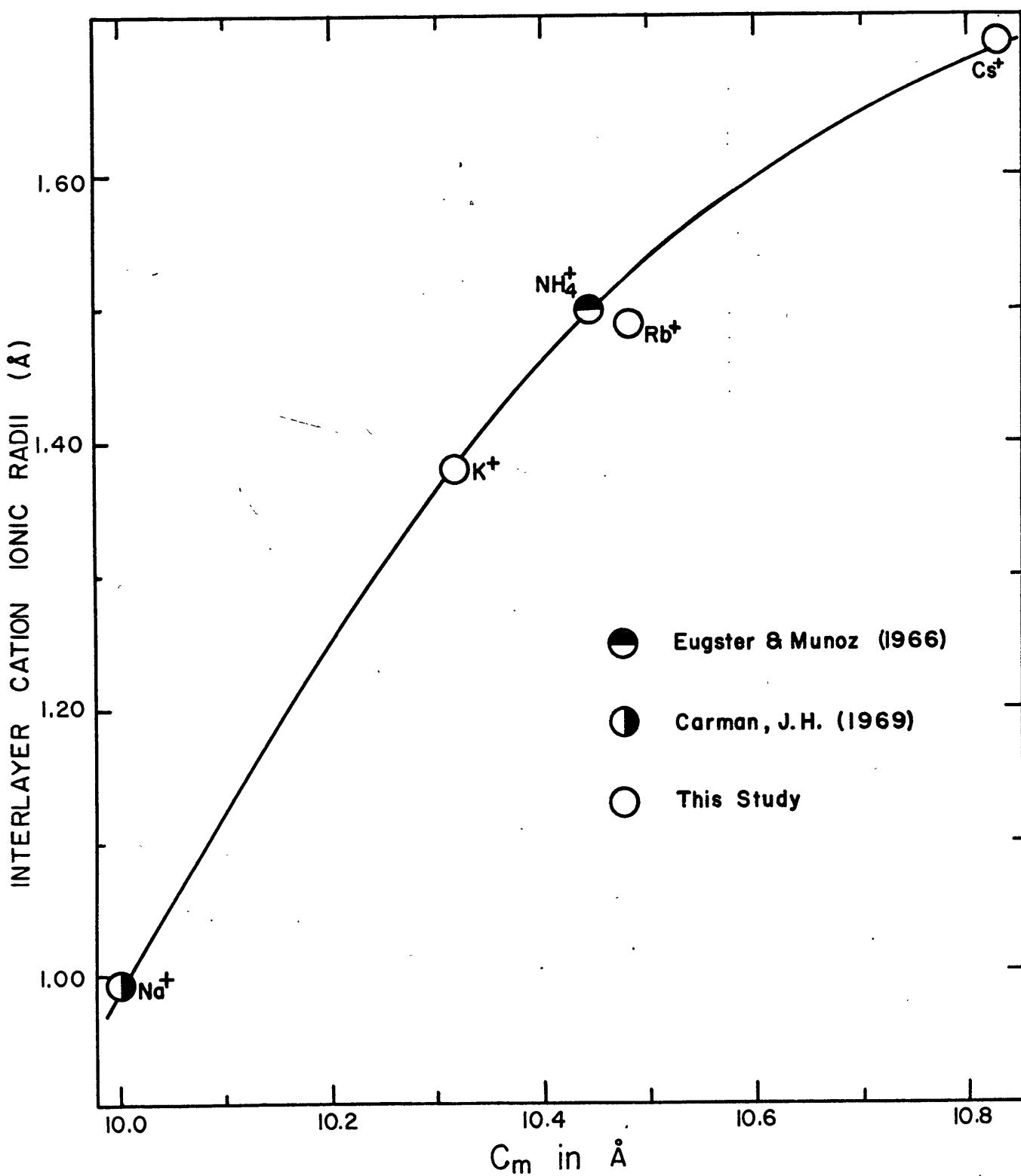
Figure #3--Monoclinic unit cell volume vs. ionic radius

of the octahedral $R^{+2}$ cation cubed, for micas

of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$. Black dots

represent biotites on the join phlogopite--

annite synthesized by Wones (1963b).

OCTAHEDRAL CATION SUBSTITUTIONS

$K R_3^{+2} AlSi_3 O_{10} (OH)_2$

IONIC RADII $R^{+2}$ CUBED ($\mathring{A}^3$)

$Fe^{+2}$

$Co^{+2}$

$Cu^{+2}$

$Mg^{+2}$

$Ni^{+2}$

• WONES (1963)

IM UNIT CELL VOLUME ($\mathring{A}^3$)
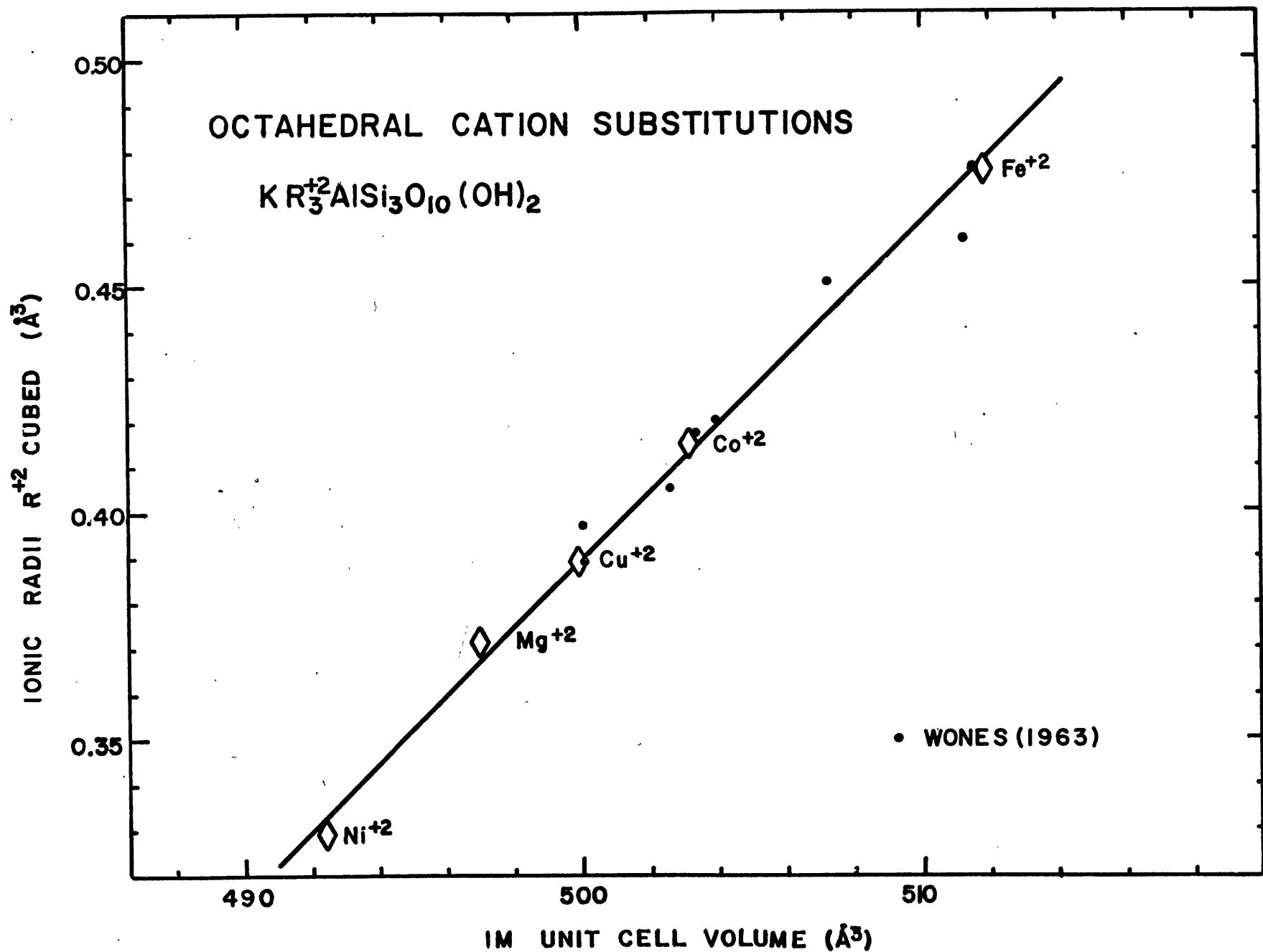
Figure #4--Monoclinic unit cell volume vs. the cube of
the interlayer $R^+$ cation radius for micas of
the form $R^+Mg_3AlSi_3O_{10}(OH)_2$, and vs. the cube
of the tetrahedral $R^{+3}$ cation radius for micas
of the form $KMg_3R^{+3}Si_3O_{10}(OH)_2$.

INTERLAYER CATION SUBSTITUTIONS

$R^+ Mg_3 AlSi_3 O_{10} (OH)_2$

IONIC RADII $R^+$ CUBED ($\text{Å}^3$)

$Cs^+$

$NH_4^+$

$Rb^+$

$K^+$

Eugster & Munoz (1966)

Carman, J. H. (1969)

This Study

$Na^+$

480    500    520

TETRAHEDRAL CATION SUBSTITUTIONS

$KMg_3 R^{+3} Si_3 O_{10} (OH)_2$

IONIC RADII $R^{+3}$ CUBED ($\text{Å}^3$)

$Fe^{+3}$

$Ga^{+3}$

$Al^{+3}$

$B^{+3}$

490    495    500    505

IM UNIT CELL VOLUME ($\text{Å}^3$)
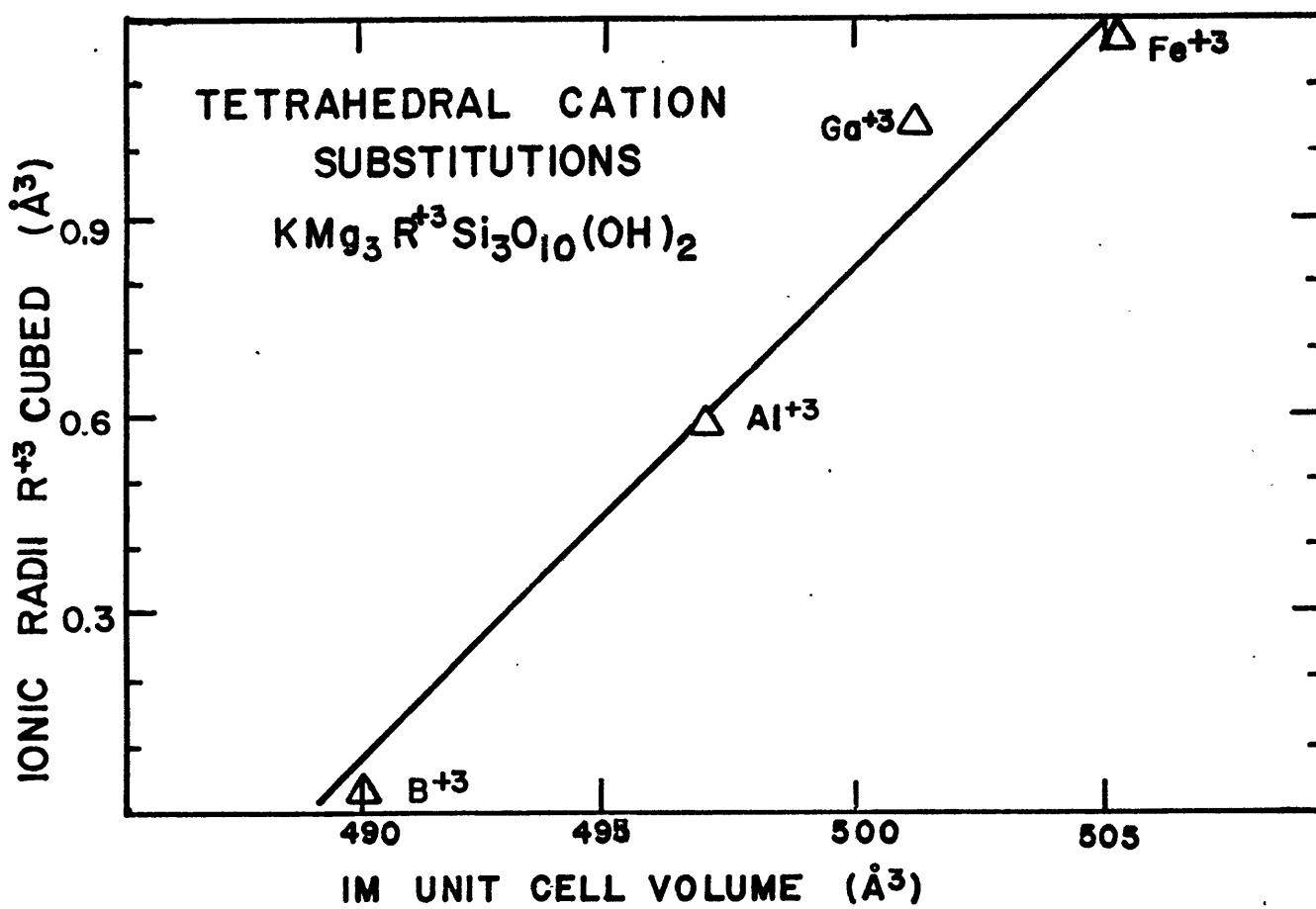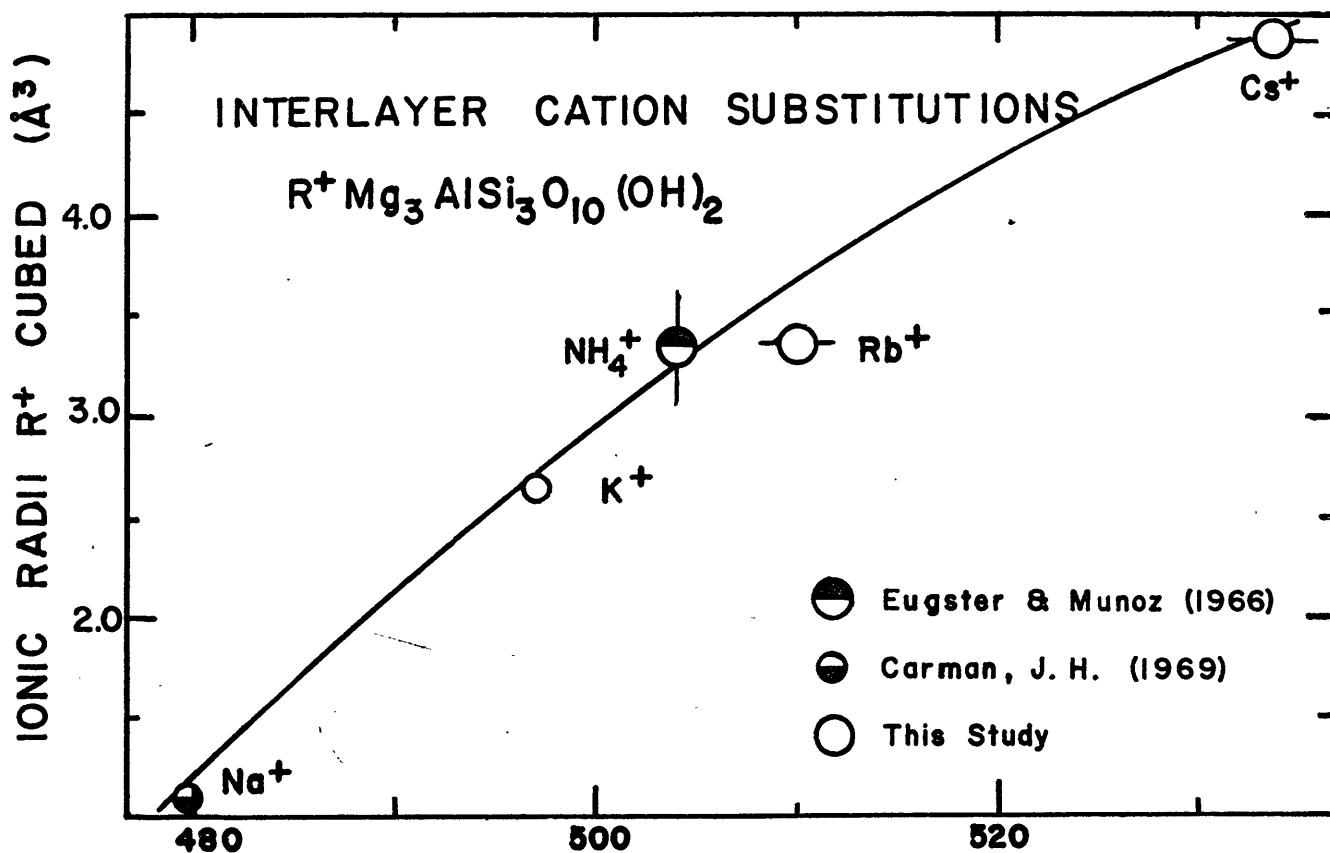
Figure #5--Monoclinic interlayer spacing $d_{001}$ vs. mono-
clinic $b_m$ cell dimension. The four lines
represent micas of the form $KMg_3AlR_3^{+4}O_{10}(OH)_2$,
$KMg_3R^{+3}Si_3O_{10}(OH)_2$, $KR_3^{+2}AlSi_3O_{10}(OH)_2$, and
$R^+Mg_3AlSi_3O_{10}(OH)_2$.
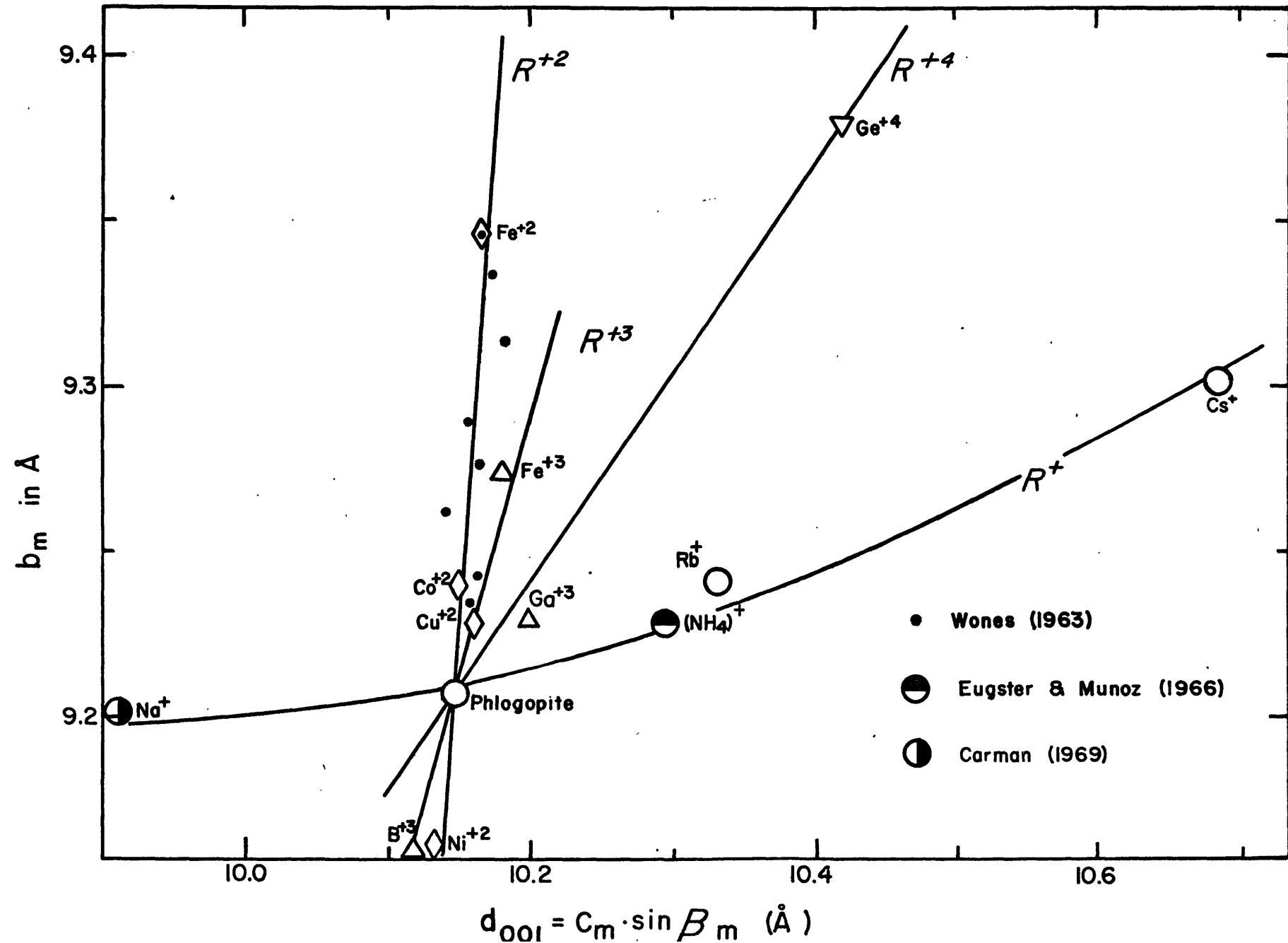
## Substitutions and Stability

Interlayer and tetrahedral cation substitutions demon-
strate that a wide range of ionic radii are possible in these
positions. Interlayer cations vary from sodium (ionic radius
= 0.98 A°) to cesium (1.70). Tetrahedral cations from boron
(0.12) to iron III (0.49) form stable micas. However, octa-
hedral cations seem far more restricted in their ability to
substitute into the phlogopite sturcture. No $R^{+2}$ cation of
radius greater than iron II (0.78), including lead (1.18)
cadmium (0.95) and manganese (0.83), was found to form a sta-
ble mica. Furthermore, Eugster and Wones (1962) have demon-
strated that the $Fe^{+2}$ mica annite is far less stable than
phlogopite. Thus, it appears that the stability of triocta-
hedral micas may be in part a function of the octahedral
cation's ionic radius.

It is well known that in phlogopite the ideal $AlSi_3$
tetrahedral layer is larger than the $Mg_3$ layer (Radoslovich
and Norrish, 1962). If the trioctahedral mica is to be sta-
ble, then these two layers must coincide, either by expansion
of the octahedral layer along $a_m$ and $b_m$ or by contraction of the
tetrahedral layer along $a_m$ and $b_m$. Radoslovich and Norrish
suggest four ways to accomplish this:

1)  Altering bond lengths of the ideal layers,

2)  tetrahedral layer tilting or corrugation,

3)  octahedral layer flattening, or

4)  tetrahedral layer rotation.

The altering of bond lengths is energetically far more
difficult than altering bond angles. Thus, while such dis-
tortions have been noted in dioctahedral mica structure
studies (Takeda and Burnham, 1969), bond stretching or con-
traction is assumed to be a minor effect. Tetrahedral
tilting or corrugation is also well documented by Takeda
and Burnham in their study of dioctahedral fluor-lithionite.
However, these authors believe that tilting of tetrahedra
will be minimized when all three octahedral positions are
filled.

Donnay, Donnay and Takeda (1963) have demonstrated that
the octahedral 001 projection may conform to the larger tetra-
hedral layer by octahedral layer flattening (See Fig. #6).
In this way bond lengths are preserved while bond angles are
altered. The amount of compression may be represented by the
angle $\Psi$, which has the value 54°44' in an ideal octahedron.
If the assumptions are made that:

1) there is no tetrahedral tilting or corrugation
   (i.e., basal oxygens in each tetrahedral sheet are
   coplanar),

2) 001 projections of tetrahedra are equilateral tri-
   angles, and

3) $a_m = b_m / \sqrt{3}$,

then $\Psi$ is a simple function of the mean octahedral bond length
$d_o$ and cell dimension $b_m$: $\sin \Psi = b_m / 3\sqrt{3} \cdot d_o$. The mean octa-
hedral bond length for Mg-(O,OH) and $Fe^{+2}$- (O,OH) are given
by Donnay, Donnay and Takeda (1963) as 2.07 A° and 2.12 A°

Figure #6--Expansion of the octahedral 001 projection by

octahedral layer compression.

# OCTAHEDRAL LAYER COMPRESSION

$$\Psi = \text{Arc sin} \left( b_m / 3\sqrt{3} \cdot d_o \right)$$

$$b_m = 3 \cdot \overline{AB}$$

$$d_o = \overline{MO}$$
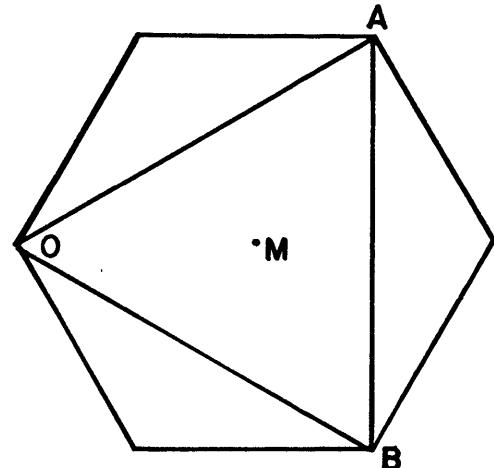
**OOl Projections**

Ideal Octahedron:
$\Psi = 54°44'$
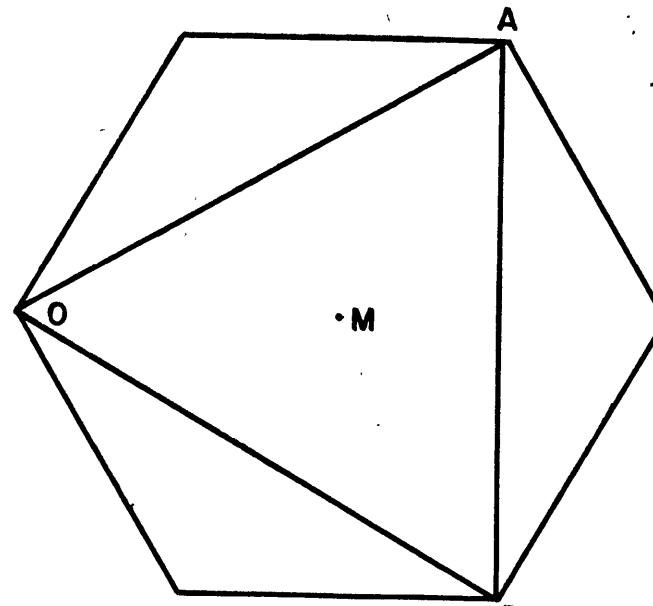
Flattened Octahedron:
$\Psi > 54°44'$

**Y Axis Projections**
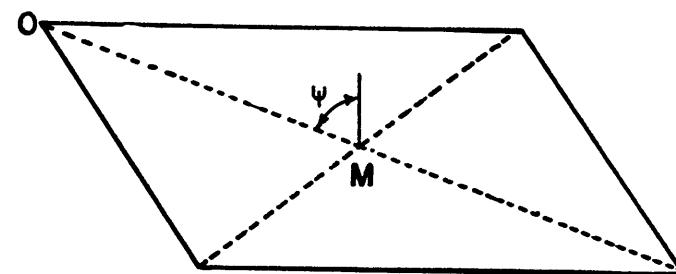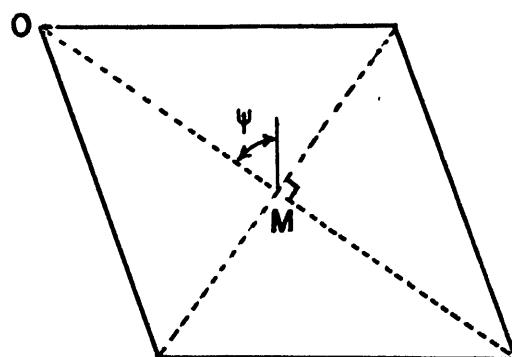
respectively. Mean bond lengths for other octahedral cations may be calculated by interpolation. Thus, knowing $b_m$, we can calculate $\Psi$ for each octahedral layer substitution. In Figure #7, $\Psi$ is plotted vs. octahedral cation ionic radius. As ionic radius increases, the value of $\Psi$ is noted to decrease slightly. Thus, larger octahedral cations require less site flattening to expand the 001 octahedral projection. While octahedral layer flattening is a real effect in hydrous trioctahedral micas, this structural parameter does not explain the instability of 100% octahedral substitutions of cations larger than iron II.

Tetrahedral layer rotation is a fourth means of fitting the non-equivalent octahedral and tetrahedral layers (see Fig. #8). Donnay, Donnay and Takeda (1963) have shown that by rotating each tetrahedron through an angle $\alpha$ about an axis perpendicular to the 001 plane, the effective size of the tetrahedral sheet is reduced. Structure studies by Steinfink (1962) and others reveal values for $\alpha$ may be greater than 10° in natural micas. Thus, in phlogopite the strain between octahedral and tetrahedral layers may be released primarily through tetrahedral layer rotation.

If the conditions assumed by Donnay, Donnay and Takeda (1963) for octahedral layer flattening are correct, then $\alpha$ is defined by the mean tetrahedral bond length $d_t$ and the cell dimension $b_m$: $\cos \alpha = b_m/4 \cdot \sqrt{2} \cdot d_t$. The mean tetrahedral bond length for the $AlSi_3$ layer is known to be 1.643 ± .002A° from studies of muscovite (Guven, 1967 and Burnham and

Figure #7--Octahedral layer compression angle Ψ vs. ionic

radius of the octahedral $R^{+2}$ cation in micas

of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$.  Black dots

represent biotites on the join phlogopite--

annite synthesized by Wones (1963b).
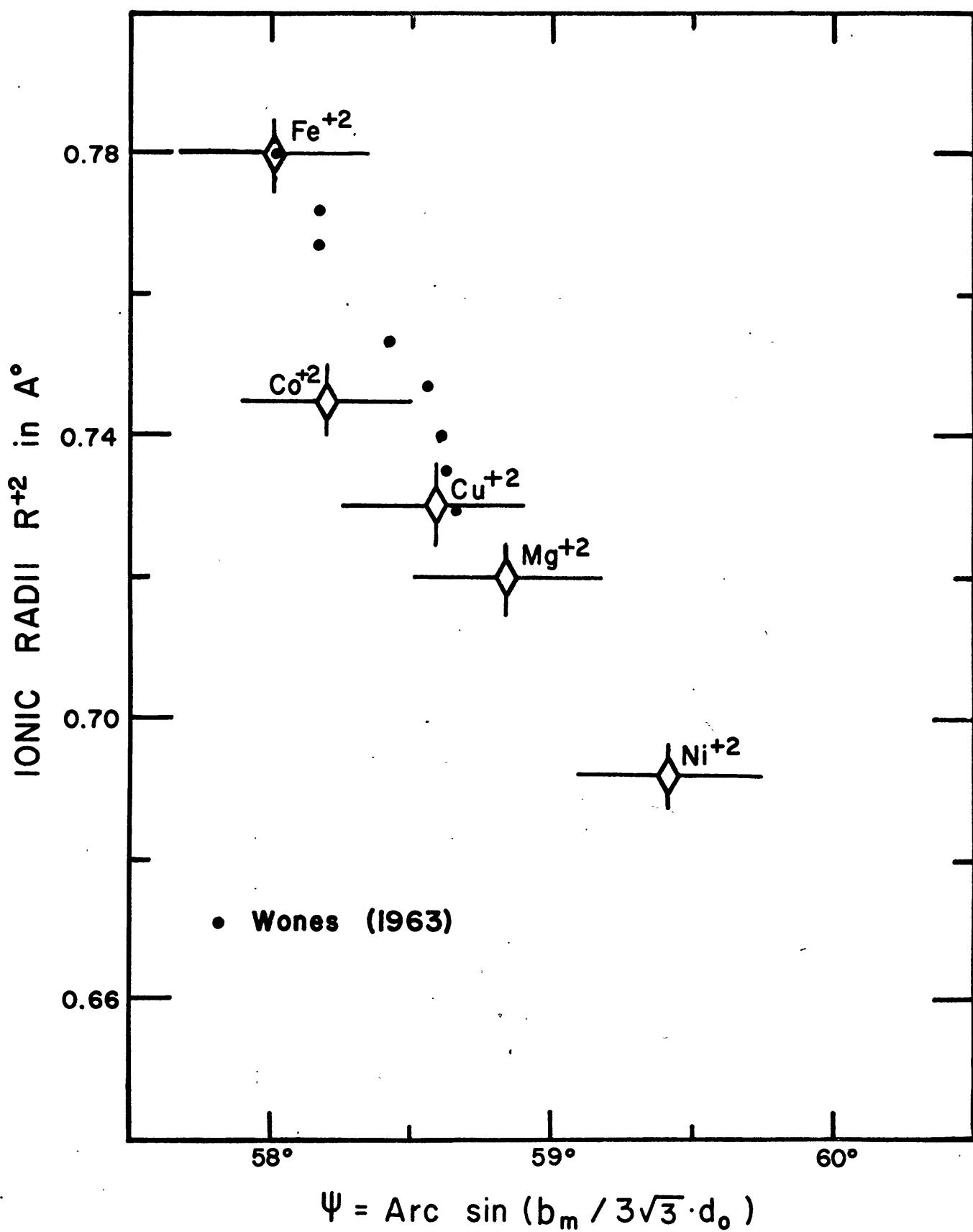
Figure #8--Contraction of the tetrahedral 001 projection
by tetrahedral layer rotation.

TETRAHEDRAL LAYER ROTATION $\alpha$

$$\alpha = \text{Arc cos}\,(b_m/4\sqrt{2}\cdot d_t)$$

$b_m = \overline{AC}$

$d_t = \overline{BT}$
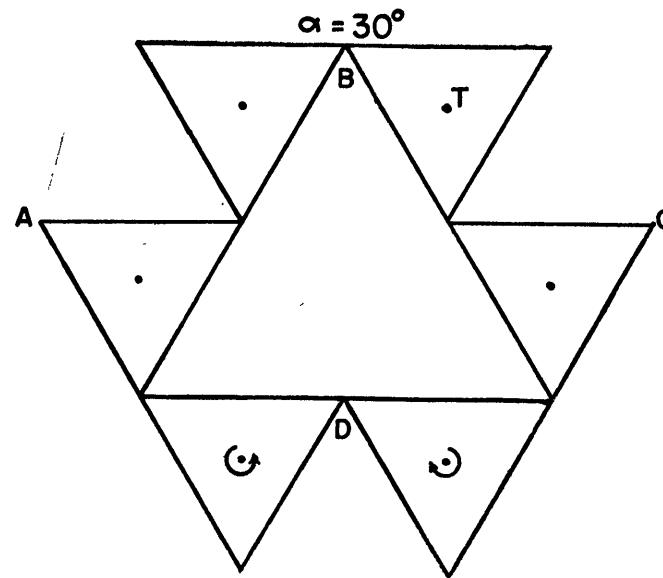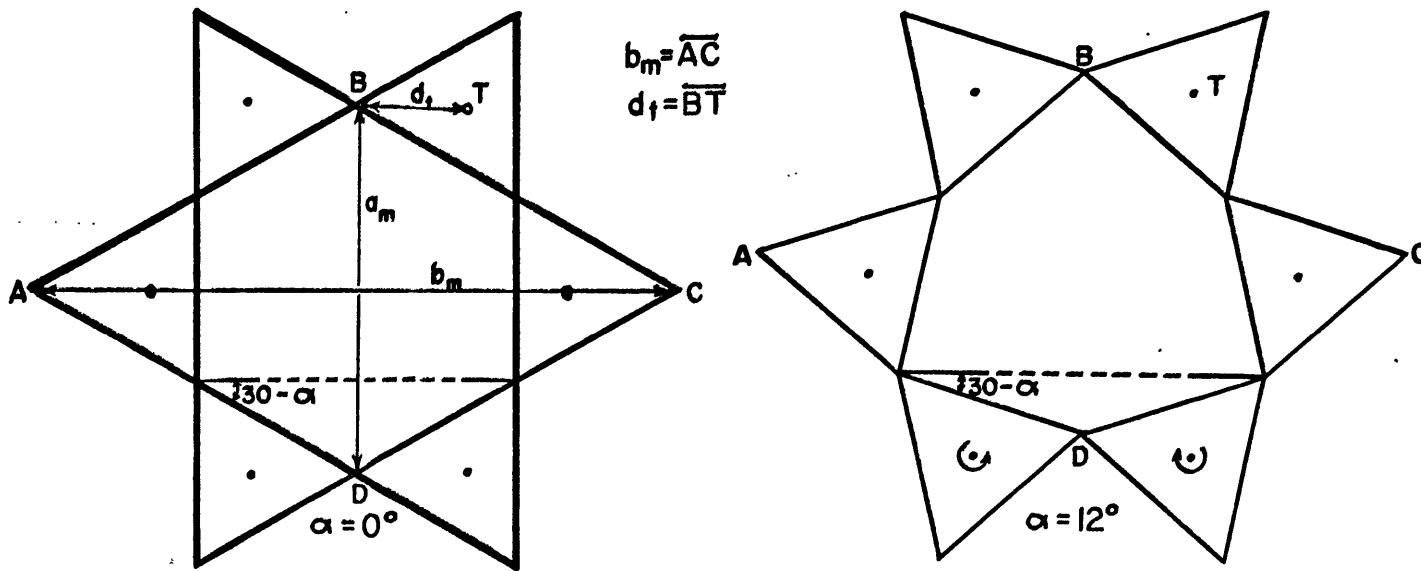
Radoslovich, 1964), biotite (Franzini, 1963) and fluor-

phlogopite (McCauley, 1968). With this value of $d_t$, and the

known values of $b_m$, a plot of $R^{+2}$ ionic radius vs. $\alpha$ has been

constructed for micas of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$ (see

Fig. #9). As the octahedral cation ionic radius increases

to 0.76 A°, $\alpha$ approaches the critical value of 0°. For octa-

hedral cations of ionic radius greater than $\sim$0.76 A°, the

tetrahedral layer cannot expand further by rotation. It

might therefore be expected that hydrous trioctahedral micas

with an $AlSi_3$ tetrahedral layer would not be stable for an

octahedral layer cation of radius greater than about 0.76 A°.

Figure #9--Tetrahedral layer rotation angle α vs. ionic

   radius of the octahedral $R^{+2}$ cation for micas

   of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$.  Black dots

   represent biotites on the join phlogopite--

   annite synthesized by Wones (1963b).

$$\alpha = \text{Arc } \cos \left( b_m / 4\sqrt{2} \cdot d_t \right)$$
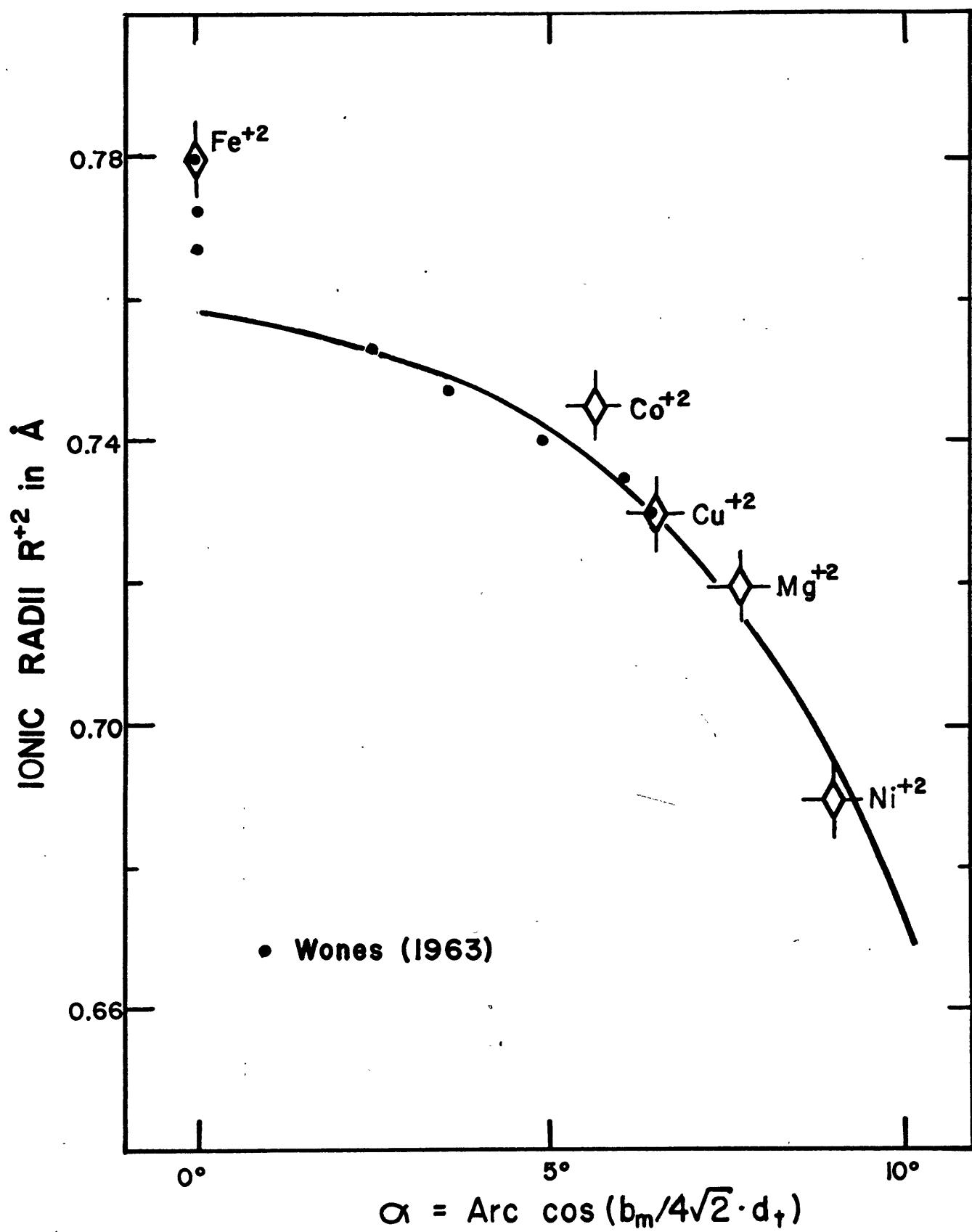
## Octahedral Cation Distribution in Natural Micas

Foster (1960) has plotted the octahedral cation distribution for over 200 natural phlogopites, biotites and siderophyllites (Fig. #10). As the iron II content of these micas increases, so does the octahedral aluminum content. Trivalent aluminum in $R^{+2}$ sites requires a corresponding substitution of aluminum for silicon in the tetrahedral layer. Thus, aluminum has the dual effect of increasing the size of the tetrahedral layer, while decreasing the effective octahedral cation radius. The maximum observed effective octahedral ionic radius, for the most iron-rich, aluminum-poor specimens, is 0.74 $A^{\circ}$. Similarly, manganophyllites are known with almost 20% MnO substituting for MgO (Jakob, 1925), resulting in an effective octahedral ionic radius of 0.74 $A^{\circ}$. Thus, while octahedral cations in natural micas of the form $KR_3{}^2AlSi_3O_{10}(OH)_2$ approach the critical ionic radius of 0.76 $A^{\circ}$, they are not observed to exceed this value.

Figure #10--The composition of the octahedral layer of
          more than 200 natural phlogopites, biotites
          and siderophyllites from Foster (1960).

Mg

EXPLANATION
• Phlogopites
○ Mg biotites
x Fe$^{+2}$ biotites
● Mg–Fe$^{+2}$ biotites
★ Siderophyllites and lepidomelanes

Foster, 1960

Phlogopites

Mg biotites

Fe$^{+2}$ biotites

Siderophyllites and lepidomelanes

R$^{+3}$

Fe$^{+2}$ (+Mn$^{+2}$)
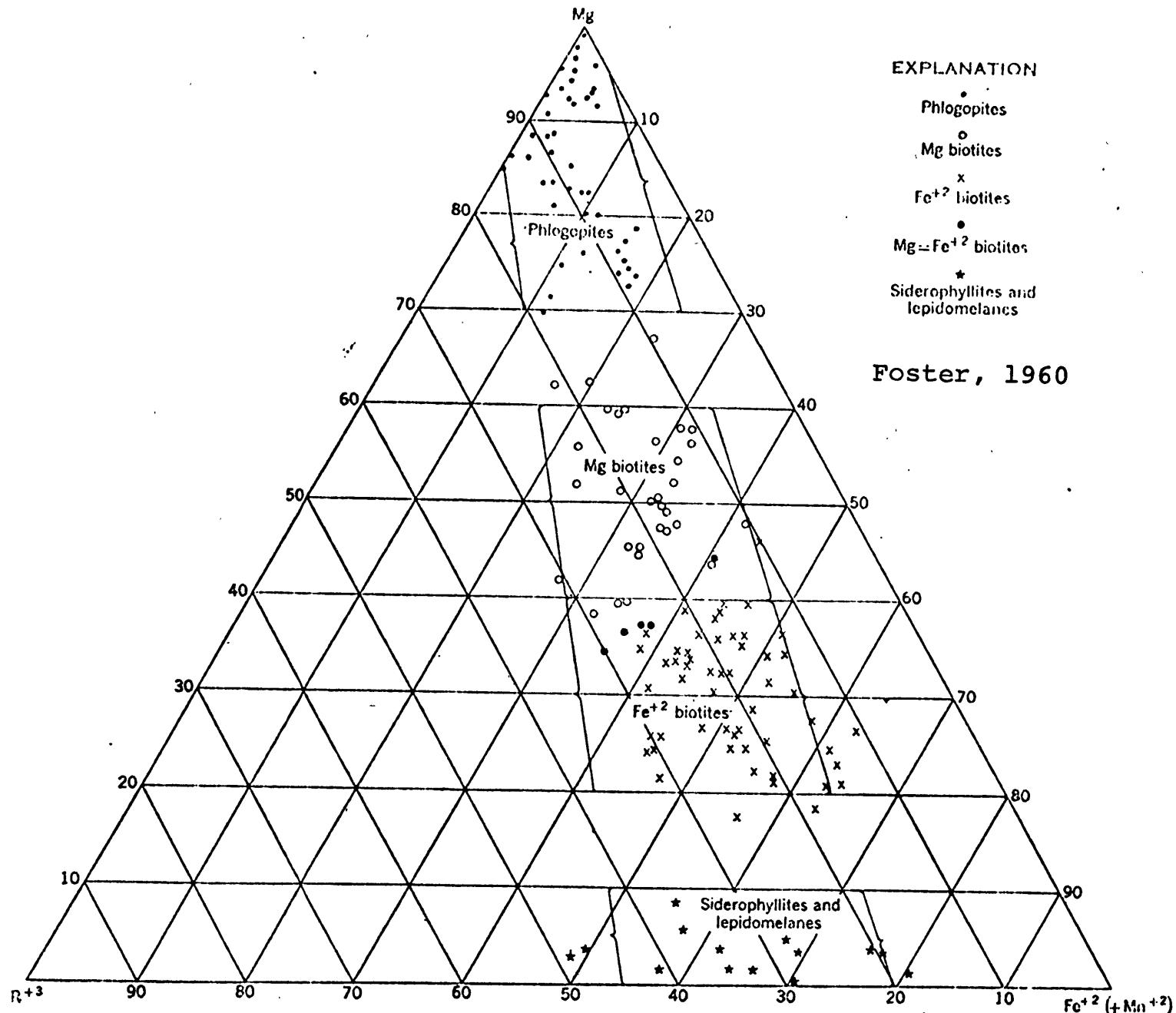
## The Composition of Annite

Synthetic annite was noted to be the only hydrous trioctahedral mica of the form $KR_3^{+2}AlSi_3O_{10}(OH)_2$ which appears to have an average octahedral ionic radius greater than the critical value of 0.76 A°. Eugster and Wones (1962) have demonstrated that trivalent iron (VI ionic radius = 0.63 A°) may substitute for octahedral divalent iron (0.78 A°) in annite as expressed by the oxyannite reaction:

$$KFe_3^{+2}AlSi_3O_{10}(OH)_2 \rightleftharpoons K(Fe^{+2}Fe_2^{+3}) AlSi_3O_{12} + H_2.$$
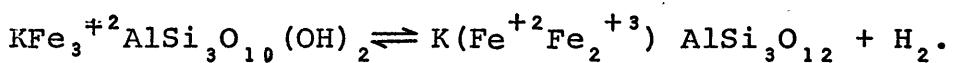
An annite with $\sim$12 mole percent octahedral $Fe^{+3}$ (i.e. $\sim$18 mole percent oxyannite) has an average octahedral cation radius of 0.76 A°, and it was thus predicted that even the most reduced synthetic annites may have appreciable oxyannite content. Subsequent study by Wones, Burns and Carroll (1971) employing Mössbauer and analytical chemistry techniques have confirmed that at least 10 mole % of octahedral iron in all synthetic annnites is in the trivalent state. It therefore appears that octahedral cation size restrictions, resulting from the misfit between octahedral and tetrahedral mica layers, may have a profound effect on the valency of iron in annite.

From Fig. #9 it can be seen that for synthetic biotites of high iron content, tetrahedral rotation (i.e., $\alpha$) is zero. Therefore, from Donnay, Donnay and Takeda (1963):

$$\cos \alpha = 1 = b_m/4 \cdot \sqrt{2} \cdot d_t \text{ for these micas.}$$

However, Wones (1963b) has shown that values for $b_m$ increase

with increasing Fe content, in these high-iron biotites.
It must therefore be assumed that $d_t$ is also increasing in
order to maintain the relation $b_m/d_t = 4\sqrt{2}$ for these micas.
One possible way to increase the mean tetrahedral bond
length $d_t$ is by substitution of $Fe^{+3}$ for $Al^{+3}$ in the tetra-
hedral layer. Since $b_m$ for annite = 9.348 A°, then $d_t$ =
9.348/4$\sqrt{2}$ = 1.652 A°. Donnay, Donnay and Takeda (1963) have
suggested a value of 1.68 A° for $d_t$ of the $FeSi_3$ tetrahedral
layer, as opposed to the smaller 1.643 A° mean tetrahedral
bond length for an $AlSi_3$ sheet. Therefore, $d_t$ = 1.652 im-
plies a composition of $(Fe^{+3}_{0.2}, Al^{+3}_{0.8})$ $Si_3$ (i.e. $\sim$7% total
iron is trivalent and in tetrahedral sites) for annites'
tetrahedral layer. Indeed, Mössbauer studies by Burns
(see Wones, Burns and Carroll, 1971) confirm that 6.5% total
Fe is tetrahedral $Fe^{+3}$!

## Prediction of Trioctahedral Mica Stability

It has been shown that $b_m$ is proportional to the octahedral cation ionic radius (Fig. #1). But we know that $\cos \alpha$ is proportional to $b_m/d_t$. Therefore, $\cos \alpha$ is proportional to octahedral ionic radius/$d_t$. This linear relation is demonstrated in Figure #11, a plot of $\cos \alpha$ vs. $R^{+2}$ ionic radii for varying mean tetrahedral bond length $d_t$. The line for an $AlSi_3$ tetrahedral layer ($d_t = 1.643$) has been developed previously (Fig. #9). Donnay, Donnay and Takeda (1963) suggest a value of $d_t = 1.68$ A° for the $FeSi_3$ tetrahedral layer, and this value has been used to obtain a second line on Figure #11 defined by $Ni^{+2}$, $Mg^{+2}$, $Co^{+2}$ and $Fe^{+2}$ ferri-phlogopites. By noting that these two lines are parallel, and by calculating additional mean tetrahedral bond lengths from data of Shannon and Prewitt (rev. 1970), additional lines can be drawn for the $BSi_3$, $GaSi_3$ and $AlGe_3$ tetrahedral layers. The resulting nomogram is found in Figure #12. The intersection of any line with $\cos \alpha = 1.00$ defines the critical octahedral cation radius for a hydrous trioctahedral mica with a mean tetrahedral bond length corresponding to that line. Thus, if the composition of a hydrous trioctahedral mica is known, systematic relations between composition and ionic radii enable us to predict unit cell dimensions, structural parameters, and even the stability of the mica.

Figure #11--Cosine of the tetrahedral layer rotation
angle $\alpha$ vs. octahedral cation radius for
micas of the form $KR_3^{+2}(AlSi_3)O_{10}(OH)_2$
$[d_t = 1.643 \ A^O]$ and of the form $KR_3^{+2}(FeSi_3)$-
$O_{10}(OH)_2 \ [d_t = 1.68 \ A^O]$.

Figure axes: IONIC RADII $R^{+2}$ (Å) versus $b_m / 4\sqrt{2} \cdot d_t$ ($= \cos \alpha$)

Legend: • Wones (1963)

$(Fe^{+3}Si_3)$ TETRAHEDRA $d_t = 1.68$

$(AlSi_3)$ TETRAHEDRA $d_t = 1.643$

Labels: $Fe^{+2}$, $Co^{+2}$, $Cu^{+2}$, $Mg^{+2}$, $Ni^{+2}$
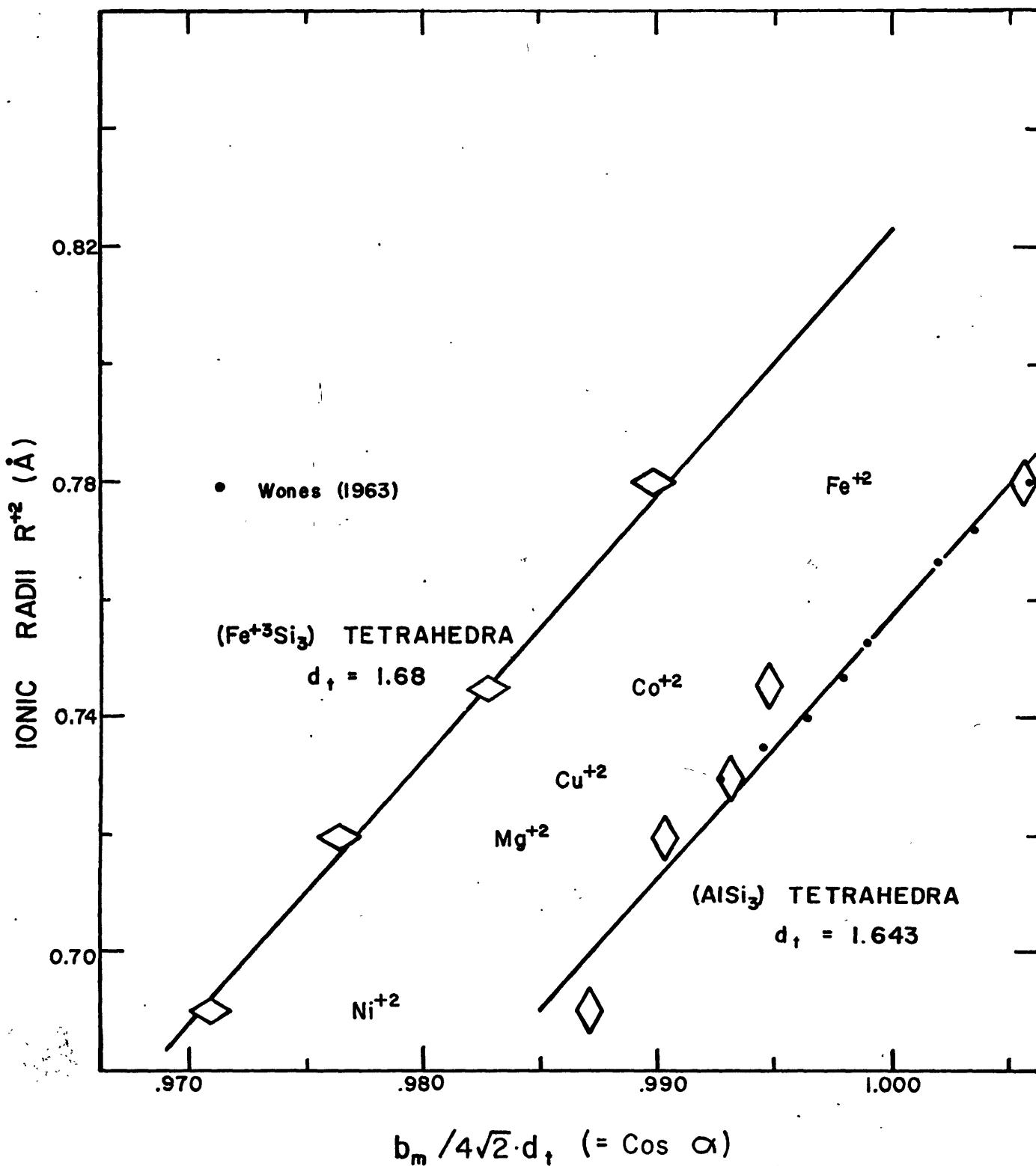
Figure #12--A nomogram for cos $\alpha$ vs. octahedral $R^{+2}$
cation radius vs. mean tetrahedral bond
length $d_t$ for all hydrous, potassic, tri-
octahedral micas.

Mean Tetrahedral → Bond Length $d_t$ in Å

1.78  1.76  1.74  1.72  1.70

1.68

1.66

1.64

1.62

Octahedral Cation Ionic Radius (Å)

0.84

0.80

0.76

0.72

0.68

0.94    0.96    0.98    1.00

$b \ /4 \cdot \sqrt{3} \cdot d_t \quad (= \cos \alpha)$
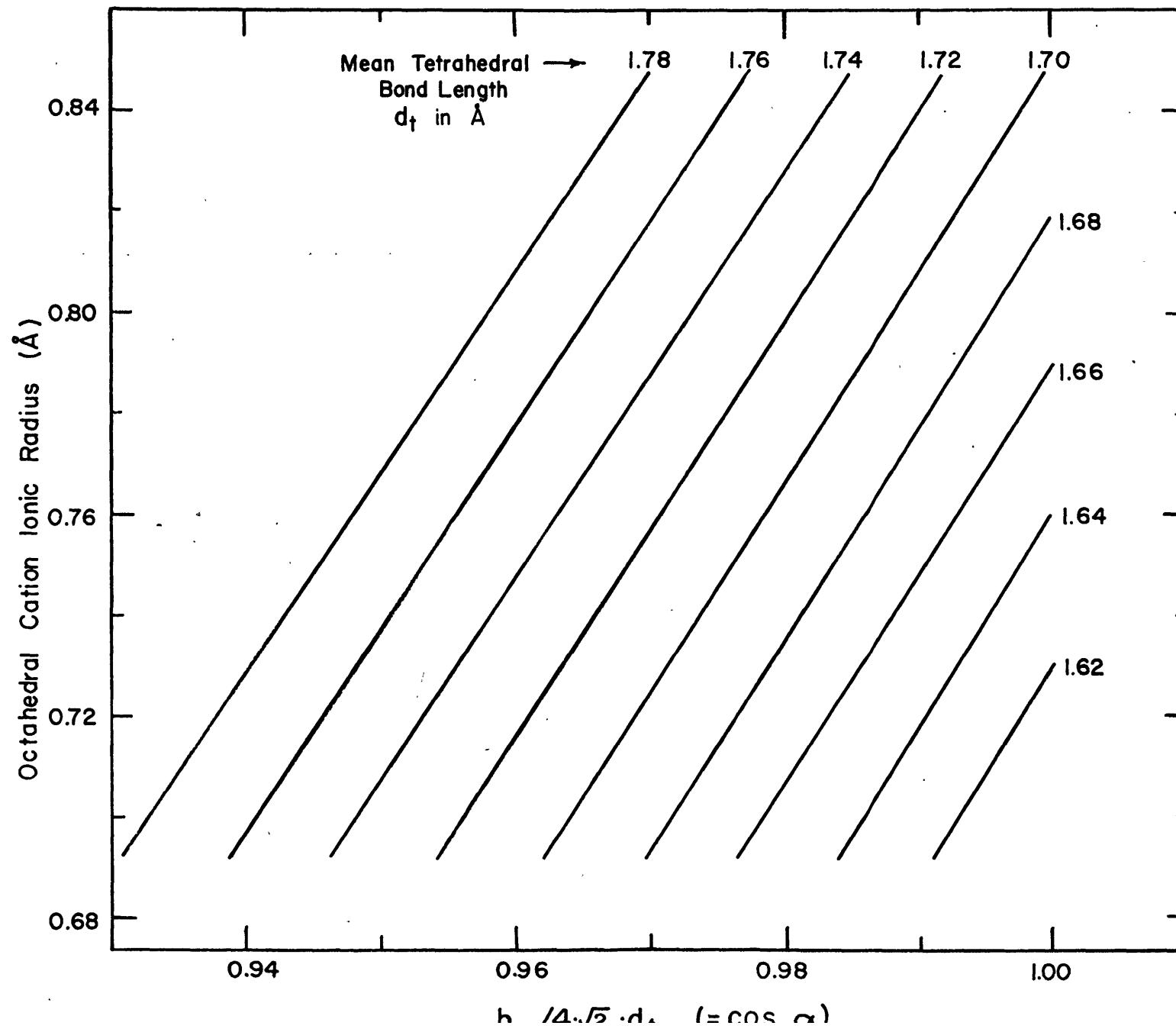
## FUTURE STUDIES

Several future studies are suggested by the present work. Of primary importance is the need for a structure determination of a hydrous trioctahedral mica. While nearly pure specimens of natural hydrous phlogopite exist (Foster, 1960), no x-ray crystal structural study of such a mica has been published. Structure studies of natural Zn and Mn micas would enhance our understanding of both mica structure and the role of Zn and Mn in these hydrous silicates.

It is well known that transition metal cations may induce site distortions in silicates. Examinations of the absorption spectra of Ni, Cu, Co, Fe and Mn-bearing micas might provide information regarding the nature and extent of such distortions.

The greatest difficulty in performing x-ray and spectral single crystal work on synthetic hydrous micas is that such crystallites rarely exceed 20$\mu$ in diameter. A technique for growing larger crystals under hydrothermal conditions would benefit both this and many other researches. Several alterations in the standard hydrothermal apparatus might facilitate single crystal growth. The use of higher ratios of $H_2O$ to starting material might increase mobility of solids while decreasing the number of nucleation sites. A larger volume of starting materials, requiring a larger capsule, might also aid in macrocrystal development. A third technique for increasing crystallite size might be to super-

impose a directional stress onto the hydrothermal system. Such a directional stress field might lower the surface free energy of large crystals.

As mentioned previously, the refractive energies of water and transition metals in silicates are not well known. A systematic study of hydrous silicate indices of refraction vs. composition would enable more meaningful applications of the rule of Gladstone and Dale.

The present study by no means has considered all possible end-member micas. Rather, it demonstrates the vast number of synthetic micas, of both end-member and intermediate compositions, that may be produced with relative ease. Future studies on the effects of cation substitutions on the physical properties of dioctahedral micas and fluor-trioctahedral micas would enhance our present understanding of the sheet silicate structure. Indeed, the method of cation substitution in silicate minerals can provide useful information about virtually every silicate structure.

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APPENDIX A--The stability of hydrous trioctahedral

micas and their related hydroxides.

## Introduction

It has been demonstrated that mica stability is closely
related to the ionic radius of the octahedral cation. Rado-
slovich (1963) and others have noted that the octahedral
layer of trioctahedral micas possesses a structure analagous
to that of brucite--$Mg(OH)_2$. Therefore, in conjunction with
studies on the physical properties of hydrous trioctahedral
micas, stability relations of nickel and cobalt micas and
hydroxides are now being determined. While this work is
not finalized, a preliminary report follows.

Several studies on the stabilities of hydrous triocta-
hedral micas and their related hydroxides have been pre-
sented by previous investigators. Brucite--$Mg(OH)_2$ sta-
bilities have been examined by several authors, the most
frequently cited being that of Barnes and Ernst (1963).
The hydroxide stabilities of cobalt and nickel have been
determined by Pistorius (1962) for pressures from 5 to 100
kilobars. Van My (1964) and Figlarz and Vincent (1968) pro-
vide additional data on these stabilities. As mentioned
previously (see Table One), several authors have examined
stabilities of hydrous trioctahedral micas of the form
$KR_3^{+2}AlSi_3O_{10}(OH)_2$. The most important of these studies are,
for $Mg^{+2}$, Yoder and Eugster (1954) and Wones (1967); for
$Fe^{+2}$, Eugster and Wones (1962) and Wones, Burns & Carroll

(1971); and for $Ni^{+2}$, Klingsberg and Roy (1957).

## Experiments and Data

All stability experiments were performed in standard hydrothermal pressure apparatus as previously described. A partial list of synthesis experiments and resulting stability points thus far completed may be found in Table A-1. Slow quenching of pure CoO, $Co(OH)_2$, NiO and $Ni(OH)_2$ from stability curve temperatures and pressures revealed no development of other phases. It is therefore assumed that no anomalous phase development took place in fast-quenching of these stability determination experiments.

In order to determine thermodynamic properties of the hydroxides and oxides of cobalt and nickel, the unit cell volumes of these substances have been redetermined (see Table A-2). While volume and cell parameters of CoO, $Co(OH)_2$ and NiO are in close agreement with those reported in the ASTM File (Smith (ed.), 1967), those of $Ni(OH)_2$ are somewhat lower than ASTM values. Future work will consider this discrepancy more carefully, and determinations of the cell parameters of $Ni(OH)_2$ formed at a range of temperatures will be performed.

## Preliminary Conclusions

Data of Pistorius (1962) and of this study agree that $Co(OH)_2$ and $Ni(OH)_2$ dehydrate at much lower temperatures than $Mg(OH)_2$, but are certainly more stable than $Fe(OH)_2$

TABLE A-1--Stability Experiments

a. Cobalt Hydroxide Dehydration: $Co(OH)_2 \rightleftarrows CoO + H_2O$.

| Pressure (bars) | Temperature ($^0$C) | Duration (hrs.) | Reactants | Products |
|---|---|---|---|---|
| 200 | 208 | 36 | CoO | $CoO + Co(OH)_2$ |
| 200 | 214 | 36 | $Co(OH)_2$ | CoO |
| 2000 | 240 | 32 | CoO | $CoO + Co(OH)_2$ |
| 2000 | 244 | 48 | $Co(OH)_2$ | CoO |

Stability Points:   ($200 \pm 2$ bars, $211 \pm 3$ $^0$C)

($2000 \pm 20$ brs, $242 \pm 2$ $^0$C)

($5 \pm 1$ kbars, $258 \pm 10$ $^0$C)[*]

($15 \pm 1$ kbars, $297 \pm 5$ $^0$C)[*]

($27 \pm 1.5$ kbs, $308 \pm 10$ $^0$C)[*]

($50 \pm 2.5$ kbs, $315 \pm 5$ $^0$C)[*]

b. Nickel Hydroxide Dehydration: $Ni(OH)_2 \rightleftarrows NiO + H_2O$.

| Pressure (bars) | Temperature ($^0$C) | Duration (hrs.) | Reactants | Products |
|---|---|---|---|---|
| 200 | 265 | 48 | NiO | $NiO + Ni(OH)_2$ |
| 200 | 270 | 54 | $Ni(OH)_2$ | NiO |
| 2000 | 275 | 38 | NiO | $Ni(OH)_2$ |
| 2000 | 280 | 48 | $Ni(OH)_2$ | $NiO + Ni(OH)_2$ |
| 2000 | 285 | 48 | $Ni(OH)_2$ | NiO |

Stability Points:   ($200 \pm 2$ bars, $268 \pm 3$ $^0$C)
($2000 \pm 20$ brs, $280 \pm 5$ $^0$C)

($5 \pm 1$ kbars, $295 \pm 5$ $^0$C)[*]

($16 \pm 1$ kbars, $325 \pm 10$ $^0$C)[*]

($31.5 \pm 1.5$ kb, $330 \pm 15$ $^0$C)[*]

($50 \pm 2.5$ kb, $338 \pm 12$ $^0$C)[*]

($100 \pm 5$ kb, $345 \pm 5$ $^0$C)[*]

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[*]--Data of Pistorius (1962)

Table A-1--Continued

c. Cobalt Mica Dehydration: $KCo_3AlSi_3O_{10}(OH)_2 \rightleftharpoons$

$$CoO + Co_2SiO_4 + KAlSi_2O_6$$

| Pressure (bars) | Temperature ($^0C$) | Duration (hrs.) | Reactants | Products |
|---|---|---|---|---|
| 100 | 790 | 48 | Gel | Co Mica |
| 100 | 795 | 48 | Gel | Co Mica, CoO, $Co_2SiO_4$ & Leucite |
| 100 | 802 | 32 | Co Mica | CoO, $Co_2SiO_4$, & Leucite |
| 205 | 825 | 46 | Gel | Co Mica |
| 205 | 880 | 39 | Gel | CoO, $Co_2SiO_4$, & Leucite |
| 300 | 875 | 48 | Gel | CoO, $Co_2SiO_4$, & Leucite |

Stability Points: $(100 \pm 1$ bars, $796 \pm 6\,^0C)$

$(205 \pm 2$ bars, $850 \pm 20\,^0C)$

Table A-2--Cell Parameters and
hkl  d-spacings for the Oxides and Hydroxides
of Cobalt and Nickel

a. Oxides:

| | CoO | | NiO | |
|---|---|---|---|---|
| hkl | This Study | ASTM File | This Study | ASTM File |
| 111 | 2.4599 | 2.460 | 2.4108 | 2.410 |
| 200 | 2.1295 | 2.130 | 2.0881 | 2.088 |
| 220 | 1.5059 | 1.5062 | 1.4766 | 1.476 |
| 311 | 1.2840 | 1.2846 | 1.2596 | 1.259 |
| 222 | 1.2298 | 1.2298 | 1.2059 | 1.206 |
| a $(A^0)$ | 4.2595 | 4.260 | 4.17665 | 4.1769 |
| Vol. $(A^0)^3$ | 77.281 | 77.31 | 72.859 | 72.872 |

b. Hydroxides:

| | $Co(OH)_2$ | | $Ni(OH)_2$ | |
|---|---|---|---|---|
| hkl | This Study | ASTM File | This Study | ASTM File |
| 001 | 4.654 | 4.66 | 4.638 | 4.605 |
| 100 | 2.755 | 2.76 | 2.706 | 2.707 |
| 101 | 2.368 | 2.38 | 2.336 | 2.334 |
| 102 | 1.776 | 1.78 | 1.758 | 1.754 |
| 110 | 1.594 | 1.60 | 1.563 | 1.563 |
| 111 | 1.506 | 1.51 | 1.481 | 1.480 |
| 103 | 1.352 | 1.36 | - - - | - - - |
| a $(A^0)$ | 3.182 | 3.179 | 3.125 | 3.126 |
| c $(A^0)$ | 4.653 | 4.649 | 4.628 | 4.608 |
| Vol. $(A^0)^3$ | 40.795 | 40.688 | 39.15 | 38.97 |

Brucite--$Mg(OH)_2$:  a = 3.147 A
b = 4.769 A
Vol = 40.9026 $A^3$

which is metastable at laboratory conditions. Furthermore, $Co(OH)_2$ has a slightly lower thermal stability than $Ni(OH)_2$. This relative sequence of stabilities: $Fe(OH)_2 < Co(OH)_2 < Ni(OH)_2 < Mg(OH)_2$, is identical to the order of stabilities seen in $Fe^{+2}$, $Co^{+2}$, $Ni^{+2}$ and $Mg^{+2}$ micas. Therefore, we may conclude that the factors which control the qualitative (if not quantitative) aspects of hydroxide stabilities may also strongly influence trioctahedral mica stabilities.

Ionic radii, crystal field stabilization, and oxidation potential of the octahedral cation are all known to affect the pressure-temperature stability of micas. Furthermore, octahedral cations affect the dehydration products of micas. While nickel and cobalt phlogopite react to form monoxide plus olivine plus leucite, Mg-phlogopite reacts to form kalsilite plus olivine plus leucite, and annite dehydrates to sanidine and magnetite! Clearly, the differences in $\Delta V_{rxn}$ for the decomposition of these four micas will affect the pressure stabilities. Accurate determinations of a variety of mica dehydrations will aid in our understanding of these controls on the stability of micas.

APPENDIX B--Selected computer d-spacing
output for synthetic micas.

On the following pages are computer output d-spacings
for the micas listed below:

| Formulae | Run Number |
|---|---|
| $KMg_3AlSi_3O_{10}(OH)_2$ | M1 |
| $Ni_3$ | M7b |
| $Cu_3$ | M49 |
| $Co_3$ | M114 |
| $Zn_3$ | M101 |
| $Mn_3$ | M91 |
| $KMg_3B\ Si_3O_{10}(OH)_2$ | M108 |
| $Ga$ | M109 |
| $Fe^{+3}$ | M111 |
| $KMg_3AlGe_3O_{10}(OH)_2$ | M68 |

| N | H | K | L | | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | | 10.157771 | | 1.540500 | 8.69766 | | |
| 2 | 0 | 0 | 2 | | 5.078884 | | 1.540500 | 17.44555 | | |
| *** | 0 | 0 | 2 | | 5.076894 | 5.077721 | 1.540500 | 17.44565 | 17.4500 | -0.00404 |
| 3 | 0 | 2 | 0 | | 4.602023 | | 1.540500 | 19.27011 | | |
| *** | 0 | 2 | 0 | | 4.602023 | 4.593786 | 1.540500 | 19.27011 | 19.3050 | -0.03487 |
| 4 | 1 | 1 | 0 | | 4.551393 | | 1.540500 | 19.46656 | | |
| 5 | -1 | 1 | 1 | | 4.406263 | | 1.540500 | 20.13436 | | |
| 6 | 0 | 2 | 1 | | 4.151879 | | 1.540500 | 21.17632 | | |
| 7 | 1 | 1 | 1 | | 3.939787 | | 1.540500 | 22.54849 | | |
| *** | 1 | 1 | 1 | | 3.939787 | 3.940392 | 1.540500 | 22.54849 | 22.5450 | 0.00350 |
| *** | 1 | 1 | -2 | | 3.673047 | 3.670796 | 1.540500 | 24.20992 | 24.2250 | -0.01507 |
| 8 | -1 | 1 | 2 | | 3.673046 | | 1.540500 | 24.20992 | | |
| 9 | 0 | 2 | 2 | | 3.410279 | | 1.540500 | 26.10704 | | |
| 10 | 0 | 0 | 3 | | 3.385922 | | 1.540500 | 26.29820 | | |
| *** | 0 | 0 | 3 | | 3.385922 | 3.388861 | 1.540500 | 26.29820 | 26.2750 | 0.02321 |
| 11 | 1 | 1 | 2 | | 3.162913 | | 1.540500 | 28.18941 | | |
| 12 | -1 | 1 | 3 | | 2.934566 | | 1.540500 | 30.43391 | | |
| *** | 1 | 1 | -3 | | 2.934566 | 2.935878 | 1.540500 | 30.43391 | 30.4200 | 0.01393 |
| 13 | 0 | 2 | 3 | | 2.727283 | | 1.540500 | 32.80981 | | |
| *** | 0 | 2 | 3 | | 2.727283 | 2.727270 | 1.540500 | 32.80981 | 32.8100 | -0.00019 |
| 14 | -2 | 0 | 1 | | 2.647665 | | 1.540500 | 33.82565 | | |
| 15 | 1 | 3 | 0 R | | 2.647127 | 2.643923 | 1.540500 | 33.83276 | 33.8750 | -0.04224 |
| 16 | 2 | 0 | 0 | | 2.618215 | | 1.540500 | 34.21783 | | |
| 17 | -1 | 3 | 1 R | | 2.617649 | 2.617693 | 1.540500 | 34.22543 | 34.2250 | 0.00046 |
| 18 | 1 | 1 | 3 | | 2.541001 | | 1.540500 | 35.29120 | | |
| 19 | 0 | 0 | 4 | | 2.539441 | | 1.540500 | 35.31360 | | |
| *** | 0 | 0 | 4 | | 2.539441 | 2.539345 | 1.540500 | 35.31360 | 35.3150 | -0.00137 |
| 20 | -2 | 0 | 2 | | 2.509372 | | 1.540500 | 35.74095 | | |
| 21 | 1 | 3 | 1 R | | 2.508956 | 2.508080 | 1.540500 | 35.75708 | 35.7700 | -0.01291 |
| 22 | 2 | 0 | 1 | | 2.436212 | | 1.540500 | 36.86255 | | |
| 23 | -1 | 3 | 2 R | | 2.435718 | 2.434463 | 1.540500 | 36.87030 | 36.8900 | -0.01966 |
| 24 | -1 | 1 | 4 | | 2.373534 | | 1.540500 | 37.87250 | | |
| 25 | 0 | 4 | 0 | | 2.301011 | | 1.540500 | 39.11395 | | |
| 26 | -2 | 2 | 1 | | 2.294953 | | 1.540500 | 39.22144 | | |
| 27 | 2 | 2 | 0 | | 2.275697 | | 1.540500 | 39.56708 | | |
| 28 | -2 | 0 | 3 | | 2.268254 | | 1.540500 | 39.70053 | | |
| 29 | 1 | 3 | 2 | | 2.268078 | | 1.540500 | 39.70557 | | |
| 30 | 0 | 4 | 1 | | 2.244153 | | 1.540500 | 40.14697 | | |
| 31 | 0 | 2 | 4 | | 2.223398 | | 1.540500 | 40.53812 | | |
| 32 | -2 | 2 | 2 | | 2.203132 | | 1.540500 | 40.92764 | | |
| 33 | 2 | 0 | 2 | | 2.179675 | | 1.540500 | 41.38618 | | |
| 34 | -1 | 3 | 3 R | | 2.179295 | 2.178074 | 1.540500 | 41.39572 | 41.4200 | -0.02426 |
| 35 | 2 | 2 | 1 | | 2.153125 | | 1.540500 | 41.92242 | | |
| 36 | 0 | 4 | 2 | | 2.055940 | | 1.540500 | 43.12256 | | |
| 37 | 1 | 1 | 4 | | 2.038870 | | 1.540500 | 43.27595 | | |
| 38 | -2 | 2 | 3 | | 2.034620 | | 1.540500 | 44.45051 | | |
| 39 | 0 | 0 | 5 | | 2.031553 | | 1.540500 | 44.56125 | | |
| *** | 0 | 0 | 5 | | 2.031553 | 2.030959 | 1.540500 | 44.56125 | 44.5750 | -0.01373 |
| 40 | -2 | 0 | 4 | | 2.002924 | | 1.540500 | 45.23318 | | |
| 41 | 1 | 3 | 3 R | | 2.002753 | 2.002009 | 1.540500 | 45.23727 | 45.2550 | -0.01770 |
| 42 | 2 | 2 | 2 | | 1.969993 | | 1.540500 | 46.02482 | | |
| 43 | -1 | 1 | 5 | | 1.967715 | | 1.540500 | 46.08871 | | |
| 44 | 2 | 0 | 3 | | 1.917904 | | 1.540500 | 47.35776 | | |
| 45 | -1 | 3 | 4 | | 1.917620 | | 1.540500 | 47.36505 | | |
| 46 | 0 | 4 | 3 | | 1.903137 | | 1.540500 | 47.74796 | | |
| 47 | 0 | 2 | 5 | | 1.855919 | | 1.540500 | 48.96848 | | |
| 48 | -2 | 2 | 4 | | 1.836523 | | 1.540500 | 49.59427 | | |
| 49 | 2 | 2 | 3 | | 1.770420 | | 1.540500 | 51.59215 | | |
| 50 | 1 | 1 | 5 | | 1.769005 | | 1.540500 | 51.91006 | | |
| 51 | -2 | 0 | 5 | | 1.757957 | | 1.540500 | 51.97159 | | |
| 52 | 1 | 3 | 4 | | 1.757656 | | 1.540500 | 51.97479 | | |
| 53 | -3 | 1 | 1 | | 1.739873 | | 1.540500 | 52.55313 | | |
| 54 | -2 | 4 | 1 | | 1.736780 | | 1.540500 | 52.65393 | | |
| 55 | 1 | 5 | 0 | | 1.736620 | | 1.540500 | 52.65891 | | |
| 56 | 2 | 4 | 0 | | 1.728389 | | 1.540500 | 52.92938 | | |
| 57 | -1 | 5 | 1 | | 1.728225 | | 1.540500 | 52.93478 | | |
| 58 | 3 | 1 | 0 | | 1.714911 | | 1.540500 | 53.37814 | | |
| 59 | -3 | 1 | 2 | | 1.714886 | | 1.540500 | 53.37900 | | |
| 60 | 0 | 4 | 4 | | 1.705139 | | 1.540500 | 53.70853 | | |
| 61 | -2 | 4 | 2 | | 1.695946 | | 1.540500 | 54.02325 | | |
| 62 | 1 | 5 | 1 | | 1.695818 | | 1.540500 | 54.02765 | | |
| 63 | 0 | 0 | 6 | | 1.692961 | | 1.540500 | 54.12628 | | |
| 64 | 2 | 0 | 4 | | 1.684012 | | 1.540500 | 54.43755 | | |
| 65 | -1 | 3 | 5 R | | 1.683812 | 1.683801 | 1.540500 | 54.44458 | 54.4450 | -0.00040 |
| 66 | 2 | 4 | 1 | | 1.672616 | | 1.540500 | 54.83240 | | |
| 67 | -1 | 5 | 2 | | 1.672655 | | 1.540500 | 54.83817 | | |
| 68 | -1 | 1 | 6 | | 1.670334 | | 1.540500 | 54.92081 | | |
| 69 | 3 | 1 | 1 | | 1.645664 | | 1.540500 | 55.80316 | | |
| 70 | -3 | 1 | 3 | | 1.645147 | | 1.540500 | 55.80487 | | |
| 71 | -2 | 2 | 5 | | 1.642226 | | 1.540500 | 55.94241 | | |
| 72 | -2 | 4 | 3 | | 1.615391 | | 1.540500 | 56.95578 | | |
| 73 | 1 | 5 | 2 | | 1.615251 | | 1.540500 | 56.95563 | | |
| 74 | 0 | 2 | 6 | | 1.598151 | | 1.540500 | 57.99631 | | |
| 75 | 2 | 4 | 2 | | 1.582420 | | 1.540500 | 58.25494 | | |
| 76 | -1 | 5 | 3 | | 1.592274 | | 1.540500 | 58.26086 | | |
| 77 | 2 | 2 | 4 | | 1.581454 | | 1.540500 | 58.29388 | | |
| 78 | -2 | 0 | 6 | | 1.549076 | | 1.540500 | 59.67651 | | |
| 79 | 1 | 3 | 5 | | 1.549017 | | 1.540500 | 59.67902 | | |
| 80 | 3 | 1 | 2 | | 1.547548 | | 1.540500 | 59.69868 | | |
| 81 | -3 | 1 | 4 R | | 1.547490 | 1.547644 | 1.540500 | 59.70139 | 59.7250 | -0.02355 |
| 82 | -3 | 3 | 1 | | 1.534356 | | 1.540500 | 60.28420 | | |
| *** | 3 | 3 | 0 | | 1.544404 | 1.534243 | 1.540500 | 60.28018 | 60.2700 | 0.01018 |
| 83 | 0 | 6 | 0 | | 1.534409 | | 1.540500 | 60.28018 | | |
| 84 | 3 | 4 | 0 | | 1.532035 | | 1.540500 | 60.37460 | | |

| N | H | K | L | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 10.137272 | | 1.54050C | 8.71525 | | |
| 2 | 0 | 0 | 2 | 5.068634 | | 1.5405CC | 17.46152 | | |
| *** | 0 | 0 | 2 | 5.068634 | 5.074835 | 1.540500 | 17.48152 | 17.4600 | C.02153 |
| 3 | 0 | 2 | C | 4.545919 | | 1.5405C0 | 19.33885 | | |
| *** | 0 | 2 | C | 4.545919 | 4.584390 | 1.5405C0 | 19.33885 | 19.3450 | -C.00612 |
| 4 | 1 | 1 | C | 4.540851 | | 1.5405C0 | 19.53224 | | |
| 5 | -1 | 1 | 1 | 4.392442 | | 1.5405C0 | 20.19897 | | |
| 6 | 0 | 2 | 1 | 4.178190 | | 1.540500 | 21.24449 | | |
| 7 | 1 | 1 | 1 | 3.933608 | | 1.5405C0 | 22.58438 | | |
| 8 | -1 | 1 | 2 | 3.660636 | | 1.5405C0 | 24.29324 | | |
| *** | 1 | 1 | -2 | 3.660636 | 3.658895 | 1.5405C0 | 24.29324 | 24.3050 | -C.01174 |
| 9 | 0 | 2 | 2 | 3.400579 | | 1.5405C0 | 26.18283 | | |
| 10 | 0 | 0 | 3 | 3.379089 | | 1.5405C0 | 26.35234 | | |
| *** | 0 | 0 | 3 | 3.379089 | 3.378128 | 1.5405C0 | 26.35234 | 26.3600 | -C.00764 |
| 11 | 1 | 1 | 2 | 3.159820 | | 1.5405C0 | 28.22668 | | |
| 12 | -1 | 1 | 3 | 2.925001 | | 1.54050C | 30.53586 | | |
| *** | 1 | 1 | -3 | 2.925001 | 2.924615 | 1.5405C0 | 30.53586 | 30.5400 | -0.00413 |
| 13 | 0 | 2 | 3 | 2.720338 | | 1.5405C0 | 32.89597 | | |
| 14 | -2 | 0 | 1 | 2.640966 | | 1.540500 | 33.91406 | | |
| 15 | 1 | 3 | C | 2.639885 | | 1.540500 | 33.94162 | | |
| 16 | 2 | 0 | C | 2.613174 | | 1.5405C0 | 34.28586 | | |
| 17 | -1 | 3 | 1 | 2.608786 | 2.608074 | 1.5405C0 | 34.34534 | 34.3550 | -C.00964 |
| 18 | 1 | 1 | 3 | 2.537772 | | 1.5405C0 | 35.33759 | | |
| 19 | 0 | 0 | 4 | 2.534316 | | 1.5405C0 | 35.38736 | | |
| *** | 0 | 0 | 4 | 2.534316 | 2.534135 | 1.540500 | 35.38736 | 35.3900 | -C.00262 |
| 20 | 1 | 3 | 1 | 2.502105 | | 1.5405C0 | 35.85831 | | |
| 21 | -2 | 0 | 2 | 2.501787 | | 1.5405CC | 35.86301 | | |
| 22 | 2 | 0 | 1 | 2.432746 | | 1.540500 | 36.91696 | | |
| 23 | -1 | 3 | 2 | 2.427269 | 2.427477 | 1.5405C0 | 37.00290 | 37.0000 | C.00290 |
| 24 | -1 | 1 | 4 | 2.366238 | | 1.5405C0 | 37.99374 | | |
| 25 | 0 | 4 | C | 2.262909 | | 1.5405C6 | 39.26781 | | |
| 26 | -2 | 2 | 1 | 2.288592 | | 1.5405C0 | 39.33508 | | |
| 27 | 2 | 2 | C | 2.270426 | | 1.5405C0 | 39.66278 | | |
| 28 | 1 | 3 | 2 | 2.262695 | | 1.5405C0 | 39.80420 | | |
| 29 | -2 | 0 | 3 | 2.260906 | | 1.5405C0 | 39.83682 | | |
| 30 | 0 | 4 | 1 | 2.236415 | | 1.5405C0 | 40.29190 | | |
| 31 | 0 | 2 | 4 | 2.216130 | | 1.5405C0 | 40.63864 | | |
| 32 | -2 | 2 | 2 | 2.196221 | | 1.5405CC | 41.06223 | | |
| 33 | 2 | 0 | 2 | 2.177215 | | 1.5405C0 | 41.43707 | | |
| 34 | -1 | 3 | 3 | 2.171935 | 2.172059 | 1.540500 | 41.54248 | 41.5400 | C.00250 |
| 35 | 2 | 2 | 1 | 2.149070 | | 1.5405CC | 42.00575 | | |
| 36 | 0 | 4 | 2 | 2.039095 | | 1.540500 | 43.27094 | | |
| 37 | 1 | 1 | 4 | 2.086105 | | 1.5405C0 | 43.33609 | | |
| 38 | -2 | 2 | 3 | 2.027845 | | 1.5405C0 | 44.44713 | | |
| 39 | 0 | 0 | 5 | 2.027453 | | 1.5405C0 | 44.65822 | | |
| 40 | 1 | 3 | 3 | 1.998458 | | 1.5405C0 | 45.33896 | | |
| 41 | -2 | 0 | 4 | 1.996211 | 1.996576 | 1.5405C0 | 45.39377 | 45.3850 | 0.00879 |
| 42 | 2 | 2 | 2 | 1.966904 | | 1.5405C0 | 46.11133 | | |
| 43 | -1 | 1 | 5 | 1.961586 | | 1.5405CC | 46.23114 | | |
| 44 | 2 | 0 | 3 | 1.915966 | | 1.5405C0 | 47.40660 | | |
| 45 | -1 | 3 | 4 | 1.911434 | | 1.5405C0 | 47.52789 | | |
| 46 | 0 | 4 | 3 | 1.897339 | | 1.5405CC | 47.90302 | | |
| 47 | 0 | 2 | 5 | 1.854311 | | 1.5405C0 | 49.08691 | | |
| 48 | -2 | 2 | 4 | 1.830317 | | 1.5405C0 | 49.77383 | | |
| 49 | 2 | 2 | 3 | 1.767971 | | 1.5405C0 | 51.65887 | | |
| 50 | 1 | 1 | 5 | 1.757457 | | 1.5405C0 | 51.98779 | | |
| 51 | 1 | 3 | 4 | 1.754409 | | 1.5405C0 | 52.08487 | | |
| 52 | -2 | 0 | 5 | 1.752143 | | 1.5405C0 | 52.15729 | | |
| 53 | -3 | 1 | 1 | 1.735744 | | 1.5405CC | 52.68777 | | |
| 54 | -2 | 4 | 1 | 1.731404 | | 1.5405C0 | 52.83005 | | |
| 55 | 1 | 5 | C | 1.730818 | | 1.5405C0 | 52.84933 | | |
| 56 | 2 | 4 | C | 1.723503 | | 1.5405C0 | 53.09113 | | |
| 57 | -1 | 5 | 1 | 1.722241 | | 1.5405C0 | 53.13309 | | |
| 58 | 3 | 1 | C | 1.711515 | | 1.5405C0 | 53.49243 | | |
| 59 | -3 | 1 | 2 | 1.710179 | | 1.5405C0 | 53.53757 | | |
| 60 | 0 | 4 | 4 | 1.700289 | | 1.5405C0 | 53.87408 | | |
| 61 | 1 | 5 | 1 | 1.690458 | | 1.5405C0 | 54.21295 | | |
| 62 | -2 | 4 | 2 | 1.690361 | | 1.5405C0 | 54.21634 | | |
| 63 | 0 | 0 | 6 | 1.689545 | | 1.5405C0 | 54.24466 | | |
| 64 | 2 | 0 | 4 | 1.682337 | | 1.5405C0 | 54.49631 | | |
| 65 | -1 | 3 | 5 | 1.678635 | 1.678535 | 1.5405C0 | 54.62650 | 54.6300 | -C.00348 |
| 66 | 2 | 4 | 1 | 1.668579 | | 1.5405CC | 54.98343 | | |
| 67 | -1 | 5 | 2 | 1.666815 | | 1.5405C0 | 55.04654 | | |
| 68 | -1 | 1 | 6 | 1.665686 | | 1.5405CC | 55.08701 | | |
| 69 | 3 | 1 | 1 | 1.643310 | | 1.5405C0 | 55.90231 | | |
| 70 | -3 | 1 | 3 | 1.640946 | | 1.5405C0 | 55.98990 | | |
| 71 | -2 | 2 | 5 | 1.636742 | | 1.5405C0 | 56.14645 | | |
| 72 | 1 | 5 | 2 | 1.610535 | | 1.5405C0 | 57.14313 | | |
| 73 | -2 | 4 | 3 | 1.609598 | | 1.5405C0 | 57.16797 | | |
| 74 | 0 | 2 | 6 | 1.585369 | | 1.5405C0 | 58.13623 | | |
| 75 | 2 | 2 | 4 | 1.579410 | | 1.5405C0 | 58.37668 | | |
| 76 | 2 | 4 | 2 | 1.578840 | | 1.5405C0 | 58.39978 | | |
| 77 | -1 | 5 | 3 | 1.576923 | | 1.5405C0 | 58.48175 | | |
| 78 | 3 | 1 | 2 | 1.565437 | | 1.5405C0 | 59.78875 | | |
| 79 | 1 | 3 | 5 | 1.545115 | | 1.5405C0 | 59.80249 | | |
| 80 | 2 | 0 | 6 | 1.543070 | | 1.5405C0 | 59.80959 | | |
| 81 | -3 | 1 | 4 | 1.542491 | | 1.5405C0 | 59.91464 | | |
| 82 | -3 | 3 | 1 | 1.530290 | | 1.5405C0 | 60.44156 | | |
| 83 | 0 | 6 | C | 1.520606 | | 1.5405C0 | 60.51541 | | |
| *** | 0 | 6 | 0 | 1.520606 | 1.524730 | 1.5405C0 | 60.51541 | 60.5100 | C.00543 |
| 84 | 0 | 4 | 5 | 1.519546 | | 1.5405C0 | 60.94537 | | |
| 85 | 3 | 3 | C | 1.513517 | | 1.5405C0 | 61.17459 | | |

| N | h | k | l | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|--------|-------|--------|--------------|-------------|--------------|
| 1 | 0 | 0 | 1 | 10.161137 | | 1.540500 | 8.69477 | | |
| 2 | 0 | 0 | 2 | 5.080566 | | 1.540500 | 17.44012 | | |
| 3 | 0 | 2 | 0 | 4.616814 | | 1.540500 | 19.20779 | | |
| *** | 0 | 2 | 0 | 4.616814 | 4.617482 | 1.540500 | 19.20779 | 19.2050 | 0.00281 |
| 4 | 1 | 1 | 0 | 4.562205 | | 1.540500 | 19.43993 | | |
| *** | 1 | 1 | 0 | 4.562205 | 4.556385 | 1.540500 | 19.43993 | 19.4650 | -0.02507 |
| 5 | -1 | 1 | 1 | 4.416667 | | 1.540500 | 20.08612 | | |
| 6 | 0 | 2 | 1 | 4.203287 | | 1.540500 | 21.11816 | | |
| 7 | 1 | 1 | 1 | 3.946623 | | 1.540500 | 22.50893 | | |
| *** | 1 | 1 | 1 | 3.946623 | 3.946441 | 1.540500 | 22.50893 | 22.5100 | -0.00104 |
| 8 | -1 | 1 | 2 | 3.675962 | | 1.540500 | 24.16373 | | |
| *** | -1 | 1 | 2 | 3.675962 | 3.675774 | 1.540500 | 24.16373 | 24.1650 | -0.00126 |
| 9 | 0 | 2 | 2 | 3.416758 | | 1.540500 | 26.05635 | | |
| 10 | 0 | 0 | 3 | 3.387047 | | 1.540500 | 26.28931 | | |
| *** | 0 | 0 | 3 | 3.387047 | 3.383165 | 1.540500 | 26.28931 | 26.3200 | -0.03067 |
| 11 | 1 | 1 | 2 | 3.166563 | | 1.540500 | 28.15625 | | |
| 12 | -1 | 1 | 3 | 2.938649 | | 1.540500 | 30.39061 | | |
| *** | -1 | 1 | 3 | 2.938649 | 2.939652 | 1.540500 | 30.39061 | 30.3800 | 0.01062 |
| 13 | 0 | 2 | 3 | 2.730942 | | 1.540500 | 32.76462 | | |
| *** | 0 | 2 | 3 | 2.730942 | 2.730103 | 1.540500 | 32.76462 | 32.7750 | -0.01038 |
| 14 | 1 | 3 | 0 | 2.654885 | | 1.540500 | 33.73090 | | |
| 15 | -2 | 0 | 1 | 2.653650 | | 1.540500 | 33.74710 | | |
| 16 | -1 | 3 | 1 | 2.625316 | | 1.540500 | 34.12241 | | |
| 17 | 2 | 0 | 0 | 2.623726 | | 1.540500 | 34.14374 | | |
| *** | 2 | 0 | 0 | 2.623726 | 2.624379 | 1.540500 | 34.14374 | 34.1350 | 0.00875 |
| 18 | 1 | 1 | 3 | 2.543058 | | 1.540500 | 35.26169 | | |
| 19 | 0 | 0 | 4 | 2.540284 | | 1.540500 | 35.30148 | | |
| 20 | 1 | 3 | 1 | 2.515513 | | 1.540500 | 35.66074 | | |
| *** | 1 | 3 | 1 | 2.515513 | 2.513518 | 1.540500 | 35.66074 | 35.6900 | -0.02924 |
| 21 | -2 | 0 | 2 | 2.514810 | | 1.540500 | 35.67102 | | |
| 22 | -1 | 3 | 2 | 2.442118 | | 1.540500 | 36.77020 | | |
| *** | 2 | 0 | 1 R | 2.440521 | 2.443055 | 1.540500 | 36.79510 | 36.7550 | 0.04013 |
| 23 | 2 | 0 | 1 | 2.440521 | | 1.540500 | 36.79510 | | |
| 24 | -1 | 1 | 4 | 2.376075 | | 1.540500 | 37.83047 | | |
| 25 | 0 | 4 | 0 | 2.308407 | | 1.540500 | 38.98352 | | |
| 26 | -2 | 2 | 1 | 2.300686 | | 1.540500 | 39.11969 | | |
| 27 | 2 | 2 | 0 | 2.281103 | | 1.540500 | 39.46939 | | |
| 28 | 1 | 3 | 2 | 2.272961 | | 1.540500 | 39.61670 | | |
| 29 | -2 | 0 | 3 | 2.272658 | | 1.540500 | 39.62146 | | |
| 30 | 0 | 4 | 1 | 2.251045 | | 1.540500 | 40.01871 | | |
| 31 | 0 | 2 | 4 | 2.225627 | | 1.540500 | 40.49573 | | |
| 32 | -2 | 2 | 2 | 2.208434 | | 1.540500 | 40.82498 | | |
| 33 | -1 | 3 | 3 | 2.184106 | | 1.540500 | 41.30035 | | |
| 34 | 2 | 0 | 2 | 2.182735 | | 1.540500 | 41.32748 | | |
| *** | 2 | 0 | 2 | 2.182735 | 2.182661 | 1.540500 | 41.32748 | 41.3250 | 0.00250 |
| 35 | 2 | 2 | 1 | 2.157614 | | 1.540500 | 41.83109 | | |
| 36 | 0 | 4 | 2 | 2.101644 | | 1.540500 | 42.99969 | | |
| 37 | 1 | 1 | 4 | 2.090163 | | 1.540500 | 43.24771 | | |
| 38 | -2 | 2 | 3 | 2.039032 | | 1.540500 | 44.38907 | | |
| 39 | 0 | 0 | 5 | 2.032228 | | 1.540500 | 44.54565 | | |
| *** | 0 | 0 | 5 | 2.032228 | 2.032690 | 1.540500 | 44.54565 | 44.5350 | 0.01068 |
| 40 | 1 | 3 | 3 | 2.006155 | | 1.540500 | 45.15533 | | |
| *** | 1 | 3 | 3 | 2.006155 | 2.007053 | 1.540500 | 45.15533 | 45.1350 | 0.02136 |
| 41 | -2 | 0 | 4 | 2.006150 | | 1.540500 | 45.15549 | | |
| 42 | 2 | 2 | 2 | 1.973311 | | 1.540500 | 45.95050 | | |
| 43 | -1 | 1 | 5 | 1.969429 | | 1.540500 | 46.04630 | | |
| 44 | -1 | 3 | 4 | 1.921103 | | 1.540500 | 47.27408 | | |
| 45 | 2 | 0 | 3 | 1.920017 | | 1.540500 | 47.30243 | | |
| 46 | 0 | 4 | 3 | 1.907516 | | 1.540500 | 47.63153 | | |
| 47 | 0 | 2 | 5 | 1.860005 | | 1.540500 | 48.92676 | | |
| 48 | -2 | 2 | 4 | 1.839580 | | 1.540500 | 49.49478 | | |
| 49 | 2 | 2 | 3 | 1.772822 | | 1.540500 | 51.50397 | | |
| 50 | 1 | 1 | 5 | 1.760802 | | 1.540500 | 51.88162 | | |
| 51 | -2 | 0 | 5 | 1.760358 | | 1.540500 | 51.89444 | | |
| 52 | 1 | 3 | 4 | 1.760282 | | 1.540500 | 51.89813 | | |
| 53 | -3 | 1 | 1 | 1.743824 | | 1.540500 | 52.42502 | | |
| 54 | 1 | 5 | 0 | 1.741598 | | 1.540500 | 52.48416 | | |
| 55 | -2 | 4 | 1 | 1.741449 | | 1.540500 | 52.49548 | | |
| 56 | -1 | 5 | 1 | 1.733564 | | 1.540500 | 52.75912 | | |
| 57 | 2 | 4 | 0 | 1.733106 | | 1.540500 | 52.77411 | | |
| 58 | -3 | 1 | 2 | 1.718809 | | 1.540500 | 53.24750 | | |
| 59 | 3 | 1 | 0 | 1.718588 | | 1.540500 | 53.25491 | | |
| 60 | 0 | 4 | 4 | 1.708399 | | 1.540500 | 53.59781 | | |
| 61 | 1 | 5 | 1 | 1.700802 | | 1.540500 | 53.85648 | | |
| 62 | -2 | 4 | 2 | 1.700565 | | 1.540500 | 53.86392 | | |
| 63 | 0 | 0 | 6 | 1.693522 | | 1.540500 | 54.10684 | | |
| 64 | -1 | 3 | 5 | 1.686333 | | 1.540500 | 54.35651 | | |
| 65 | 2 | 0 | 4 | 1.685493 | | 1.540500 | 54.38583 | | |
| *** | 2 | 0 | 4 | 1.685493 | 1.685516 | 1.540500 | 54.38583 | 54.3850 | 0.00085 |
| 66 | -1 | 5 | 2 | 1.677569 | | 1.540500 | 54.66406 | | |
| 67 | 2 | 4 | 1 | 1.677052 | | 1.540500 | 54.68234 | | |
| 68 | -1 | 1 | 6 | 1.671575 | | 1.540500 | 54.87656 | | |
| 69 | -3 | 1 | 3 | 1.649565 | | 1.540500 | 55.67172 | | |
| 70 | 3 | 1 | 1 | 1.649176 | | 1.540500 | 55.68604 | | |
| 71 | -2 | 2 | 5 | 1.644675 | | 1.540500 | 55.84427 | | |
| 72 | 1 | 5 | 2 | 1.619613 | | 1.540500 | 56.79379 | | |
| 73 | -2 | 4 | 3 | 1.619517 | | 1.540500 | 56.79745 | | |
| 74 | 0 | 2 | 6 | 1.589531 | | 1.540500 | 57.95349 | | |
| 75 | -1 | 5 | 3 | 1.586520 | | 1.540500 | 58.09000 | | |
| 76 | 2 | 4 | 2 | 1.585995 | | 1.540500 | 58.11108 | | |
| 77 | 2 | 2 | 4 | 1.583202 | | 1.540500 | 58.22021 | | |
| 78 | -3 | 1 | 4 | 1.550650 | | 1.540500 | 59.56738 | | |
| 79 | 3 | 1 | 2 | 1.550161 | | 1.540500 | 59.58807 | | |
| 80 | -2 | 0 | 6 | 1.549911 | | 1.540500 | 59.59863 | | |
| 81 | 1 | 3 | 5 | 1.549759 | | 1.540500 | 59.60547 | | |
| 82 | 0 | 6 | 0 | 1.538939 | | 1.540500 | 60.06711 | | |
| *** | 0 | 6 | 0 | 1.538939 | 1.539104 | 1.540500 | 60.06711 | 60.0400 | 0.00711 |
| 83 | -3 | 3 | 1 | 1.538137 | | 1.540500 | 60.10162 | | |
| 84 | 0 | 4 | 5 | 1.525349 | | 1.540500 | 60.65823 | | |

| N. | H | K | L | D-CALC | D-OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 10.188807 | | 1.540500 | 8.67112 | | |
| 2 | 0 | 0 | 2 | 5.094403 | | 1.540500 | 17.39240 | | |
| *** | 0 | 0 | 2 | 5.094403 | 5.093653 | 1.540500 | 17.39240 | 17.3950 | -0.00259 |
| 3 | 0 | 2 | 0 | 4.623050 | | 1.540500 | 19.19420 | | |
| *** | 0 | 2 | 0 | 4.623050 | 4.619864 | 1.540500 | 19.19420 | 19.1950 | -0.00079 |
| 4 | -1 | 1 | 0 | 4.579976 | | 1.540500 | 19.40225 | | |
| *** | 1 | 1 | 0 | 4.579976 | 4.576180 | 1.540500 | 19.40225 | 19.3900 | 0.02227 |
| 5 | -1 | 1 | 1 | 4.426703 | - | 1.540500 | 20.04102 | | |
| 6 | 0 | 2 | 1 | 4.207685 | | 1.540500 | 21.09584 | | |
| 7 | 1 | 1 | 1 | 3.954204 | | 1.540500 | 22.46521 | | |
| *** | 1 | 1 | 1 | 3.954204 | 3.953377 | 1.540500 | 22.46521 | 22.4700 | -0.00477 |
| 8 | -1 | 1 | 2 | 3.689365 | | 1.540500 | 24.10123 | | |
| *** | -1 | 1 | 2 | 3.689365 | 3.686538 | 1.540500 | 24.10123 | 24.1200 | -0.01877 |
| 9 | 0 | 2 | 2 | 3.422313 | | 1.540500 | 26.01364 | | |
| *** | 0 | 2 | 2 | 3.422313 | 3.420199 | 1.540500 | 26.01364 | 26.0300 | -0.01635 |
| 10 | 0 | 0 | 3 | 3.396269 | | 1.540500 | 26.21666 | | |
| *** | 0 | 0 | 3 | 3.396269 | 3.395209 | 1.540500 | 26.21666 | 26.2250 | -0.00833 |
| 11 | 1 | 1 | 2 | 3.173136 | | 1.540500 | 28.09673 | | |
| *** | 1 | 1 | 2 | 3.173136 | 3.172775 | 1.540500 | 28.09673 | 28.1000 | -0.00326 |
| 12 | -1 | 1 | 3 | 2.946669 | | 1.540500 | 30.30591 | | |
| *** | -1 | 1 | 3 | 2.946669 | 2.948182 | 1.540500 | 30.30591 | 30.2900 | 0.01592 |
| 13 | 0 | 2 | 3 | 2.736443 | | 1.540500 | 32.69693 | | |
| *** | 0 | 2 | 3 | 2.736443 | 2.737823 | 1.540500 | 32.69693 | 32.6800 | 0.01604 |
| 14 | -2 | 0 | 1 | 2.660244 | | 1.540500 | 33.66068 | | |
| 15 | 1 | 3 | 0 | 2.657844 | | 1.540500 | 33.69226 | | |
| 16 | 2 | 0 | 0 | 2.629808 | | 1.540500 | 34.06232 | | |
| *** | 2 | 0 | 0 | 2.629808 | 2.629612 | 1.540500 | 34.06232 | 34.0650 | -0.00266 |
| 17 | -1 | 3 | 1 | 2.628569 | | 1.540500 | 34.07889 | | |
| 18 | 1 | 1 | 3 | 2.548707 | | 1.540500 | 35.18100 | | |
| 19 | 0 | 0 | 4 | 2.547202 | | 1.540500 | 35.20245 | | |
| *** | 0 | 0 | 4 | 2.547202 | 2.547377 | 1.540500 | 35.20245 | 35.2000 | 0.00247 |
| 20 | -2 | 0 | 2 | 2.521552 | | 1.540500 | 35.57245 | | |
| 21 | 1 | 3 | 1 | 2.518521 | | 1.540500 | 35.61670 | | |
| 22 | 2 | 0 | 1 | 2.445932 | 2.447917 | 1.540500 | 36.71082 | 36.6800 | 0.03082 |
| 23 | -1 | 3 | 2 | 2.445871 | | 1.540500 | 36.71252 | | |
| 24 | -1 | 1 | 4 | 2.382730 | | 1.540500 | 37.72079 | | |
| 25 | 0 | 4 | 0 | 2.310025 | | 1.540500 | 38.95514 | | |
| 26 | -2 | 2 | 1 | 2.305394 | | 1.540500 | 39.03656 | | |
| 27 | 2 | 2 | 0 | 2.285489 | | 1.540500 | 39.39050 | | |
| 28 | -2 | 0 | 3 | 2.279117 | 2.278299 | 1.540500 | 39.50522 | 39.5200 | -0.01477 |
| 29 | 1 | 3 | 2 | 2.276163 | | 1.540500 | 39.55862 | | |
| 30 | 0 | 4 | 1 | 2.252650 | | 1.540500 | 39.98535 | | |
| 31 | 0 | 2 | 4 | 2.230639 | | 1.540500 | 40.40076 | | |
| 32 | -2 | 2 | 2 | 2.213352 | | 1.540500 | 40.73022 | | |
| 33 | -1 | 3 | 3 | 2.188980 | | 1.540500 | 41.22192 | | |
| 34 | 2 | 0 | 2 | 2.187526 | | 1.540500 | 41.23295 | | |
| 35 | 2 | 2 | 1 | 2.161682 | | 1.540500 | 41.74869 | | |
| 36 | 0 | 0 | 4 | 2.133843 | | 1.540500 | 42.95251 | | |
| 37 | 1 | 1 | 4 | 2.095027 | | 1.540500 | 43.14227 | | |
| 38 | -2 | 2 | 3 | 2.043944 | | 1.540500 | 44.27673 | | |
| 39 | 0 | 0 | 5 | 2.037762 | | 1.540500 | 44.41824 | | |
| 40 | -2 | 0 | 4 | 2.012022 | 2.011912 | 1.540500 | 45.01740 | 45.0200 | -0.00259 |
| 41 | 1 | 3 | 3 | 2.009498 | | 1.540500 | 45.07706 | | |
| 42 | 2 | 2 | 2 | 1.977103 | | 1.540500 | 45.85736 | | |
| 43 | -1 | 1 | 5 | 1.974997 | | 1.540500 | 45.90906 | | |
| 44 | -1 | 3 | 4 | 1.925085 | | 1.540500 | 47.17038 | | |
| 45 | 2 | 0 | 3 | 1.924274 | | 1.540500 | 47.19144 | | |
| 46 | 0 | 4 | 3 | 1.910074 | | 1.540500 | 47.56381 | | |
| 47 | 0 | 2 | 5 | 1.864458 | | 1.540500 | 48.80228 | | |
| 48 | -2 | 2 | 4 | 1.844683 | | 1.540500 | 49.36017 | | |
| 49 | 2 | 2 | 3 | 1.776356 | | 1.540500 | 51.39407 | | |
| 50 | -2 | 0 | 5 | 1.765583 | | 1.540500 | 51.73074 | | |
| 51 | 1 | 1 | 5 | 1.765031 | | 1.540500 | 51.74814 | | |
| 52 | 1 | 3 | 4 | 1.763544 | | 1.540500 | 51.79498 | | |
| 53 | -3 | 1 | 1 | 1.747952 | | 1.540500 | 52.29178 | | |
| 54 | -2 | 4 | 1 | 1.744212 | | 1.540500 | 52.41245 | | |
| 55 | 1 | 5 | 0 | 1.743528 | | 1.540500 | 52.43457 | | |
| 56 | 2 | 4 | 0 | 1.735544 | | 1.540500 | 52.69431 | | |
| 57 | -1 | 5 | 1 | 1.735187 | | 1.540500 | 52.70599 | | |
| 58 | -3 | 1 | 2 | 1.723094 | | 1.540500 | 53.10471 | | |
| 59 | 3 | 1 | 0 | 1.722475 | | 1.540500 | 53.12531 | | |
| 60 | 0 | 0 | 4 | 1.711156 | | 1.540500 | 53.50458 | | |
| 61 | -2 | 4 | 2 | 1.703315 | | 1.540500 | 53.77066 | | |
| 62 | 1 | 5 | 1 | 1.702380 | | 1.540500 | 53.80255 | | |
| 63 | 0 | 0 | 6 | 1.698134 | | 1.540500 | 53.94797 | | |
| 64 | -1 | 3 | 5 | 1.690141 | | 1.540500 | 54.22397 | | |
| 65 | 2 | 0 | 4 | 1.689301 | | 1.540500 | 54.25317 | | |
| 66 | 2 | 4 | 1 | 1.679427 | | 1.540500 | 54.59854 | | |
| 67 | -1 | 5 | 2 | 1.679390 | | 1.540500 | 54.59985 | | |
| 68 | -1 | 1 | 6 | 1.676312 | | 1.540500 | 54.70847 | | |
| 69 | -3 | 1 | 3 | 1.653888 | | 1.540500 | 55.51373 | | |
| 70 | 3 | 1 | 1 | 1.652792 | | 1.540500 | 55.55371 | | |
| 71 | -2 | 2 | 5 | 1.649254 | | 1.540500 | 55.68326 | | |
| 72 | -2 | 4 | 3 | 1.622396 | | 1.540500 | 56.68756 | | |
| 73 | 1 | 5 | 2 | 1.621330 | | 1.540500 | 56.72818 | | |
| 74 | 0 | 2 | 6 | 1.593879 | | 1.540500 | 57.79642 | | |
| 75 | -1 | 5 | 3 | 1.588568 | | 1.540500 | 58.00800 | | |
| 76 | 2 | 4 | 2 | 1.588356 | | 1.540500 | 58.01645 | | |
| 77 | 2 | 2 | 4 | 1.586568 | | 1.540500 | 58.08807 | | |
| 78 | -3 | 1 | 4 | 1.554573 | | 1.540500 | 59.28934 | | |
| 79 | -2 | 0 | 6 | 1.554496 | | 1.540500 | 59.40521 | | |
| 80 | 3 | 1 | 2 | 1.553510 | | 1.540500 | 59.47336 | | |
| 81 | 1 | 1 | 5 | 1.552877 | | 1.540500 | 59.96957 | | |
| 82 | -3 | 3 | 1 | 1.541208 | | 1.540500 | 59.96957 | | |
| *** | 0 | 6 | 0 | 1.540017 | 1.542131 | 1.540500 | 60.02072 | 59.9300 | 0.09073 |
| 83 | 0 | 6 | 0 | 1.540017 | | 1.540500 | 60.02072 | | |
| 84 | 0 | 4 | 5 | 1.528153 | | 1.540500 | 60.53525 | | |

| N | H | K | L | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|--------|-------|--------|--------------|-------------|--------------|
| 1 | 0 | 0 | 1 | 10.151373 | | 1.540500 | 8.70316 | | |
| 2 | 0 | 0 | 2 | 5.075686 | | 1.540500 | 17.45703 | | |
| *** | 0 | 0 | 2 | 5.075686 | 5.071955 | 1.540500 | 17.45703 | 17.4700 | -0.01295 |
| 3 | 0 | 2 | 0 | 4.612772 | | 1.540500 | 19.22478 | | |
| *** | 0 | 2 | 0 | 4.612772 | 4.625160 | 1.540500 | 19.22478 | 19.2400 | -0.01521 |
| 4 | 1 | 1 | 0 | 4.560875 | | 1.540500 | 19.44565 | | |
| *** | 1 | 1 | 0 | 4.560875 | 4.555171 | 1.540500 | 19.44565 | 19.4530 | -0.00734 |
| 5 | -1 | 1 | 1 | 4.416381 | | 1.540500 | 20.08835 | | |
| 6 | 0 | 2 | 1 | 4.199546 | | 1.540500 | 21.13719 | | |
| 7 | 1 | 1 | 1 | 3.944102 | | 1.540500 | 22.52350 | | |
| 8 | -1 | 1 | 2 | 3.679170 | | 1.540500 | 24.16902 | | |
| *** | -1 | 1 | 2 | 3.679170 | 3.676776 | 1.540500 | 24.16902 | 24.1850 | -0.01597 |
| 9 | 0 | 2 | 2 | 3.413674 | | 1.540500 | 26.08061 | | |
| 10 | 0 | 0 | 3 | 3.383792 | | 1.540500 | 26.31505 | | |
| *** | 0 | 0 | 3 | 3.383792 | 3.383802 | 1.540500 | 26.31505 | 26.3150 | 0.00007 |
| 11 | 1 | 1 | 2 | 3.163815 | | 1.540500 | 28.18121 | | |
| 12 | -1 | 1 | 3 | 2.937512 | | 1.540500 | 30.40265 | | |
| 13 | 0 | 2 | 3 | 2.728399 | | 1.540500 | 32.79602 | | |
| 14 | -2 | 0 | 1 | 2.653856 | | 1.540500 | 33.74435 | | |
| 15 | 1 | 3 | 0 | 2.653085 | | 1.540500 | 33.75449 | | |
| 16 | -1 | 3 | 1 | 2.623126 | | 1.540500 | 34.14374 | | |
| 17 | 2 | 0 | 0 | 2.623456 | | 1.540500 | 34.14734 | | |
| 18 | 1 | 1 | 3 | 2.540579 | | 1.540500 | 35.29727 | | |
| 19 | 0 | 0 | 4 | 2.537843 | | 1.540500 | 35.33655 | | |
| 20 | -2 | 0 | 2 | 2.515105 | | 1.540500 | 35.66669 | | |
| 21 | 1 | 3 | 1 | 2.513553 | | 1.540500 | 35.68945 | | |
| 22 | -1 | 3 | 2 | 2.440650 | | 1.540500 | 36.79248 | | |
| 23 | 2 | 0 | 1 | 2.439654 | | 1.540500 | 36.80865 | | |
| *** | 2 | 0 | 1 | 2.439654 | 2.438100 | 1.540500 | 36.80865 | 36.8330 | -0.02432 |
| 24 | -1 | 1 | 4 | 2.374637 | | 1.540500 | 37.85092 | | |
| 25 | 0 | 4 | 0 | 2.306386 | | 1.540500 | 39.01910 | | |
| 26 | -2 | 2 | 1 | 2.300320 | | 1.540500 | 39.12616 | | |
| 27 | 2 | -2 | 0 | 2.280437 | | 1.540500 | 39.48141 | | |
| 28 | -2 | 0 | 3 | 2.272784 | | 1.540500 | 39.61990 | | |
| 29 | 1 | 3 | 2 | 2.270980 | | 1.540500 | 39.65268 | | |
| *** | 1 | 3 | 2 | 2.270980 | 2.270306 | 1.540500 | 39.65268 | 39.6650 | -0.01230 |
| 30 | 0 | 4 | 1 | 2.249069 | | 1.540500 | 40.05545 | | |
| 31 | 0 | 2 | 4 | 2.223523 | | 1.540500 | 40.53552 | | |
| 32 | -2 | 2 | 2 | 2.208151 | | 1.540500 | 40.82968 | | |
| 33 | -1 | 3 | 3 | 2.182783 | | 1.540500 | 41.32654 | | |
| *** | 2 | 0 | 2 | 2.181458 | 2.182609 | 1.540500 | 41.35278 | 41.3300 | 0.02280 |
| 34 | 2 | 0 | 2 | 2.181458 | | 1.540500 | 41.35278 | | |
| 35 | 2 | 2 | 1 | 2.156602 | | 1.540500 | 41.85165 | | |
| 36 | 0 | 4 | 2 | 2.099772 | | 1.540500 | 43.03992 | | |
| 37 | 1 | 1 | 4 | 2.088031 | | 1.540500 | 43.29413 | | |
| 38 | -2 | 2 | 3 | 2.038746 | | 1.540500 | 44.39563 | | |
| 39 | 0 | 0 | 5 | 2.030274 | | 1.540500 | 44.59082 | | |
| 40 | -2 | 0 | 4 | 2.006005 | | 1.540500 | 45.15979 | | |
| 41 | 1 | 3 | 3 | 2.004314 | | 1.540500 | 45.20004 | | |
| *** | 1 | 3 | 3 | 2.004314 | 2.004548 | 1.540500 | 45.20004 | 45.1850 | 0.01505 |
| 42 | 2 | 2 | 2 | 1.972052 | | 1.540500 | 45.98157 | | |
| 43 | -1 | 1 | 5 | 1.968219 | | 1.540500 | 46.07626 | | |
| 44 | -1 | 3 | 4 | 1.919868 | | 1.540500 | 47.30637 | | |
| 45 | 2 | 0 | 3 | 1.918568 | | 1.540500 | 47.34036 | | |
| 46 | 0 | 4 | 3 | 1.905794 | | 1.540500 | 47.67728 | | |
| 47 | 0 | 2 | 5 | 1.858244 | | 1.540500 | 48.97620 | | |
| 48 | -2 | 2 | 4 | 1.835584 | | 1.540500 | 49.59616 | | |
| 49 | 2 | 2 | 3 | 1.771452 | | 1.540500 | 51.54675 | | |
| 50 | -2 | 0 | 5 | 1.760011 | | 1.540500 | 51.90671 | | |
| 51 | 1 | 1 | 5 | 1.758574 | | 1.540500 | 51.93958 | | |
| 52 | 1 | 3 | 4 | 1.758559 | | 1.540500 | 51.95273 | | |
| 53 | -3 | 1 | 1 | 1.743824 | | 1.540500 | 52.42502 | | |
| 54 | -2 | 4 | 1 | 1.740639 | | 1.540500 | 52.52173 | | |
| 55 | 1 | 5 | 0 | 1.740621 | | 1.540500 | 52.52884 | | |
| 56 | -1 | 5 | 1 | 1.732251 | | 1.540500 | 52.80222 | | |
| 57 | 2 | 4 | 0 | 1.732174 | | 1.540500 | 52.80475 | | |
| 58 | -3 | 1 | 2 | 1.718937 | | 1.540500 | 53.24326 | | |
| 59 | 3 | 1 | 0 | 1.718365 | | 1.540500 | 53.26239 | | |
| 60 | 0 | 4 | 4 | 1.706837 | | 1.540500 | 53.65082 | | |
| 61 | -2 | 4 | 2 | 1.699868 | | 1.540500 | 53.88849 | | |
| 62 | 1 | 5 | 1 | 1.699385 | | 1.540500 | 53.90494 | | |
| 63 | 0 | 0 | 6 | 1.691895 | | 1.540500 | 54.16315 | | |
| 64 | -1 | 3 | 5 | 1.685179 | | 1.540500 | 54.39679 | | |
| 65 | 2 | 0 | 4 | 1.684031 | | 1.540500 | 54.43695 | | |
| *** | 2 | 0 | 4 | 1.684031 | 1.683944 | 1.540500 | 54.43695 | 54.4400 | -0.00302 |
| 66 | -1 | 5 | 2 | 1.676331 | | 1.540500 | 54.70782 | | |
| 67 | 2 | 4 | 1 | 1.675596 | | 1.540500 | 54.71967 | | |
| 68 | -1 | 1 | 6 | 1.670439 | | 1.540500 | 54.91702 | | |
| 69 | -3 | 1 | 3 | 1.649711 | | 1.540500 | 55.66647 | | |
| 70 | 3 | 1 | 1 | 1.648701 | | 1.540500 | 55.70358 | | |
| 71 | -2 | 2 | 5 | 1.644381 | | 1.540500 | 55.86270 | | |
| 72 | -2 | 4 | 3 | 1.618851 | | 1.540500 | 56.82294 | | |
| 73 | 1 | 5 | 2 | 1.618158 | | 1.540500 | 56.84793 | | |
| 74 | 0 | 2 | 6 | 1.588420 | | 1.540500 | 58.01389 | | |
| 75 | -1 | 5 | 3 | 1.585357 | | 1.540500 | 58.13669 | | |
| 76 | 2 | 4 | 2 | 1.584649 | | 1.540500 | 58.15710 | | |
| 77 | 2 | 2 | 4 | 1.581906 | | 1.540500 | 58.27570 | | |
| 78 | -3 | 1 | 4 | 1.550722 | | 1.540500 | 59.56433 | | |
| *** | 3 | 1 | -4 | 1.550722 | 1.550542 | 1.540500 | 59.56433 | 59.5550 | 0.00334 |
| 79 | 3 | 1 | 2 | 1.549464 | | 1.540500 | 59.61758 | | |
| 80 | -2 | 0 | 6 | 1.549357 | | 1.540500 | 59.62042 | | |
| 81 | 1 | 3 | 5 | 1.548158 | | 1.540500 | 59.67133 | | |
| 82 | -3 | 3 | 1 | 1.537837 | | 1.540500 | 60.11459 | | |
| 83 | 0 | 6 | 0 | 1.537591 | | 1.540500 | 60.12521 | | |
| *** | 0 | 6 | 0 | 1.537591 | 1.537711 | 1.540500 | 60.12521 | 60.1200 | 0.00522 |
| 84 | 0 | 4 | 5 | 1.523940 | | 1.540500 | 60.72025 | | |
| 85 | -3 | 3 | 2 | 1.520667 | | 1.540500 | 60.86386 | | |

| N | H | K | L | | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | | 10.156191 | | 1.540500 | 8.69902 | | |
| 2 | 0 | 0 | 2 | | 5.078055 | | 1.540500 | 17.44868 | | |
| *** | 0 | 0 | 2 | | 5.078055 | 5.105682 | 1.540500 | 17.44868 | 17.3400 | 0.10869 |
| 3 | 0 | 2 | 0 | | 4.683037 | | 1.540500 | 18.93364 | | |
| *** | 0 | 2 | 0 | R | 4.683037 | 4.595688 | 1.540500 | 18.93364 | 19.2800 | -0.34635 |
| 4 | 1 | 1 | 0 | | 4.535029 | | 1.540500 | 19.55756 | | |
| *** | 1 | 1 | 0 | | 4.535029 | 4.531028 | 1.540500 | 19.55756 | 19.5750 | -0.01744 |
| 5 | -1 | 1 | 1 | | 4.442572 | | 1.540500 | 19.96689 | | |
| 6 | 0 | 2 | 1 | | 4.252714 | | 1.540500 | 20.86995 | | |
| 7 | 1 | 1 | 1 | | 3.853166 | | 1.540500 | 22.82201 | | |
| 8 | -1 | 1 | 2 | | 3.724612 | | 1.540500 | 23.86977 | | |
| *** | -1 | 1 | 2 | | 3.724612 | 3.723043 | 1.540500 | 23.86977 | 23.8300 | -0.01922 |
| 9 | 0 | 2 | 2 | | 3.442612 | | 1.540500 | 25.85757 | | |
| 10 | 0 | 0 | 3 | | 3.385357 | | 1.540500 | 26.30235 | | |
| *** | 0 | 0 | 3 | | 3.385357 | 3.386961 | 1.540500 | 26.30235 | 26.2900 | 0.01237 |
| 11 | 1 | 1 | 2 | | 3.120129 | | 1.540500 | 28.58411 | | |
| *** | 1 | 1 | 2 | R | 3.120129 | 3.170012 | 1.540500 | 28.58411 | 28.1250 | 0.45912 |
| 12 | -1 | 1 | 3 | | 2.976154 | | 1.540500 | 29.99857 | | |
| 13 | 0 | 2 | 3 | | 2.743581 | | 1.540500 | 32.60947 | | |
| *** | 0 | 2 | 3 | | 2.743581 | 2.744769 | 1.540500 | 32.60947 | 32.5950 | 0.01450 |
| 14 | 1 | 3 | 0 | | 2.674347 | | 1.540500 | 33.47821 | | |
| 15 | -1 | 3 | 1 | | 2.655087 | | 1.540500 | 33.72827 | | |
| 16 | -2 | 0 | 1 | | 2.641937 | | 1.540500 | 33.90121 | | |
| *** | -2 | 0 | 1 | | 2.641937 | 2.642788 | 1.540500 | 33.90121 | 33.8900 | 0.01123 |
| *** | 2 | 0 | 0 | R | 2.591567 | 2.621025 | 1.540500 | 34.58066 | 34.1800 | 0.40067 |
| 17 | 2 | 0 | 0 | | 2.591567 | | 1.540500 | 34.58066 | | |
| 18 | 0 | 0 | 4 | | 2.539047 | | 1.540500 | 35.31924 | | |
| 19 | -2 | 0 | 2 | | 2.523481 | | 1.540500 | 35.54434 | | |
| 20 | 1 | 3 | 1 | | 2.522388 | | 1.540500 | 35.56027 | | |
| 21 | 1 | 1 | 3 | | 2.509010 | | 1.540500 | 35.75626 | | |
| 22 | -1 | 3 | 2 | | 2.474766 | | 1.540500 | 36.26813 | | |
| *** | 2 | 0 | 1 | R | 2.357964 | 2.456326 | 1.540500 | 37.47220 | 36.5500 | 0.92221 |
| 23 | -1 | 1 | 4 | | 2.403518 | | 1.540500 | 37.38242 | | |
| 24 | 2 | 0 | 1 | | 2.357964 | | 1.540500 | 37.47220 | | |
| 25 | 0 | 4 | 0 | | 2.341518 | | 1.540500 | 38.41049 | | |
| 26 | -2 | 2 | 1 | | 2.301023 | | 1.540500 | 39.11371 | | |
| 27 | -2 | 0 | 3 | | 2.292558 | | 1.540500 | 39.25623 | | |
| 28 | 0 | 4 | 1 | | 2.281665 | | 1.540500 | 39.45929 | | |
| 29 | 1 | 3 | 2 | | 2.270877 | | 1.540500 | 39.65457 | | |
| 30 | 2 | 2 | 0 | | 2.261515 | | 1.540500 | 39.71582 | | |
| 31 | 0 | 2 | 4 | | 2.232085 | | 1.540500 | 40.37344 | | |
| 32 | -2 | 2 | 2 | | 2.221487 | | 1.540500 | 40.57452 | | |
| 33 | -1 | 3 | 3 | | 2.213525 | | 1.540500 | 40.72693 | | |
| *** | 2 | 0 | 2 | R | 2.140250 | 2.178827 | 1.540500 | 42.18661 | 41.4050 | 0.78162 |
| 34 | 2 | 0 | 2 | | 2.140250 | | 1.540500 | 42.18661 | | |
| 35 | 2 | 2 | 1 | | 2.134416 | | 1.540500 | 42.33743 | | |
| 36 | 0 | 4 | 2 | | 2.126357 | | 1.540500 | 42.47552 | | |
| 37 | 1 | 1 | 4 | | 2.065585 | | 1.540500 | 43.78867 | | |
| 38 | -2 | 2 | 3 | | 2.059384 | | 1.540500 | 43.92743 | | |
| 39 | 0 | 0 | 5 | | 2.031239 | | 1.540500 | 44.56851 | | |
| *** | 0 | 0 | 5 | | 2.031239 | 2.029015 | 1.540500 | 44.56851 | 44.6200 | -0.05148 |
| 40 | -2 | 0 | 4 | | 2.029658 | | 1.540500 | 44.60416 | | |
| 41 | 1 | 3 | 3 | | 1.999805 | | 1.540500 | 45.30762 | | |
| *** | 1 | 3 | 3 | | 1.999805 | 1.999706 | 1.540500 | 45.30762 | 45.3100 | -0.00238 |
| 42 | -1 | 1 | 5 | | 1.989258 | | 1.540500 | 45.56036 | | |
| 43 | 2 | 2 | 2 | | 1.946593 | | 1.540500 | 46.61816 | | |
| 44 | -1 | 3 | 4 | | 1.945147 | | 1.540500 | 46.65491 | | |
| 45 | 0 | 4 | 3 | | 1.925769 | | 1.540500 | 47.15259 | | |
| 46 | 2 | 0 | 3 | | 1.882773 | | 1.540500 | 48.29709 | | |
| 47 | 0 | 2 | 5 | | 1.863495 | | 1.540500 | 48.82916 | | |
| 48 | -2 | 2 | 4 | | 1.862306 | | 1.540500 | 48.86237 | | |
| 49 | -2 | 0 | 5 | | 1.782668 | | 1.540500 | 51.19988 | | |
| 50 | 1 | 5 | 0 | | 1.761694 | | 1.540500 | 51.85342 | | |
| 51 | -1 | 5 | 1 | | 1.756154 | | 1.540500 | 52.02924 | | |
| 52 | 1 | 3 | 4 | | 1.752577 | | 1.540500 | 52.14340 | | |
| 53 | -2 | 4 | 1 | | 1.752334 | | 1.540500 | 52.15118 | | |
| 54 | 2 | 2 | 3 | | 1.746880 | | 1.540500 | 52.32632 | | |
| 55 | 1 | 1 | 5 | | 1.742655 | | 1.540500 | 52.46271 | | |
| 56 | 2 | 4 | 0 | | 1.737398 | | 1.540500 | 52.63376 | | |
| 57 | -3 | 1 | 1 | | 1.732587 | | 1.540500 | 52.79120 | | |
| 58 | 0 | 4 | 4 | | 1.721306 | | 1.540500 | 53.16422 | | |
| 59 | -3 | 1 | 2 | | 1.716920 | | 1.540500 | 53.31076 | | |
| 60 | -2 | 4 | 2 | | 1.716431 | | 1.540500 | 53.32715 | | |
| 61 | 1 | 5 | 1 | | 1.716066 | | 1.540500 | 53.33868 | | |
| 62 | -1 | 3 | 5 | | 1.705251 | | 1.540500 | 53.70468 | | |
| 63 | -1 | 5 | 2 | | 1.700655 | | 1.540500 | 53.85455 | | |
| 64 | 3 | 1 | 0 | | 1.699046 | | 1.540500 | 53.91666 | | |
| 65 | 0 | 0 | 6 | | 1.692658 | | 1.540500 | 54.13531 | | |
| 66 | -1 | 1 | 6 | | 1.688264 | | 1.540500 | 54.35889 | | |
| *** | 2 | 0 | 4 | R | 1.654572 | 1.685659 | 1.540500 | 55.48880 | 54.3900 | 1.10983 |
| 67 | 2 | 4 | 1 | | 1.675304 | | 1.540500 | 54.74417 | | |
| 68 | -2 | 2 | 5 | | 1.666041 | | 1.540500 | 55.07425 | | |
| 69 | -3 | 1 | 3 | | 1.655822 | | 1.540500 | 55.44333 | | |
| 70 | 2 | 0 | 4 | | 1.654572 | | 1.540500 | 55.48880 | | |
| 71 | -2 | 4 | 3 | | 1.638280 | | 1.540500 | 56.08905 | | |
| 72 | 1 | 5 | 2 | | 1.630155 | | 1.540500 | 56.39355 | | |
| 73 | 3 | 1 | 1 | | 1.624179 | | 1.540500 | 56.61969 | | |
| 74 | -1 | 5 | 3 | | 1.608544 | | 1.540500 | 57.22052 | | |
| 75 | 0 | 2 | 6 | | 1.591900 | | 1.540500 | 57.87503 | | |
| 76 | 2 | 4 | 2 | | 1.579757 | | 1.540500 | 58.36261 | | |
| 77 | -2 | 0 | 6 | | 1.569417 | | 1.540500 | 58.78467 | | |
| 78 | -3 | 1 | 4 | | 1.562467 | | 1.540500 | 59.07199 | | |
| 79 | 0 | 6 | 0 | | 1.561012 | | 1.540500 | 59.13248 | | |
| 80 | 2 | 2 | 4 | | 1.560064 | | 1.540500 | 59.17263 | | |
| 81 | -2 | 6 | 1 | | 1.542854 | | 1.540500 | 59.89734 | | |
| 82 | 1 | 3 | 5 | | 1.542147 | | 1.540500 | 59.92935 | | |
| *** | 0 | 6 | 0 | R | 1.561012 | 1.534934 | 1.540500 | 59.13248 | 60.2400 | -1.10751 |
| 83 | -3 | 2 | 1 | | 1.535153 | | 1.540500 | 60.23053 | | |
| 84 | 0 | 2 | 5 | | 1.534361 | | 1.540500 | 60.26483 | | |
| 85 | -2 | 4 | 4 | | 1.533657 | | 1.540500 | 60.29364 | | |

| N | H | K | L | D-CALC | D-OBS | LAMBDA | 2-THETA-CALC | 2-THETA-OBS | 2-THETA-DIFF |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 10.130881 | | 1.540500 | 8.72079 | | |
| 2 | 0 | 0 | 2 | 5.065442 | | 1.540500 | 17.49261 | | |
| *** | 0 | 0 | 2 | 5.065442 | 5.066198 | 1.540500 | 17.49261 | 17.4900 | 0.00263 |
| 3 | 0 | 2 | 0 | 4.588264 | | 1.540500 | 19.32845 | | |
| *** | 0 | 2 | 0 | 4.598264 | 4.584380 | 1.540500 | 19.32845 | 19.3450 | -0.01653 |
| 4 | -1 | 1 | 0 | 4.544901 | | 1.540500 | 19.51466 | | |
| 5 | -1 | 1 | 1 | 4.363264 | | 1.540500 | 20.33548 | | |
| 6 | 0 | 2 | 1 | 4.179591 | | 1.540500 | 21.23929 | | |
| 7 | 1 | 1 | 1 | 3.959539 | | 1.540500 | 22.43454 | | |
| *** | 1 | 1 | 1 | R | 3.959539 | 3.885965 | 1.540500 | 22.43454 | 22.8650 | -0.43044 |
| 8 | -1 | 1 | 2 | 3.624347 | | 1.540500 | 24.54025 | | |
| 9 | 0 | 2 | 2 | 3.400610 | 3.512424 | 1.540500 | 26.18259 | 25.3350 | -0.84760 |
| *** | 0 | 2 | 2 | R | 3.400610 | 3.408618 | 1.540500 | 26.18259 | 26.1200 | 0.06260 |
| 10 | 0 | 0 | 3 | 3.376962 | | 1.540500 | 26.36923 | | |
| *** | 0 | 0 | 3 | 3.376962 | 3.376238 | 1.540500 | 26.36923 | 26.3750 | -0.00576 |
| 11 | 1 | 1 | 2 | 3.183963 | | 1.540500 | 27.99922 | | |
| 12 | -1 | 1 | 3 | 2.896240 | | 1.540500 | 30.84659 | | |
| 13 | 0 | 2 | 3 | R | 2.719737 | 2.766659 | 1.540500 | 32.90344 | 32.3300 | -0.57346 |
| 14 | 1 | 3 | 0 | 2.640612 | | 1.540500 | 33.91876 | | |
| 15 | -2 | 0 | 1 | R | 2.629469 | 2.624751 | 1.540500 | 34.06686 | 34.1300 | -0.06311 |
| 16 | 2 | 0 | 0 | 2.615809 | | 1.540500 | 34.25021 | | |
| *** | 2 | 0 | 0 | 2.615809 | 2.615828 | 1.540500 | 34.25021 | 34.2500 | 0.00021 |
| 17 | -1 | 3 | 1 | 2.603528 | | 1.540500 | 34.41684 | | |
| 18 | 1 | 1 | 3 | 2.556653 | | 1.540500 | 35.06812 | | |
| 19 | 0 | 0 | 4 | 2.532721 | | 1.540500 | 35.41040 | | |
| *** | 0 | 0 | 4 | 2.532721 | 2.532749 | 1.540500 | 35.41040 | 35.4100 | 0.00043 |
| 20 | 1 | 3 | 1 | 2.509540 | 2.509436 | 1.540500 | 35.74844 | 35.7500 | -0.00156 |
| 21 | -2 | 0 | 2 | 2.479900 | | 1.540500 | 36.19043 | | |
| 22 | 2 | 0 | 1 | R | 2.445968 | 2.455675 | 1.540500 | 36.71027 | 36.5600 | 0.15027 |
| 23 | -1 | 3 | 2 | 2.417339 | | 1.540500 | 37.16083 | | |
| 24 | -1 | 1 | 4 | 2.345395 | | 1.540500 | 38.34451 | | |
| 25 | 0 | 4 | 0 | 2.294131 | | 1.540500 | 39.23602 | | |
| 26 | -2 | 2 | 1 | 2.281388 | | 1.540500 | 39.46426 | | |
| 27 | 1 | 3 | 2 | 2.272466 | | 1.540500 | 39.62570 | | |
| 28 | 2 | 0 | 2 | R | 2.272450 | 2.265645 | 1.540500 | 39.62598 | 39.7500 | -0.12402 |
| 29 | 0 | 4 | 1 | 2.237481 | | 1.540500 | 40.27188 | | |
| 30 | -2 | 0 | 3 | 2.235716 | | 1.540500 | 40.30502 | | |
| 31 | 0 | 2 | 4 | 2.217336 | | 1.540500 | 40.65384 | | |
| 32 | 2 | 0 | 2 | 2.194574 | | 1.540500 | 41.09442 | | |
| 33 | -2 | 2 | 2 | 2.181633 | | 1.540500 | 41.34930 | | |
| 34 | -1 | 3 | 3 | 2.160593 | | 1.540500 | 41.77072 | | |
| 35 | 2 | 2 | 1 | 2.158423 | | 1.540500 | 41.81467 | | |
| 36 | 1 | 1 | 4 | 2.099712 | | 1.540500 | 43.04120 | | |
| 37 | 0 | 4 | 2 | 2.089795 | | 1.540500 | 43.25571 | | |
| 38 | 0 | 0 | 5 | 2.026176 | 2.026429 | 1.540500 | 44.68588 | 44.6800 | 0.00589 |
| 39 | -2 | 2 | 3 | 2.009816 | | 1.540500 | 45.06952 | | |
| 40 | 1 | 3 | 3 | 2.008090 | | 1.540500 | 45.11041 | | |
| 41 | 2 | 2 | 2 | 1.979274 | | 1.540500 | 45.79208 | | |
| 42 | -2 | 0 | 4 | 1.972543 | | 1.540500 | 45.96945 | | |
| 43 | -1 | 1 | 5 | 1.946820 | | 1.540500 | 46.61292 | | |
| 44 | 2 | 0 | 3 | 1.933081 | | 1.540500 | 46.96353 | | |
| 45 | -1 | 3 | 4 | 1.900745 | | 1.540500 | 47.81180 | | |
| 46 | 0 | 4 | 3 | 1.897654 | | 1.540500 | 47.89456 | | |
| 47 | 0 | 2 | 5 | 1.853496 | | 1.540500 | 49.10992 | | |
| 48 | -2 | 2 | 4 | 1.812173 | | 1.540500 | 50.30667 | | |
| 49 | 2 | 2 | 3 | 1.781432 | | 1.540500 | 51.23700 | | |
| 50 | 1 | 1 | 5 | 1.767385 | | 1.540500 | 51.67407 | | |
| 51 | 1 | 3 | 4 | 1.762757 | | 1.540500 | 51.81982 | | |
| 52 | 1 | 5 | 0 | 1.731831 | | 1.540500 | 52.81601 | | |
| 53 | -2 | 0 | 5 | 1.731772 | | 1.540500 | 52.81793 | | |
| 54 | -3 | 1 | 1 | 1.731460 | | 1.540500 | 52.82822 | | |
| 55 | -2 | 4 | 1 | 1.728676 | | 1.540500 | 52.91989 | | |
| 56 | 2 | 4 | 0 | 1.724779 | | 1.540500 | 53.04880 | | |
| 57 | -1 | 5 | 1 | 1.721243 | | 1.540500 | 53.16629 | | |
| 58 | 3 | 1 | 0 | 1.713213 | | 1.540500 | 53.43524 | | |
| 59 | 0 | 4 | 4 | 1.709305 | | 1.540500 | 53.87350 | | |
| 60 | -3 | 1 | 2 | 1.700286 | | 1.540500 | 53.87418 | | |
| 61 | 2 | 0 | 4 | 1.697431 | | 1.540500 | 53.97214 | | |
| 62 | 1 | 5 | 1 | 1.693238 | | 1.540500 | 54.11667 | | |
| 63 | 0 | 0 | 6 | 1.688480 | 1.688385 | 1.540500 | 54.28168 | 54.2850 | -0.00330 |
| 64 | -2 | 4 | 2 | 1.684045 | | 1.540500 | 54.43643 | | |
| 65 | 2 | 4 | 1 | 1.673301 | | 1.540500 | 54.81519 | | |
| 66 | -1 | 3 | 5 | 1.669331 | | 1.540500 | 54.95657 | | |
| 67 | -1 | 5 | 2 | 1.666048 | | 1.540500 | 55.14584 | | |
| 68 | -1 | 1 | 6 | 1.654311 | | 1.540500 | 55.49829 | | |
| 69 | 3 | 1 | 1 | 1.644946 | | 1.540500 | 55.55787 | | |
| 70 | -3 | 1 | 3 | 1.627071 | | 1.540500 | 56.50998 | | |
| 71 | -2 | 2 | 5 | 1.670200 | | 1.540500 | 56.77103 | | |
| 72 | 1 | 5 | 2 | 1.614482 | | 1.540500 | 56.99075 | | |
| 73 | -2 | 4 | 3 | 1.601144 | | 1.540500 | 57.50958 | | |
| 74 | 2 | 2 | 4 | 1.591981 | | 1.540500 | 57.87183 | | |
| 75 | 2 | 4 | 2 | 1.585927 | | 1.540500 | 58.11783 | | |
| 76 | 0 | 2 | 6 | 1.584590 | | 1.540500 | 58.16751 | | |
| 77 | -1 | 5 | 3 | 1.572862 | | 1.540500 | 58.64337 | | |
| 78 | 3 | 1 | 2 | 1.555208 | | 1.540500 | 59.37527 | | |
| 79 | 1 | 3 | 5 | 1.552039 | | 1.540500 | 59.50870 | | |
| 80 | 0 | 6 | 0 | 1.529422 | | 1.540500 | 60.47977 | | |
| *** | 0 | 6 | 0 | 1.529422 | 1.529531 | 1.540500 | 60.47977 | 60.4750 | 0.00479 |
| 81 | -3 | 3 | 1 | 1.527540 | | 1.540500 | 60.56207 | | |
| 82 | -3 | 3 | 0 | 1.526671 | | 1.540500 | 60.60016 | | |
| 83 | -2 | 0 | 6 | 1.526123 | | 1.540500 | 60.62421 | | |
| 84 | 1 | 1 | 6 | 1.519794 | | 1.540500 | 60.90344 | | |
| 85 | 2 | 4 | 5 | 1.518665 | | 1.540500 | 60.95349 | | |
| 86 | 3 | 3 | 0 | 1.514967 | | 1.540500 | 61.11819 | | |
| 87 | 0 | 6 | 1 | 1.512286 | | 1.540500 | 61.23816 | | |
| 88 | -1 | 5 | 4 | 1.511065 | 1.511020 | 1.540500 | 61.29565 | 61.2950 | 0.00067 |
| 89 | -3 | 3 | 2 | 1.506016 | | 1.540500 | 61.52118 | | |
| 90 | 2 | 2 | 5 | 1.497355 | | 1.540500 | 61.91568 | | |
| 91 | -2 | 4 | 4 | 1.495685 | | 1.540500 | 61.99243 | | |

| N | H | K | L | | D-CALC | D-OBS | LAMBDA | 2-THETA-CALC | 2-THETA-OBS | 2-THETA-DIFF |
|---|---|---|---|---|--------|-------|--------|--------------|-------------|--------------|
| 1 | 0 | 0 | 1 | | 10.207149 | | 1.540500 | 8.65551 | | |
| *** | 0 | 0 | 1 | R | 10.207149 | 10.266965 | 1.540500 | 8.65551 | 8.6050 | 0.05051 |
| 2 | 0 | 0 | 2 | | 5.103574 | | 1.540500 | 17.36090 | | |
| *** | 0 | 0 | 2 | | 5.103574 | 5.111147 | 1.540500 | 17.36090 | 17.3350 | 0.02591 |
| 3 | 0 | 2 | 0 | | 4.608973 | | 1.540500 | 19.24078 | | |
| *** | 0 | 2 | 0 | | 4.608973 | 4.609160 | 1.540500 | 19.24078 | 19.2400 | -0.00079 |
| 4 | 1 | 1 | 0 | | 4.561342 | | 1.540500 | 19.44363 | | |
| *** | 1 | 1 | 0 | | 4.561342 | 4.566840 | 1.540500 | 19.44363 | 19.4200 | 0.02364 |
| 5 | -1 | 1 | 1 | | 4.415116 | 4.425837 | 1.540500 | 20.09416 | 20.0450 | 0.04918 |
| 6 | 0 | 2 | -1 | | 4.201593 | | 1.540500 | 21.13187 | | |
| 7 | 1 | 1 | 1 | | 3.952124 | | 1.540500 | 22.47719 | | |
| *** | 1 | 1 | 1 | | 3.952124 | 3.955983 | 1.540500 | 22.47719 | 22.4550 | 0.02221 |
| 8 | -1 | 1 | 2 | | 3.692734 | | 1.540500 | 24.14528 | | |
| *** | -1 | 1 | 2 | | 3.692734 | 3.683527 | 1.540500 | 24.14528 | 24.1400 | 0.00528 |
| 9 | 0 | 2 | 2 | | 3.420568 | | 1.540500 | 26.02713 | | |
| 10 | 0 | 0 | 3 | | 3.402384 | | 1.540500 | 26.16870 | | |
| *** | 0 | 0 | 3 | | 3.402384 | 3.402858 | 1.540500 | 26.16870 | 26.1650 | 0.00371 |
| 11 | 1 | 1 | 2 | | 3.175323 | | 1.540500 | 28.07697 | | |
| *** | 1 | 1 | 2 | | 3.175323 | 3.173328 | 1.540500 | 28.07697 | 28.0950 | -0.01801 |
| 12 | -1 | 1 | 3 | | 2.944212 | | 1.540500 | 30.33180 | | |
| *** | -1 | 1 | 3 | | 2.944212 | 2.944385 | 1.540500 | 30.33180 | 30.3300 | 0.00182 |
| 13 | 0 | 2 | 3 | | 2.737323 | | 1.540500 | 32.68610 | | |
| *** | 0 | 2 | 3 | | 2.737323 | 2.736692 | 1.540500 | 32.68610 | 32.6950 | -0.00888 |
| 14 | -2 | 0 | 1 | | 2.653230 | | 1.540500 | 33.75262 | | |
| *** | -2 | 0 | 1 | | 2.653230 | 2.652667 | 1.540500 | 33.75262 | 33.7600 | -0.00735 |
| 15 | 1 | 3 | 0 | R | 2.651731 | 2.645061 | 1.540500 | 33.77225 | 33.8600 | -0.08774 |
| 16 | 2 | 0 | 0 | | 2.624513 | | 1.540500 | 34.13318 | | |
| *** | 2 | 0 | 0 | | 2.624513 | 2.624005 | 1.540500 | 34.13318 | 34.1400 | -0.00681 |
| 17 | -1 | 3 | 1 | | 2.622063 | | 1.540500 | 34.16605 | | |
| 18 | -1 | 1 | 4 | | 2.552100 | | 1.540500 | 35.13266 | | |
| 19 | 0 | 0 | 4 | | 2.551787 | | 1.540500 | 35.13715 | | |
| *** | 0 | 0 | 4 | | 2.551787 | 2.551589 | 1.540500 | 35.13715 | 35.1400 | -0.00284 |
| 20 | -2 | 0 | 2 | | 2.514787 | 2.514881 | 1.540500 | 35.67136 | 35.6700 | 0.00137 |
| 21 | 1 | 3 | 1 | R | 2.514391 | 2.482249 | 1.540500 | 35.67719 | 36.1550 | -0.47781 |
| 22 | 2 | 0 | 1 | | 2.443385 | | 1.540500 | 36.75043 | | |
| 23 | -1 | 3 | 2 | R | 2.443401 | 2.441940 | 1.540500 | 36.79385 | 36.7730 | 0.02087 |
| 24 | -1 | 1 | 4 | | 2.392398 | | 1.540500 | 37.72641 | | |
| 25 | 0 | 4 | 0 | | 2.304486 | | 1.540500 | 39.05255 | | |
| 26 | -2 | 2 | 1 | | 2.299439 | | 1.540500 | 39.14175 | | |
| 27 | 2 | 2 | 0 | | 2.280671 | | 1.540500 | 39.47720 | | |
| 28 | 1 | 3 | 2 | R | 2.274313 | 2.274267 | 1.540500 | 39.59216 | 39.5930 | -0.00082 |
| 29 | -2 | 0 | 3 | | 2.273952 | | 1.540500 | 39.59869 | | |
| 30 | 0 | 4 | 1 | | 2.247908 | | 1.540500 | 40.07706 | | |
| 31 | 0 | 2 | 4 | | 2.232461 | | 1.540500 | 40.36636 | | |
| 32 | -2 | 2 | 2 | | 2.207559 | | 1.540500 | 40.84189 | | |
| 33 | 2 | 0 | 2 | | 2.187204 | | 1.540500 | 41.23743 | | |
| 34 | -1 | 1 | 3 | | 2.194718 | | 1.540500 | 41.28824 | | |
| 35 | -2 | 2 | 1 | | 2.158788 | | 1.540500 | 41.80728 | | |
| 36 | 0 | 4 | 2 | | 2.100296 | | 1.540500 | 43.02866 | | |
| 37 | 1 | 1 | 4 | R | 2.098496 | 2.098376 | 1.540500 | 43.06741 | 43.0700 | -0.00256 |
| 38 | 0 | 0 | 5 | | 2.041430 | | 1.540500 | 44.33417 | | |
| *** | 0 | 0 | 5 | | 2.041430 | 2.041394 | 1.540500 | 44.33417 | 44.3350 | -0.00082 |
| 39 | -2 | 2 | 3 | | 2.039261 | | 1.540500 | 44.38385 | | |
| 40 | -1 | 1 | 3 | | 2.049332 | | 1.540500 | 45.08099 | | |
| 41 | -2 | 0 | 4 | R | 2.008635 | 2.008740 | 1.540500 | 45.09747 | 45.0950 | 0.00250 |
| 42 | 2 | 2 | 2 | | 1.976062 | | 1.540500 | 45.88290 | | |
| 43 | -1 | 1 | 5 | | 1.975615 | | 1.540500 | 45.89386 | | |
| 44 | 2 | 0 | 3 | | 1.925450 | | 1.540500 | 47.16089 | | |
| 45 | -1 | 3 | 4 | | 1.923298 | | 1.540500 | 47.21686 | | |
| 46 | 0 | 4 | 3 | | 1.909022 | | 1.540500 | 47.61819 | | |
| 47 | 0 | 2 | 5 | | 1.866533 | | 1.540500 | 48.74451 | | |
| 48 | -2 | 2 | 4 | | 1.841367 | | 1.540500 | 49.45505 | | |
| 49 | 2 | 2 | 3 | | 1.776649 | | 1.540500 | 51.38495 | | |
| 50 | 1 | 1 | 5 | | 1.768241 | | 1.540500 | 51.64725 | | |
| 51 | 1 | 3 | 4 | | 1.764372 | | 1.540500 | 51.76889 | | |
| 52 | -2 | 3 | 5 | R | 1.743596 | 1.763449 | 1.540500 | 51.79337 | 51.7980 | -0.00461 |
| 53 | -3 | 1 | 1 | | 1.743597 | | 1.540500 | 52.43234 | | |
| 54 | -2 | 4 | 1 | R | 1.739844 | 1.740124 | 1.540500 | 52.55408 | 52.5450 | 0.00909 |
| 55 | 1 | 5 | 0 | | 1.739422 | | 1.540500 | 52.56784 | | |
| 56 | 2 | 4 | 0 | | 1.731672 | | 1.540500 | 52.82123 | | |
| 57 | -1 | 5 | 1 | | 1.730968 | | 1.540500 | 52.84439 | | |
| 58 | -3 | 1 | 0 | | 1.718984 | | 1.540500 | 53.24170 | | |
| 59 | -3 | 1 | 2 | | 1.718420 | | 1.540500 | 53.26053 | | |
| 60 | 1 | 4 | 4 | | 1.710283 | | 1.540500 | 53.53406 | | |
| 61 | 0 | 0 | 6 | | 1.701191 | | 1.540500 | 53.84317 | | |
| 62 | -2 | 4 | 2 | | 1.699109 | | 1.540500 | 53.91794 | | |
| 63 | 1 | 5 | 1 | | 1.698887 | | 1.540500 | 53.92215 | | |
| 64 | 2 | 0 | 4 | | 1.691166 | | 1.540500 | 54.18839 | | |
| 65 | -1 | 3 | 5 | | 1.689440 | 1.689304 | 1.540500 | 54.24832 | 54.2530 | -0.00467 |
| 66 | -1 | 1 | 6 | | 1.677351 | | 1.540500 | 54.67175 | | |
| 67 | 2 | 4 | 1 | | 1.676473 | | 1.540500 | 54.70279 | | |
| 68 | -1 | 5 | 2 | | 1.675572 | | 1.540500 | 54.73465 | | |
| 69 | 3 | 1 | 1 | | 1.650461 | | 1.540500 | 55.63898 | | |
| 70 | -3 | 1 | 3 | | 1.649465 | | 1.540500 | 55.67554 | | |
| 71 | -2 | 2 | 5 | | 1.647129 | | 1.540500 | 55.76135 | | |
| 72 | 1 | 5 | 2 | | 1.618745 | | 1.540500 | 56.82700 | | |
| 73 | -2 | 4 | 3 | | 1.618614 | | 1.540500 | 56.83200 | | |
| 74 | 2 | 2 | 6 | | 1.595947 | | 1.540500 | 57.71442 | | |
| 75 | 2 | 2 | 4 | | 1.587662 | | 1.540500 | 58.04422 | | |
| 76 | -2 | 4 | 2 | R | 1.586464 | 1.586320 | 1.540500 | 58.09225 | 58.0980 | -0.00574 |
| 77 | -1 | 5 | 3 | | 1.585480 | | 1.540500 | 58.13177 | | |
| 78 | 1 | 3 | 5 | | 1.554214 | | 1.540500 | 59.41705 | | |
| 79 | -2 | 0 | 6 | R | 1.553376 | 1.552957 | 1.540500 | 59.44812 | 59.4700 | -0.02185 |
| 80 | 3 | 1 | 2 | | 1.552330 | | 1.540500 | 59.49643 | | |
| 81 | -3 | 3 | 4 | | 1.551097 | | 1.540500 | 59.54892 | | |
| 82 | -3 | 3 | 1 | | 1.537409 | | 1.540500 | 60.13342 | | |
| 83 | 0 | 6 | 0 | | 1.536325 | | 1.540500 | 60.17987 | | |
| 84 | 0 | 4 | 5 | | 1.528998 | | 1.540500 | 60.53817 | | |
| 85 | 1 | 1 | 6 | | 1.521955 | | 1.540500 | 60.81219 | | |
| | | | | | | | 1.540500 | | 60.8800 | -0.03552 |

| N | H | K | L | D-CALC | D-OBS | LAMBDA | 2-THETA-CALC | 2-THETA-OBS | 2-THETA-DIFF |
|---|---|---|---|--------|-------|--------|--------------|-------------|--------------|
| 1 | 0 | 0 | 1 | 10.163612 | | 1.540500 | 8.69094 | | |
| 2 | 0 | 0 | 2 | 5.082806 | | 1.540500 | 17.43240 | | |
| *** | 0 | 0 | 2 | 5.082806 | 5.087847 | 1.540500 | 17.43240 | 17.4150 | 0.01741 |
| 3 | 0 | 2 | 0 | 4.638136 | | 1.540500 | 19.11865 | | |
| *** | 0 | 2 | 0 | 4.638136 | 4.627028 | 1.540500 | 19.11865 | 19.1650 | -0.04633 |
| 4 | -1 | 1 | 0 | 4.586522 | | 1.540500 | 19.33586 | | |
| 5 | -1 | 1 | 1 | 4.438571 | | 1.540500 | 19.98689 | | |
| 6 | 0 | 2 | -1 | 4.219679 | | 1.540500 | 21.03520 | | |
| 7 | 1 | 1 | 1 | 3.963113 | | 1.540500 | 22.41406 | | |
| *** | 1 | 1 | -1 | 3.963113 | 3.963824 | 1.540500 | 22.41406 | 22.4100 | 0.00407 |
| 8 | -1 | 1 | 2 | 3.692713 | | 1.540500 | 24.07904 | | |
| *** | -1 | 1 | 2 | 3.692713 | 3.696352 | 1.540500 | 24.07904 | 24.0550 | -0.02406 |
| 9 | 0 | 2 | 2 | 3.426100 | | 1.540500 | 25.98438 | | |
| *** | 0 | 2 | 2 | 3.426100 | 3.421492 | 1.540500 | 25.98438 | 26.0200 | -0.03561 |
| 10 | 0 | 0 | 3 | 3.388538 | | 1.540500 | 26.27753 | | |
| *** | 0 | 0 | 3 | 3.388538 | 3.389496 | 1.540500 | 26.27753 | 26.2700 | 0.00755 |
| 11 | 1 | 1 | 2 | 3.175736 | | 1.540500 | 28.07324 | | |
| *** | 1 | 1 | 2 | 3.175736 | 3.173551 | 1.540500 | 28.07324 | 28.0930 | -0.01974 |
| 12 | -1 | 1 | 3 | 2.945463 | | 1.540500 | 30.31862 | | |
| *** | -1 | 1 | 3 | 2.945463 | 2.942016 | 1.540500 | 30.31862 | 30.3550 | -0.03637 |
| 13 | 0 | 2 | 3 | 2.736120 | | 1.540500 | 32.70087 | | |
| *** | 0 | 2 | 3 | 2.736120 | 2.735379 | 1.540500 | 32.70087 | 32.7100 | -0.00912 |
| 14 | -2 | 0 | 1 | 2.668512 | | 1.540500 | 33.55356 | | |
| 15 | -1 | 1 | 4 | 2.667786 | | 1.540500 | 33.56296 | | |
| *** | -2 | 0 | 1 R | 2.668512 | 2.652286 | 1.540500 | 33.55356 | 33.7650 | -0.21143 |
| 16 | 2 | 0 | 0 | 2.638315 | | 1.540500 | 33.94916 | | |
| *** | 2 | 0 | 0 | 2.638315 | 2.638254 | 1.540500 | 33.94916 | 33.9500 | -0.00082 |
| 17 | -1 | 3 | 1 | 2.637713 | | 1.540500 | 33.95715 | | |
| 18 | 1 | 1 | 3 | 2.548292 | | 1.540500 | 35.18692 | | |
| 19 | 0 | 2 | 4 | 2.541403 | | 1.540500 | 35.28543 | | |
| *** | 0 | 2 | 4 | 2.541403 | 2.542131 | 1.540500 | 35.28543 | 35.2750 | 0.01044 |
| 20 | -2 | 0 | 2 | 2.527388 | | 1.540500 | 35.48758 | | |
| 21 | 1 | 3 | 1 | 2.526681 | | 1.540500 | 35.49786 | | |
| 22 | -2 | 0 | 1 R | 2.452557 | 2.485240 | 1.540500 | 36.60815 | 36.1100 | 0.49817 |
| 23 | -1 | 3 | 2 R | 2.452154 | 2.451144 | 1.540500 | 36.61435 | 36.6300 | -0.01563 |
| 23 | -1 | 3 | 2 R | 2.452154 | 2.426212 | 1.540500 | 36.61435 | 37.0200 | -0.40564 |
| 24 | -1 | 1 | 4 | 2.379964 | | 1.540500 | 37.76630 | | |
| 25 | 0 | 4 | 0 | 2.319368 | | 1.540500 | 38.79712 | | |
| 26 | -2 | 2 | 1 | 2.313908 | 2.313459 | 1.540500 | 38.90286 | 38.8950 | 0.00787 |
| 27 | 2 | 2 | 0 | 2.293262 | | 1.540500 | 39.25153 | | |
| 28 | -2 | 0 | 3 | 2.282026 | | 1.540500 | 39.45276 | | |
| 29 | -1 | 3 | 2 R | 2.281440 | 2.278299 | 1.540500 | 39.46335 | 39.5200 | -0.05664 |
| 30 | 0 | 4 | 1 | 2.260982 | | 1.540500 | 39.83545 | | |
| 31 | -3 | 2 | 4 | 2.228758 | | 1.540500 | 40.43634 | | |
| 32 | -2 | 2 | 2 | 2.219286 | | 1.540500 | 40.61655 | | |
| 33 | 2 | 0 | 2 | 2.191642 | | 1.540500 | 41.15189 | | |
| 34 | -1 | 3 | 3 | 2.191414 | | 1.540500 | 41.15637 | | |
| 35 | 2 | 0 | 1 | 2.168106 | | 1.540500 | 41.61923 | | |
| 36 | 0 | 4 | 2 | 2.109839 | | 1.540500 | 42.82440 | | |
| 37 | 1 | 1 | 4 | 2.093416 | | 1.540500 | 43.17712 | | |
| 38 | -2 | 2 | 3 | 2.047606 | | 1.540500 | 44.19339 | | |
| 39 | 0 | 0 | 5 | 2.033122 | | 1.540500 | 44.52502 | | |
| *** | 0 | 0 | 5 | 2.033122 | 2.033557 | 1.540500 | 44.52502 | 44.5150 | 0.01004 |
| 40 | 0 | 2 | 4 | 2.017796 | | 1.540500 | 45.00128 | | |
| 41 | 1 | 3 | 3 R | 2.012259 | 2.012463 | 1.540500 | 45.01178 | 45.0070 | 0.00479 |
| 42 | 2 | 2 | 2 | 1.981557 | | 1.540500 | 45.74844 | | |
| 43 | -1 | 1 | 5 | 1.971872 | | 1.540500 | 45.98596 | | |
| 44 | 2 | 0 | 3 | 1.926341 | | 1.540500 | 47.13773 | | |
| 45 | -1 | 3 | 4 | 1.926226 | | 1.540500 | 47.14072 | | |
| 46 | 0 | 4 | 3 | 1.913788 | | 1.540500 | 47.46588 | | |
| 47 | 0 | 2 | 5 | 1.862080 | | 1.540500 | 48.86868 | | |
| 48 | -2 | 2 | 4 | 1.846456 | | 1.540500 | 49.31244 | | |
| 49 | 2 | 2 | 3 | 1.779007 | | 1.540500 | 51.31189 | | |
| 50 | -2 | 0 | 5 | 1.764915 | | 1.540500 | 51.75174 | | |
| 51 | 1 | 3 | 4 | 1.764583 | | 1.540500 | 51.76224 | | |
| 52 | 1 | 1 | 5 | 1.763001 | | 1.540500 | 51.81210 | | |
| 53 | -3 | 1 | 1 | 1.753640 | | 1.540500 | 52.10941 | | |
| 54 | -2 | 4 | 1 | 1.750429 | | 1.540500 | 52.21219 | | |
| 55 | 1 | 5 | 0 R | 1.750223 | 1.750187 | 1.540500 | 52.21681 | 52.2200 | -0.00116 |
| 56 | 2 | 4 | 0 | 1.741823 | | 1.540500 | 52.48981 | | |
| 57 | -1 | 5 | 1 | 1.741650 | | 1.540500 | 52.49545 | | |
| 58 | 3 | 3 | 2 | 1.728145 | | 1.540500 | 52.93744 | | |
| 59 | 3 | 1 | 0 | 1.728087 | | 1.540500 | 52.93933 | | |
| 60 | 0 | 4 | 4 | 1.713049 | | 1.540500 | 53.44077 | | |
| 61 | -2 | 4 | 2 | 1.708737 | | 1.540500 | 53.58636 | | |
| 62 | -1 | 5 | 1 | 1.708519 | | 1.540500 | 53.59375 | | |
| 63 | 0 | 0 | 6 | 1.694269 | | 1.540500 | 54.08105 | | |
| 64 | 2 | 0 | 5 | 1.689989 | | 1.540500 | 54.22922 | | |
| 65 | -1 | 3 | 5 R | 1.689939 | 1.689679 | 1.540500 | 54.23099 | 54.2400 | -0.00900 |
| 66 | 2 | 4 | 1 | 1.685045 | | 1.540500 | 54.40146 | | |
| 67 | -1 | 5 | 2 | 1.684915 | | 1.540500 | 54.40604 | | |
| 68 | -1 | 1 | 6 | 1.673248 | | 1.540500 | 54.81708 | | |
| 69 | -3 | 1 | 3 | 1.657330 | | 1.540500 | 55.37149 | | |
| 70 | 3 | 1 | 1 | 1.657099 | | 1.540500 | 55.37515 | | |
| 71 | -2 | 2 | 5 | 1.649528 | | 1.540500 | 55.67319 | | |
| 72 | -2 | 4 | 3 | 1.626575 | | 1.540500 | 56.52881 | | |
| 73 | 1 | 5 | 2 | 1.626362 | | 1.540500 | 56.53687 | | |
| 74 | -2 | 4 | 2 | 1.592869 | | 1.540500 | 57.83649 | | |
| 75 | -1 | 5 | 3 | 1.592781 | | 1.540500 | 57.84000 | | |
| 76 | 0 | 2 | 6 | 1.591415 | | 1.540500 | 57.89435 | | |
| 77 | 2 | 2 | 4 | 1.587968 | | 1.540500 | 58.03598 | | |
| 78 | -2 | 1 | 6 | 1.557420 | | 1.540500 | 59.27921 | | |
| 79 | 3 | 1 | 2 | 1.557374 | | 1.540500 | 59.28442 | | |
| 80 | -2 | 0 | 6 | 1.553105 | | 1.540500 | 59.46371 | | |
| 81 | 1 | 3 | 5 | 1.552858 | | 1.540500 | 59.47415 | | |
| 82 | 3 | 3 | 1 R | 1.546450 | 1.546581 | 1.540500 | 59.74541 | 59.7400 | 0.00562 |
| *** | 0 | 5 | 0 | 1.546045 | 1.546581 | 1.540500 | 59.76282 | 59.7400 | 0.02283 |
| 83 | 0 | 6 | 0 | 1.546045 | | 1.540500 | 59.76282 | | |
| *** | 0 | 5 | 0 R | 1.546045 | 1.529646 | 1.540500 | 59.76282 | 60.4700 | -0.70715 |
| 84 | -3 | 1 | 2 | 1.528880 | | 1.540500 | 60.50345 | | |
| 84 | -3 | 1 | 2 R | 1.528880 | 1.529646 | 1.540500 | 60.50345 | 60.4700 | 0.03346 |

| N | H | K | L | D CALC | D OBS | LAMBDA | 2-THETA CALC | 2-THETA OBS | 2-THETA DIFF |
|---|---|---|---|--------|-------|--------|--------------|-------------|--------------|
| 1 | 0 | 0 | 1 | 10.440727 | | 1.540500 | 8.46151 | | |
| 2 | 0 | 0 | 2 | 5.220366 | | 1.540500 | 16.96960 | | |
| *** | 0 | 0 | 2 | 5.220366 | 5.223304 | 1.540500 | 16.96960 | 16.9600 | 0.00962 |
| 3 | 0 | 2 | 0 | 4.689141 | | 1.540500 | 18.90878 | | |
| 4 | 1 | 1 | 0 | 4.620929 | | 1.540500 | 19.19052 | | |
| *** | 1 | 1 | 0 | 4.620929 | 4.625833 | 1.540500 | 19.19052 | 19.1700 | 0.02053 |
| 5 | -1 | 1 | 1 | 4.475566 | | 1.540500 | 19.81821 | | |
| 6 | 0 | 2 | 1 | 4.277537 | | 1.540500 | 20.74750 | | |
| 7 | 1 | 1 | 1 | 4.012979 | | 1.540500 | 22.13200 | | |
| *** | 1 | 1 | 1 | 4.012979 | 4.009761 | 1.540500 | 22.13200 | 22.1500 | -0.01799 |
| 8 | -1 | 1 | 2 | 3.743870 | | 1.540500 | 23.74519 | | |
| *** | -1 | 1 | 2 | 3.743870 | 3.744680 | 1.540500 | 23.74519 | 23.7400 | 0.00521 |
| 9 | 0 | 2 | 2 | 3.488463 | | 1.540500 | 25.51195 | | |
| 10 | 0 | 0 | 3 | 3.480244 | | 1.540500 | 25.57321 | | |
| *** | 0 | 0 | 3 | 3.480244 | 3.475339 | 1.540500 | 25.57321 | 25.5800 | -0.00676 |
| 11 | 1 | 1 | 2 | 3.232404 | | 1.540500 | 27.57127 | | |
| *** | 1 | 1 | 2 | 3.232404 | 3.230828 | 1.540500 | 27.57127 | 27.5850 | -0.01371 |
| 12 | -1 | 1 | 3 | 2.959866 | | 1.540500 | 29.75594 | | |
| *** | -1 | 1 | 3 | 2.959866 | 2.959962 | 1.540500 | 29.75594 | 29.7550 | 0.00096 |
| 13 | 0 | 2 | 3 | 2.794634 | | 1.540500 | 31.99762 | | |
| 14 | 1 | 3 | 0 | 2.653557 | | 1.540500 | 33.22742 | | |
| 15 | -2 | 0 | 1 | 2.683756 | | 1.540500 | 33.35739 | | |
| *** | -2 | 0 | 1 | 2.683756 | 2.683162 | 1.540500 | 33.35739 | 33.3650 | -0.00760 |
| 16 | -1 | 3 | 1 | 2.664215 | | 1.540500 | 33.60794 | | |
| 17 | 2 | 0 | 0 | 2.655143 | | 1.540500 | 33.72754 | | |
| 18 | 0 | 0 | 4 | 2.610182 | | 1.540500 | 34.32635 | | |
| *** | 0 | 0 | 4 | 2.610182 | 2.609916 | 1.540500 | 34.32635 | 34.3390 | -0.00363 |
| 19 | 1 | 1 | 3 | 2.602306 | | 1.540500 | 34.43350 | | |
| 20 | 1 | 3 | 1 | 2.556052 | | 1.540500 | 35.07605 | | |
| 21 | -2 | 0 | 2 | 2.546760 | | 1.540500 | 35.20877 | | |
| 22 | -1 | 3 | 2 | 2.482203 | | 1.540500 | 36.15567 | | |
| 23 | 2 | 0 | 1 | 2.475341 | | 1.540500 | 36.25940 | | |
| 24 | -1 | 1 | 4 | 2.430160 | | 1.540500 | 36.94821 | | |
| 25 | 0 | 4 | 0 | 2.344570 | | 1.540500 | 38.35855 | | |
| 26 | -2 | 2 | 1 | 2.329244 | | 1.540500 | 38.62091 | | |
| 27 | 1 | 3 | 2 | 2.314551 | | 1.540500 | 38.87589 | | |
| 28 | 2 | 2 | 0 | 2.310465 | | 1.540500 | 38.94742 | | |
| 29 | -2 | 0 | 3 | 2.307160 | | 1.540500 | 39.00546 | | |
| 30 | 0 | 4 | 1 | 2.287601 | | 1.540500 | 39.35263 | | |
| 31 | 0 | 2 | 4 | 2.280656 | | 1.540500 | 39.47748 | | |
| 32 | -2 | 2 | 2 | 2.237564 | | 1.540500 | 40.26242 | | |
| 33 | -1 | 3 | 3 | 2.224533 | | 1.540500 | 40.51651 | | |
| 34 | 2 | 0 | 2 | 2.219955 | | 1.540500 | 40.60297 | | |
| 35 | 2 | 2 | 1 | 2.189055 | | 1.540500 | 41.20273 | | |
| 36 | 1 | 1 | 4 | 2.141857 | | 1.540500 | 42.15262 | | |
| 37 | 0 | 4 | 2 | 2.138766 | | 1.540500 | 42.21722 | | |
| 38 | 0 | 0 | 5 | 2.088145 | | 1.540500 | 43.29163 | | |
| 39 | -2 | 2 | 3 | 2.070150 | | 1.540500 | 43.68719 | | |
| 40 | 1 | 3 | 3 | 2.047112 | | 1.540500 | 44.20459 | | |
| *** | 0 | 0 | 5 R | 2.088145 | 2.042270 | 1.540500 | 43.29163 | 44.3150 | -1.02335 |
| 41 | -2 | 0 | 4 | 2.041677 | | 1.540500 | 44.32849 | | |
| 42 | -1 | 1 | 5 | 2.017355 | | 1.540500 | 44.89182 | | |
| 43 | 2 | 2 | 2 | 2.006490 | | 1.540500 | 45.14838 | | |
| 44 | -1 | 3 | 4 | 1.960354 | | 1.540500 | 46.27081 | | |
| 45 | 2 | 0 | 3 | 1.957565 | | 1.540500 | 46.34158 | | |
| 46 | 0 | 4 | 3 | 1.944464 | | 1.540500 | 46.67175 | | |
| 47 | 0 | 2 | 5 | 1.907555 | | 1.540500 | 47.63055 | | |
| 48 | -2 | 2 | 4 | 1.871935 | | 1.540500 | 48.59476 | | |
| 49 | 2 | 2 | 3 | 1.806469 | | 1.540500 | 50.47662 | | |
| 50 | 1 | 1 | 5 | 1.805907 | | 1.540500 | 50.49344 | | |
| 51 | 1 | 3 | 4 | 1.799157 | | 1.540500 | 50.69623 | | |
| 52 | -2 | 0 | 5 | 1.795245 | | 1.540500 | 50.81445 | | |
| 53 | 1 | 5 | 0 | 1.768576 | | 1.540500 | 51.63675 | | |
| 54 | -2 | 4 | 1 | 1.765680 | | 1.540500 | 51.72769 | | |
| 55 | -3 | 1 | 1 | 1.763833 | | 1.540500 | 51.78586 | | |
| 56 | -1 | 5 | 1 | 1.760111 | | 1.540500 | 51.90353 | | |
| 57 | 2 | 4 | 0 | 1.757456 | | 1.540500 | 51.98773 | | |
| 58 | 0 | 4 | 4 | 1.744221 | | 1.540500 | 52.41183 | | |
| 59 | 0 | 0 | 6 | 1.740121 | | 1.540500 | 52.54507 | | |
| 60 | 3 | 1 | 0 | 1.739386 | | 1.540500 | 52.56900 | | |
| 61 | -3 | 1 | 2 | 1.738955 | | 1.540500 | 52.58173 | | |
| 62 | 1 | 5 | 1 | 1.727810 | | 1.540500 | 52.94849 | | |
| 63 | -2 | 4 | 2 | 1.724918 | | 1.540500 | 53.04416 | | |
| 64 | -1 | 3 | 5 | 1.723434 | | 1.540500 | 53.09341 | | |
| 65 | 2 | 0 | 4 | 1.721701 | | 1.540500 | 53.15106 | | |
| *** | 2 | 0 | 4 | 1.721701 | 1.722034 | 1.540500 | 53.15106 | 53.1400 | 0.01108 |
| 66 | -1 | 1 | 6 | 1.713639 | | 1.540500 | 53.42090 | | |
| 67 | -1 | 5 | 2 | 1.704442 | | 1.540500 | 53.73224 | | |
| 68 | 2 | 4 | 1 | 1.702216 | | 1.540500 | 53.80817 | | |
| 69 | -2 | 2 | 5 | 1.676577 | | 1.540500 | 54.69913 | | |
| 70 | 3 | 1 | 1 | 1.671375 | | 1.540500 | 54.88364 | | |
| 71 | -3 | 1 | 3 | 1.670662 | | 1.540500 | 54.90836 | | |
| 72 | 1 | 5 | 2 | 1.647146 | | 1.540500 | 55.76071 | | |
| 73 | -2 | 4 | 3 | 1.644476 | | 1.540500 | 55.85916 | | |
| 74 | 0 | 2 | 6 | 1.631411 | | 1.540500 | 56.34625 | | |
| 75 | 2 | 2 | 4 | 1.616202 | | 1.540500 | 56.92453 | | |
| 76 | -1 | 5 | 3 | 1.613750 | | 1.540500 | 57.01898 | | |
| 77 | 2 | 4 | 2 | 1.612016 | | 1.540500 | 57.08594 | | |
| 78 | 1 | 3 | 5 | 1.585935 | | 1.540500 | 58.11349 | | |
| 79 | -2 | 0 | 6 | 1.583109 | | 1.540500 | 58.22714 | | |
| 80 | 3 | 1 | 2 | 1.573144 | | 1.540500 | 58.60730 | | |
| 81 | -3 | 1 | 4 | 1.572876 | | 1.540500 | 58.64279 | | |
| 82 | 0 | 6 | 0 | 1.563047 | | 1.540500 | 59.04785 | | |
| 83 | 0 | 4 | 5 | 1.559351 | | 1.540500 | 59.20178 | | |
| *** | 0 | 6 | 0 R | 1.563047 | 1.557599 | 1.540500 | 59.04785 | 59.2750 | -0.22714 |
| 84 | -3 | 3 | 1 | 1.557210 | | 1.540500 | 59.29129 | | |
| 85 | 1 | 1 | 6 | 1.554676 | | 1.540500 | 59.38919 | | |
| 86 | 0 | 6 | 1 | 1.545621 | | 1.540500 | 59.77237 | | |
| 87 | 1 | 5 | 3 | 1.543038 | | 1.540500 | 59.93399 | | |

# VITA

The author was born in Rockville Center, Long Island, New York on November 1, 1948. He graduated with high honors from Ridgewood High School, Ridgewood, New Jersey where he concentrated in science and music. He entered the Massachusetts Institute of Technology in September of 1966, and subsequently enrolled in the five-year Masters degree program in the Department of Earth and Planetary Sciences.

In addition to his scientific studies, the author has studied trumpet privately for four years with Andre Come of the Boston Symphony Orchestra. He has been principle trumpet of the M. I. T. Symphony Orchestra for five years, and has appeared as soloist with the M. I. T. Concert Band, Symphony Orchestra, and many other groups in more than a dozen states.

Among the author's academic awards are the Harvard Alumni Award (1965), the New Jersey Science Teachers' Award (1966), Outstanding Musician--New York State Music Festival (1966), and the Phi Sigma Kappa Foundation Award (1968). He is a member of Sigma Xi, Phi Lambda Upsilon, and Baton honorary societies.

Professional experience includes summer work with Isotopes, Inc. of Westwood, New Jersey (1968) and as field assistant for the United States Geological Survey (1970). Next year the author will continue his studies at Harvard University, and will receive for a second year a National Science Foundation Fellowship.

The author was married to Margaret Joan Hindle on August 9, 1969.