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X-RAY CRYSTALLOGRAPHY OF WEGSCHEIDERITE ($Na_2CO_3 \cdot 3NaHCO_3$)[1]

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The *x*-ray crystallography of the new mineral wegscheiderite, $Na_2CO_3 \cdot 3NaHCO_3$, has been determined by single-crystal and powder-diffraction techniques. The material used in the study came from the drill core of the Grierson Well No. 1, Green River formation (Eocene), Wyoming, and is described in the preceding paper by Fahey and Yorks. Figure 2 of that paper is a photograph of the actual sample from which the material was taken. In this sample the wegscheiderite occurs as bladed or fibrous aggregates with individual crystals as much as five cm long, without any well-developed crystal faces or cleavages. The specimen was chosen for *x*-ray study because it contained the most perfectly crystalline and least fibrous material available.

Small fragments, approximately 0.2×0.2×0.5 mm, chipped from the specimen described above, were investigated by the Buerger precession technique, using MoKα and CuKα radiation. A study of the *hk*0, *hk*1, *h*0*l* and *h*1*l* reciprocal lattice nets and of the [001] and [010] cone-axis photographs yielded the unit-cell data given in Table 1. The optic axial angle $2V$ was measured on a universal stage in sodium light, using optic-axis interference figures.

X-ray powder-diffraction patterns were made of wegscheiderite from all the localities mentioned in the paper by Fahey and Yorks, as well as of synthetic Wegscheider's salt prepared by Yorks. All the patterns were identical. Indexed powder-diffraction data for wegscheiderite are given

TABLE 1. CRYSTALLOGRAPHIC DATA FOR WEGSCHEIDERITE
Space group: triclinic, $P\bar{1}$, (non-piezoelectric)

Direct Cell	Reciprocal Cell
$a=10.04$ Å ± 0.03 Å	$a^*=0.10588$ Å^{-1}
$b=15.56$ ± 0.04	$b^*=0.68002$
$c=3.466$ ± 0.01	$c^*=0.29072$
$\alpha=91°55'$ $\pm 05'$	$\alpha^*=86°00'$
$\beta=95°49'$ $\pm 05'$	$\beta^*=83°12'$
$\gamma=108°40'$ $\pm 05'$	$\gamma^*=71°01'$
$V=509.1$ Å ± 2.6 Å^3	$V^*=0.001964$ Å^{-3}
$a:b:c=0.6452:1:0.2228$	

Cell contents: $2[Na_2CO_3 \cdot 3NaHCO_3]$

[1] Publication authorized by the Director, U. S. Geol. Survey.

TABLE 2. INDEXED *X*-RAY POWDER DIFFRACTION DATA FOR WEGSCHEIDERITE[1]

h	*k*	*l*	$d_{calc.}$[2]	$d_{meas.}$	I
0	1	0	14.71	14.7_8	13
−1	1	0	9.47	9.44	6
1	0	0	9.45		
0	2	0	7.35		
−1	2	0	7.01		
1	1	0	6.98	6.99	3
−1	3	0	5.08	5.05	2 *b*
1	2	0	5.06		
−2	1	0	4.99		
0	3	0	4.90		
−2	2	0	4.74	4.73	9
2	0	0	4.72		
−2	3	0	4.14	4.13	15
2	1	0	4.12		
−1	4	0	3.87_8		
1	3	0	3.86_7		
0	4	0	3.67_6	3.68	60
−2	4	0	3.50_6	3.49	25
2	2	0	3.49_1		
0	0	1	3.44_0	3.45	2
0	−1	1	3.40_2		
−1	0	1	3.36_3		
−1	1	1	3.31_2	3.31	6
−3	2	0	3.31_0		
−3	1	0	3.30_7		
0	1	1	3.29_9		
−1	−1	1	3.24_5	2.25	15
0	−2	1	3.20_3		
1	−1	1	3.15_9	3.15_7	4
−3	3	0	3.15_7		
3	0	0	3.14_8		
1	0	1	3.11_6		
−1	2	1	3.11_4		
−1	5	0	3.11_0	3.108	21
1	4	0	3.10_2		
1	−2	1	3.06_3	3.07_7	30
0	2	1	3.03_5	3.04_2	9
−1	−2	1	3.00_4	3.00_4	5
−2	1	1	2.977		
−2	5	0	2.967		
2	3	0	2.954	2.95_4	100 *b*
−2	0	1	2.952		
1	1	1	2.948		
0	5	0	2.941		
0	5	0	2.942		
0	−3	1	2.913	2.91_4	42
−3	4	0	2.903		
3	1	0	2.892		
−2	2	1	2.886		
1	−3	1	2.860	2.85_8	6
−1	3	1	2.836	2.83_2	35
−2	−1	1	2.817	2.79_9	50
0	3	1	2.727	2.72_8	30
−1	−3	1	2.713		
1	2	1	2.708		
2	−1	1	2.707		
−2	3	1	2.706		
2	−2	1	2.690	2.66_0	42
2	0	1	2.636	2.64_2	60
−3	5	0	2.615	2.62_1	4
−2	−2	1	2.613		
1	−4	1	2.606		
0	−4	1	2.604		
3	2	0	3.604		
2	−3	1	2.589	2.59_1	5
−1	6	0	2.586		
1	5	0	2.580		
−1	4	1	2.542	2.54_5	21
−2	6	0	2.539		
2	4	0	2.529		
−3	1	1	2.525	2.51_7	2
−3	2	1[3]	2.504		
−3	0	1	2.473	2.473	42 *b*
1	3	1	2.447	2.446	30
−3	3	1	2.416	2.397	4 *b*
−2	−3	1	2.382		
−4	4	0	2.368	2.372	4 *b*
3	3	0	2.327	3.329	18 *b*
−4	5	0	2.229	2.224	15
4	1	0	2.221	2.224	15

[1] CrKα radiation, camera diameter 114.6 mm, upper limit of d measurable = 15.5 Å, Wilson technique.

[2] Calculated from cell parameters of Table 1.

[3] All calculated d spacings listed down to d = 2.5 Å; only values corresponding to observed lines listed below d = 2.5 Å.

TABLE 2—*Continued*

h	*k*	*l*	$d_{calc.}$[2]	$d_{meas.}$	I
−3	2	1	2.211	2.214	60
3	0	1	2.197	2.193	2
2	5	0	2.196		
−4	1	1	2.116	2.113	5
1	−6	1	2.109		
−4	3	1	2.092		
3	1	1	2.091	2.089	30
−3	7	0	2.089		
3	4	0	2.080	2.084	30
0	−6	1	2.065		
−4	0	1	2.064	2.063	5
4	2	0	2.061		
−5	3	0	1.994	2.000	15
−5	2	0	1.992	1.986	4 *b*
−4	−1	1	1.979		
1	5	1	1.977	1.973	4
−2	−5	1	1.948	1.945	5
−1	8	0	1.926	1.925	6
3	−6	1	1.914	1.911	15
−4	7	0	1.908		
4	−1	1	1.903	1.902	7
4	3	0	1.899		
				1.881	3 *b*
				1.848	3 *b*
				1.809	4
				1.801	4
				1.786	5
				1.770	6 *b*
				1.757	5
				1.742	7
				1.628	42

in Table 2. A film taken with CrKα radiation was selected for publication, since it gave the best resolution of the many doublets and triplets which occur on the diffraction pattern; however, films taken with FeKα and CuKα radiations and diffractometer patterns taken with CuKα radiation were also measured and gave similar values. The results are in general agreement with the pattern given in the ASTM X-ray Powder Data File under Sodium Carbonate Hydrate, $5Na_2O \cdot 8CO_2 \cdot 3H_2O$, Wegscheider's Salt (Card No. 2-0696).

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A RAPID CHANGE ROTATING SAMPLE HOLDER FOR *X*-RAY DIFFRACTION OF POWDERS

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Deviations in the *x*-ray diffraction intensity from a flat powdered sample are due principally to inhomogeneities from orientation of crystallites and segregation of crystalline mixtures (Klug and Alexander, 1954; Parrish, 1956; de Wolff *et al.*, 1959). Rotation of the powder sample about an axis perpendicular to its face reduces these deviations by a