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Tabular data of layer structure factors for clay minerals.

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In order to obtain either the complete diffraction diagram or the distribution of interlayer distances from the observed diffraction intensities in the calculation of X-ray diffraction effects of interstratified clay minerals a knowledge is required of the structure factor of the layers. This represents the contribution of the layer structure to the variation of scattered amplitude in the [00*l*] direction in reciprocal space, and is a continuous function for random structures. The layer structure per Å^2 is given by (MacEwan, Ruiz Amil & Brown, 1961):

$$F_l = \sum_s N_s f_s \exp(2\pi i r^* Z_s) ,$$

where N_s is the number of atoms of type s per layer per Å^2, f_s is the atomic scattering factor of atoms s, Z_s is the co-ordinate (Å) in a direction perpendicular to layers of atoms s and r^* ($=2 \sin\theta/\lambda$) is the reciprocal spacing coordinate (Å) measured along the [00*l*] direction. The calculations for interstratified minerals require a knowledge of $|F_l|^2 = F_l F_l^*$ where F_l^* is the complex conjugate of F_l. Where the

Table 1. *Layer structure factors* (SF), *and squared moduli of layer structure factors* (SFL) *per* Å^2 *for various types of layer*

	Mica Type Layer $(Si_6Al_2)O_{20}(OH)_4$								Montmorillonite Type Layer (Al_{6-}, Mg_1) $Si_8O_{20}(OH)_4$						Kaolinite Type Layer				Chlorite Type Layer	
	Without Interlayer				Dioctahedral 4Al															
r^* ($Å^{-1} \times 100$)	Dioctahedral 4Al		Trioctahedral 6Mg		Interlayer $2K^+$		Interlayer $1K^+1H_2O$		Interlayer 1.34 Na^+		Interlayer 0.67 Ca^{2+}		Interlayer 0.67 Mg^{2+}		Dioctahedral $Al_4Si_4O_{10}(OH)_8$		Trioctahedral $Fe_6Si_4O_{10}(OH)_8$		$Mg_{12}Si_8O_{20}(OH)_{16}$	
	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL	SF	SFL
1	353.54	57.39	373.40	64.02	387.70	69.02	380.13	66.35	417.86	80.95	416.68	80.49	413.13	79.12	255.97	31.23	357.71	44.98	540.57	120.48
2	341.75	53.63	361.37	59.96	370.77	63.12	364.31	60.94	401.77	74.83	401.02	74.55	398.74	73.71	244.95	28.60	339.78	40.58	487.03	97.80
3	322.13	47.65	341.63	53.59	343.18	54.07	338.49	52.61	376.14	65.59	375.99	65.53	375.50	65.37	227.13	24.59	311.14	34.03	406.35	68.08
4	296.18	40.28	315.68	45.76	307.20	43.33	304.75	42.64	343.88	54.82	344.34	54.97	345.78	55.43	204.00	19.84	273.94	26.38	310.20	39.67
5	264.29	32.07	283.79	36.98	264.25	32.06	264.25	32.06	306.85	43.65	307.75	43.91	310.80	44.78	176.45	14.84	229.35	18.49	210.31	18.24
6	228.24	23.92	247.74	28.18	217.19	21.66	219.66	22.15	267.97	33.29	269.09	33.57	273.05	34.56	146.47	10.23	180.25	11.42	119.56	5.89
7	189.21	16.44	208.59	19.98	168.31	13.01	172.99	13.74	229.07	24.33	230.13	24.55	234.09	25.40	115.67	6.38	129.09	5.86	47.80	0.94
8	148.07	10.07	167.31	12.85	119.44	6.55	125.86	7.27	190.77	16.87	191.51	17.00	194.58	17.55	85.41	3.48	78.05	2.14	1.10	0.00
9	106.71	5.23	125.95	7.28	73.17	2.46	80.73	2.99	154.36	11.05	154.70	11.09	156.14	11.30	57.46	1.57	29.82	0.31	-18.71	0.14
10	66.59	2.04	85.69	3.37	31.51	0.46	39.43	0.71	120.02	6.68	119.91	6.67	119.39	6.61	33.13	0.52	-13.46	0.06	-14.75	0.09
11	28.88	0.38	47.96	1.06	-4.32	0.01	1.20	0.00	87.51	3.55	87.07	3.51	84.69	3.32	13.29	0.08	-50.09	0.88	6.79	0.02
12	-5.17	0.01	13.93	0.09	-33.22	0.51	-26.86	0.33	56.80	1.50	56.18	1.46	52.49	1.28	-1.21	0.00	-78.50	2.17	36.92	0.56
13	-34.67	0.55	-15.55	0.11	-54.90	1.38	-50.29	1.16	27.72	0.36	27.17	0.34	23.01	0.25	-9.95	0.05	-97.74	3.36	65.95	1.79
14	-58.74	1.58	-39.66	0.72	-69.26	2.20	-66.86	2.05	1.19	0.00	0.79	0.00	-2.89	0.00	-13.21	0.08	-107.94	4.10	85.63	3.02
15	-76.79	2.71	-57.93	1.54	-76.67	2.70	-76.70	2.70	-21.88	0.22	-22.10	0.23	-24.45	0.28	-11.22	0.06	-108.68	4.15	89.60	3.31
16	-88.50	3.60	-69.52	2.22	-77.92	2.79	-80.35	2.96	-40.08	0.74	-40.11	0.75	-40.58	0.76	-4.88	0.01	-100.89	3.58	76.88	2.44
17	-94.15	4.07	-75.05	2.59	-74.27	2.53	-78.86	2.86	-52.56	1.28	-52.50	1.28	-50.98	1.21	5.01	0.01	-85.55	2.57	48.05	0.95
18	-93.69	4.03	-74.63	2.56	-69.59	2.04	-72.87	2.44	-57.82	1.55	-57.81	1.55	-54.64	1.38	17.14	0.14	-64.50	1.45	7.91	0.03
19	-87.56	3.52	-68.52	2.16	-55.98	1.44	-63.35	1.84	-55.20	1.41	-55.34	1.42	-51.24	1.22	30.29	0.44	-38.56	0.52	-36.10	0.54
20	-76.16	2.66	-57.16	1.50	-43.16	0.86	-50.98	1.19	-44.55	0.92	-44.81	0.93	-40.72	0.77	43.13	0.89	-30.53	0.04	-75.83	2.37
21	-61.14	1.72	-42.34	0.82	-30.23	0.42	-37.58	0.65	-27.85	0.36	-28.17	0.37	-25.06	0.29	55.14	1.45	18.76	0.12	-104.54	4.51
22	-42.91	0.85	-24.17	0.27	-16.92	0.13	-23.14	0.25	-6.19	0.02	-6.38	0.02	-4.94	0.01	65.29	2.03	47.43	0.79	-116.07	5.55
23	-22.22	0.23	-3.60	0.01	-3.59	0.01	-8.07	0.03	18.98	0.17	19.07	0.17	18.52	0.16	72.84	2.53	74.06	1.93	-107.58	4.77
24	-0.53	0.00	17.95	0.15	9.05	0.04	6.73	0.02	44.73	0.93	45.18	0.95	42.79	0.85	77.62	2.87	97.61	3.35	-79.90	2.63
25	21.43	0.21	39.67	0.72	21.25	0.21	21.29	0.21	69.54	2.24	70.35	2.29	66.86	2.06	79.46	3.01	116.99	4.81	-36.28	0.54
26	42.60	0.83	60.72	1.69	32.89	0.50	35.26	0.57	91.73	3.90	92.72	3.99	88.62	3.64	78.61	2.95	132.17	6.14	17.37	0.12
27	62.11	1.77	80.09	2.94	44.01	0.89	48.45	1.08	110 30	5.64	111.26	5.74	107.68	5.37	75.37	2.71	141.76	7.06	74.35	2.28
28	79.16	2.88	96.98	4.32	54.62	1.37	60.69	1.69	124 71	7.21	125.37	7.29	123.12	7.03	70.29	2.36	146.89	7.59	127.38	6.69
29	93.16	3.98	110.78	5.63	64.64	1.92	71.75	2.36	135.19	8.47	135.33	8.49	134.90	8.44	64.01	1.95	147.35	7.63	170.23	11.95
30	103.44	4.91	120.90	6.71	73.88	2.51	81.30	3.04	141.99	9.35	141.50	9.28	142.96	9.47	57.10	1.55	143.60	7.25	198.59	16.26
31	109.93	5.55	127.35	7.45	82.16	3.10	89.15	3.65	146.04	9.89	144.94	9.77	147.91	10.14	50.23	1.20	135.91	6.49	211.22	18.39
32	112.44	5.80	129.76	7.73	89.10	3.65	95.01	4.14	147.79	10.13	146.29	9.92	150.05	10.44	44.16	0.93	125.69	5.55	207.97	17.83
33	110.59	5.62	127.67	7.48	93.94	4.05	98.17	4.43	146.99	10.02	145.39	9.80	149.10	10.31	39.34	0.73	113.07	4.49	190.54	14.97
34	104.98	5.06	121.90	6.82	96.40	4.27	98.60	4.46	144.14	9.63	142.86	9.46	145.66	9.84	35.69	0.61	99.16	3.46	163.74	11.05
35	95.73	4.21	112.37	5.80	95.95	4.23	95.89	4.22	138.75	8.92	138.09	8.84	139.38	9.01	33.94	0.55	84.57	2.51	131.51	7.13
36	83.56	3.21	100.06	4.60	92.36	3.92	90.08	3.73	130.78	7.93	131.05	7.96	130.54	7.90	33.81	0.55	69.69	1.71	98.81	4.03
37	68.57	2.16	84.85	3.31	84.96	3.31	80.67	2.99	119.18	6.58	120.42	6.72	118.25	6.48	35.09	0.59	55.06	1.07	67.98	1.91
38	51.57	1.22	67.77	2.11	73.71	2.49	67.91	2.12	104 14	5.03	106.15	5.22	102.85	4.90	37.55	0.67	41.24	0.60	41.73	0.72
39	33.05	0.50	49.19	1.11	58.76	1.59	51.97	1.24	85.64	3.40	87.96	3.59	84.32	3.30	40.79	0.79	28.37	0.28	20.42	0.17
40	13.85	0.09	29.89	0.41	40.45	0.75	33.41	0.51	64.58	1.93	66.63	2.06	63.48	1.87	44.47	0.94	16.81	0.10	3.83	0.01
41	-4.97	0.01	10.89	0.05	20.02	0.18	13.36	0.08	42.18	0.82	43.55	0.88	41.60	0.80	47.85	1.09	6.28	0.01	-8.78	0.03
42	-23.54	0.25	-7.94	0.03	-2.66	0.00	-8.25	0.03	19.05	0.17	19.31	0.17	18.96	0.17	50.86	1.23	-2.23	0.00	-19.98	0.16
43	-40.70	0.76	-25.38	0.30	-25.74	0.30	-29.77	0.41	-2.91	0.00	-3.90	0.01	-2.61	0.00	52.71	1.32	-9.47	0.03	-30.29	0.38
44	-56.60	1.47	-41.42	0.79	-48.96	1.10	-51.02	1.20	-23.14	0.25	-25.19	0.29	-22.60	0.24	53.68	1.37	-14.90	0.08	-41.07	0.70
45	-69.55	2.22	-54.49	1.36	-69.81	2.24	-69.74	2.23	-39.38	0.72	-42.09	0.82	-38.81	0.70	52.65	1.32	-19.38	0.13	-50.98	1.07
46	-80.47	2.97	-65.67	1.98	-88.46	3.59	-86.26	3.42	-52.23	1.26	-54.95	1.40	-51.75	1.24	50.44	1.21	-21.76	0.17	-61.23	1.55
47	-88.09	3.56	-73.39	2.47	-102.87	4.86	-98.79	4.48	-60.61	1.70	-62.74	1.82	-60.34	1.69	46.52	1.03	-23.08	0.19	-69.43	1.99
48	-93.38	4.00	-78.90	2.86	-113.38	5.90	-107.83	5.34	-65.70	2.00	-66.68	2.06	-65.60	2.00	41 77	0.83	-22.27	0.17	-75.59	2.36
49	-95.30	4.17	-80.86	3.00	-118.48	6.45	-112.00	5.76	-67.05	2.08	-66.61	2.06	-67.07	2.09	35.90	0.61	-20.18	0.14	-77.82	2.50
50	-94.42	4.09	-80.20	2.95	-118.38	6.43	-111.67	5.73	-65.62	2.00	-63.84	1.89	-65.69	2.00	29.56	0.42	-16.23	0.09	-76.22	2.40
51	-90.99	3.80	-76.95	2.72	-113.42	5.91	+107.11	5.27	-62.38	1.80	+59.58	1.65	-62.37	1.80	23.08	0.25	-10.85	0.04	-71.18	2.09
52	-85.03	3.32	-71.27	2.33	-103.86	4.95	-98.53	4.46	-57.41	1.53	-54.24	1.36	-57.33	1.52	16.89	0.14	-3.92	0.01	-63.46	1.66
53	-77.07	2.73	-63.43	1.85	-90.48	3.76	-86.67	3.45	-51.32	1.22	-48.52	1.09	-51.19	1.21	11.47	0.06	4.33	0.01	-54.52	1.23
54	-67.20	2.07	-53.58	1.32	-74.04	2.52	-72.08	2.39	-43.97	0.90	-42.18	0.82	-43.83	0.89	6.97	0.02	13.57	0.06	-45.68	0.86
55	-55.99	1.44	-42.51	0.83	-55.70	1.42	-55.78	1.43	-35.49	0.58	-35.18	0.57	-35.46	0.58	3.70	0.01	23.51	0.19	-38.65	0.62
56	-43.66	0.88	-30.34	0.42	-36.42	0.61	-38.50	0.68	-25.44	0.30	-26.70	0.33	-25.58	0.30	1.72	0.00	33.60	0.40	-33.90	0.47
57	-30.76	0.43	-17.56	0.14	-17.41	0.14	-21.27	0.21	-14.04	0.09	-16.61	0.13	-14.38	0.10	1.07	0.00	43.46	0.66	-31.39	0.41
58	-17.71	0.14	-4.67	0.01	0.29	0.00	-4.94	0.01	-1.46	0.00	-4.74	0.01	-1.90	0.00	1.53	0.00	52.48	0.97	-10.32	0.38
59	-4.51	0.01	8.21	0.03	16.31	0.12	10.24	0.05	12.78	0.08	9.53	0.04	12.29	0.07	3.14	0.00	60.19	1.27	-28.99	0.35
60	7.82	0.03	20.32	0.19	29.42	0.40	23.08	0.24	27.25	0.34	24.76	0.28	26.83	0.33	5.21	0.01	66.15	1.54	-25.51	0.27
61	19.48	0.17	31.84	0.47	39.70	0.72	33.73	0.52	41.73	0.81	40.60	0.76	41.52	0.80	7.47	0.03	69.71	1.71	-18.06	0.13
62	30.25	0.42	42.49	0.83	47.17	1.02	42.15	0.82	55.60	1.43	56.11	1.46	55.69	1.44	9.59	0.04	70.59	1.75	-5.24	0.01
63	40.01	0.73	52.03	1.24	52.07	1.24	48.48	1.08	68.35	2.17	70.38	2.30	68.76	2.19	11.19	0.06	68.10	1.63	13.05	0.07
64	48.39	1.08	60.27	1.67	54.49	1.36	52.67	1.27	79.16	2.91	82.21	3.13	79.80	2.95	11.80	0.07	62.49	1.37	35.83	0.53
65	55.35	1.41	66.99	2.06	55.04	1.39	55.13	1.40	87.47	3.55	90.87	3.83	88.20	3.61	11.08	0.06	53 50	1.01	61.04	1.54
66	61.17	1.72	72.59	2.42	54.64	1.37	56.61	1.47	93.62	4.06	96.59	4.33	94.28	4.12	8 96	0.04	41 53	0.61	86.36	3.08
67	65.61	1.98	76.97	2.72	53.61	1.32	57.25	1.50	94.45	4.20	99.29	4.57	97.87	4.44	5.26	0.01	26.69	0.25	108.00	4.81
68	68.99	2.19	80.19	2.95	52.78	1.28	57.72	1.53	99.56	4.60	99.86	4.62	99.63	4.60	0.06	0.00	9.74	0.03	123.29	6.27
69	71.17	2.33	82.19	3.10	52.43	1.26	58.16	1.55	100.11	4.65	98.80	4.53	99.79	4.62	-6.41	0.02	-8.71	0.03	129.55	6.92
70	72.40	2.41	83.22	3.18	53.00	1.29	58.95	1.60	99.83	4.62	97.23	4.38	99.17	4.56	-13.89	0.09	-27.91	0.27	125.86	6.53
71	72.77	2.43	83.47	3.20	54.57	1.37	60.17	1.66	99.05	4.55	95.77	4.25	98.20	4.47	-21.95	0.23	-46.88	0.77	112.73	5.24
72	72.47	2.41	82.99	3.16	57.23	1.50	61.94	1.76	98.12	4.46	94.92	4.18	97.28	4.39	-30.20	0.43	-64.91	1.48	91.95	3.49
73	71.71	2.36	82.07	3.09	60.88	1.70	64.24	1.89	97.24	4.38	94.83	4.17	96.59	4.32	-38.17	0.69	-81.00	2.31	67.18	1.86
74	70.46	2.28	80.70	2.99	64.99	1.94	66.69	2.04	96.18	4.29	95.11	4.19	95.88	4.26	-45.24	0.98	-94.35	3.13	41.92	0.72
75	68.89	2.18	79.09	2.87	69.21	2.20	69.11	2.19	94.85	4.17	95.36	4.22	94.99	4.18	-50.98	1.24	-104.14	3.81	20.64	0.18
76	67.38	2.08	77.36	2.75	73.33	2.47	71.46	2.35	93.30	4.04	95.27	4.21	93.87	4.08	-55.08	1.45	-110.00	4.25	7.00	0.02
77	65.48	1.97	75.28	2.60	76.41	2.68	72.96	2.44	90.82	3.82	93.77	4.08	91.66	3.90	-56.92	1.54	-111.13	4.34	2.71	0.00
78	63.56	1.85	73.36	2.47	78.34	2.82	73.66	2.49	87.67	3.56	90.93	3.83	88.63	3.64	-56.54	1.52	-108.03	4.10	8.45	0.03
79	61.58	1.74	71.02	2.32	78.65	2.84	73.22	2.46	83.76	3.25	86.58	3.48	84.58	3.32	-53.74	1.38	-100.37	3.54	23.25	0.22
80	59.70	1.64	69.00	2.19	77.37	2.75	71.72	2.36	79.56	2.93	81.31	3.06	80.08	2.97	-48.68	1.13	-88.51	2.75	44.27	0.81
81	57.63	1.53	66.91	2.06	74.23	2.53	68.90	2.18	74.96	2.60	75.22	2.62	75.04	2.61	-41.33	0.81	-72.88	1.87	67.66	1.89
82	55.63	1.42	64.65	1.92	69.49	2.22	65.02	1.94	70.77	2.32	69.51	2.24	70.39	2.30	-32.42	0.50	-54.41	1.04	88.90	3.26
83	53.51	1.31	62.51	1.79	63.37	1.84	60.17	1.66	66.92	2.08	64.46	1.93	66.18	2.03	-22.14	0.23	-33.87	0.40	104.35	4.49
84	51.39	1.21	60.14	1.66	56.27	1.45	54.65	1.37	63.90	1.89	60.79	1.71	62.96	1.84	-11.06	0.06	-12.10	0.05	110.73	5.05
85	49.10	1.11	57.74	1.53	48.77	1.09	48.88	1.10	61.69	1.76	58.63	1.59	60.77	1.71	0.27	0.00	9.78	0.03	106.69	4.69
86	46.59	1.00	55.07	1.39	41.08	0.77	42.90	0.85	60.24	1.68	57.95	1.56	59.55	1.64	11.14	0.06	30.69	0.33	92.54	3.53
87	44.38	0.90	52.70	1.28	34.26	0.54	37.61	0.65	59.75	1.66	58.76	1.60	59.46	1.64	21.36	0.22	49.98	0.88	71.07	2.08
88	41.89	0.81	49.97	1.15	28.22	0.37	32.78	0.49	59.55	1.64	60.07	1.67	59.71	1.65	30.06	0.43	66.48	1.55	44.90	0.83
89	39.16	0.70	47.16	1.02	23.33	0.25	28.62	0.38	59.01	1.61	60.92	1.72	59.58	1.65	36.77	0.64	79.54	2.22	18.46	0.14
90	36.34	0.61	44.28	0.90	19.91	0.18	25.45	0.30	58.20	1.57	61.08	1.73	59.08	1.62	41.25	0.81	88.30	2.74	-3.89	0.01

layer projects on the Z axis with a centre of symmetry, F_l is real. Calculated curves of $|F_l|^2$ have been given for a number of types of clay layer by MacEwan, Ruiz Amil & Brown (1961).

From enlarged copies of these curves it is possible to obtain values of $|F_l|^2$ sufficiently accurate to determine interlayer distances, but not always of sufficient accuracy to estimate precise quantities of the interstratified components by the Fourier-transform method. This partly arises from the fact that diffraction lines of appreciable intensity frequently occur at near zero values of $|F_l|^2$, and these terms tend to dominate the Fourier transform from which the distribution of interlayer distance is derived. MacEwan (1956) has suggested that in order to remove this difficulty the layer structure factor curve be averaged over 4 units of r^* so that $|F_l|^2$ is never zero, but there still remains a need for numerical values of $|F_l|^2$ more accurate than can be obtained by interpolation from an enlargement of a published curve. Furthermore, recent work by one of us (W.F.C.) on a long-spacing mica-like mineral from Surges Bay, Tasmania, has shown the necessity of using layer structure factors based on an individual mineral composition rather than on idealized compositions.

Consequently the authors have computed and tabulated (1) numerical data (Table 1) for the layer structure factors of the common clay mineral types, of idealized compositions, including those given by the curves of MacEwan, Ruiz Amil & Brown (1961), and (2) numerical data (Table 2) for the contribution of the various parts of the mica layer (the most common layer type involved in interstratifaction) to the layer structure factor over the composition ranges treated by Brown (1955). The calculations were based on the Z_s atomic coordinates and lattice constants set out in Table 3 and atomic scattering factors taken from Klug & Alexander (1954). They were made on a CDC 3200 digital computer.

Table 2. *Contribution of the various parts of the mica layer to the layer structure factor for micas of different composition*

r^*		Octahedral												Interlayer				
($Å^{-1}$ × 100)	Skeleton	4Al	3Al 1Fe	2Al 2Fe	1Al 3Fe	4Fe	6Mg	5Mg 1Fe	4Mg 2Fe	3Mg 3Fe	2Mg 4Fe	1Mg 5Fe	6Fe	2K	1½K ½H_2O	1K 1H_2O	½K 1½H_2O	2H_2O
1	301.58	51.96	64.95	77.94	90.93	103.92	71.82	85.83	99.84	113.85	127.86	141.87	155.88	34.16	30.37	26.59	22.80	19.02
2	289.79	51.96	64.87	77.78	90.69	103.60	71.58	85.55	99.52	113.49	127.46	141.43	155.40	29.02	25.79	22.56	19.34	16.11
3	270.29	51.84	64.68	77.52	90.36	103.20	71.34	85.25	99.16	113.07	126.98	140.89	154.80	21.05	18.70	16.36	14.02	11.67
4	246.58	51.60	64.42	77.24	90.06	102.88	71.10	84.97	98.84	112.71	126.58	140.45	154.32	11.03	9.80	8.57	7.35	6.12
5	212.93	51.36	64.13	76.90	89.67	102.44	70.86	84.66	98.46	112.26	126.06	139.86	153.66	-0.04	-0.04	-0.03	-0.03	-0.02
6	177.12	51.12	63.84	76.56	89.28	102.00	70.62	84.35	98.08	111.81	125.54	139.27	153.00	-11.04	-9.81	-8.57	-7.34	-6.11
7	138.33	50.88	63.56	76.24	88.92	101.60	70.26	83.95	97.64	111.33	125.02	138.71	152.40	-20.90	-18.56	-16.22	-13.88	-11.55
8	97.59	50.48	63.13	75.78	88.43	101.08	69.72	83.37	97.02	110.67	124.32	137.97	151.62	-28.63	-25.42	-22.20	-18.99	-15.78
9	56.59	50.12	62.71	75.30	87.89	100.48	69.36	82.92	96.48	110.04	123.60	137.16	150.72	-33.54	-29.75	-25.97	-22.19	-18.41
10	16.87	49.72	62.27	74.82	87.37	99.92	68.82	82.33	95.84	109.35	122.86	136.37	149.88	-35.08	-31.12	-27.16	-23.20	-19.24
11	-20.44	49.32	61.82	74.32	86.82	99.32	68.40	81.83	95.26	108.69	122.12	135.55	148.98	-33.20	-29.44	-25.69	-21.93	-18.17
12	-54.05	48.88	61.32	73.76	86.20	98.64	67.98	81.31	94.64	107.97	121.30	134.63	147.96	-28.05	-24.87	-21.69	-18.52	-15.34
13	-82.99	48.32	60.71	73.10	85.49	97.88	67.44	80.67	93.90	107.13	120.36	133.59	146.82	-20.23	-17.93	-15.63	-13.33	-11.03
14	-106.50	47.76	60.14	72.52	84.90	97.28	66.84	80.02	93.20	106.38	119.56	132.74	145.94	-10.52	-9.32	-8.12	-6.93	-5.73
15	-123.99	47.20	59.54	71.88	84.22	96.56	66.06	79.19	92.32	105.45	118.58	131.71	144.84	0.12	0.10	0.09	0.08	0.06
16	-135.10	46.60	58.89	71.18	83.47	95.76	65.58	78.59	91.60	104.61	117.62	130.63	143.64	10.59	9.37	8.16	6.94	5.72
17	-140.03	45.88	58.13	70.38	82.63	94.88	64.98	77.87	90.76	103.65	116.54	129.43	142.32	19.88	17.59	15.29	13.00	10.71
18	-138.89	45.20	57.42	69.64	81.86	94.08	64.26	77.07	89.88	102.69	115.50	128.31	141.12	27.10	23.96	20.82	17.68	14.54
19	-132.12	44.56	56.71	68.86	81.01	93.16	63.60	76.29	88.98	101.67	114.36	127.05	139.74	31.58	27.90	24.21	20.52	16.84
20	-120.16	44.00	56.10	68.20	80.30	92.40	63.00	75.60	88.20	100.80	113.40	126.00	138.60	33.00	29.09	25.18	21.27	17.36
21	-104.62	43.48	55.51	67.54	84.90	91.28	66.84	80.02	93.20	106.38	119.56	132.74	145.94	30.92	27.24	23.57	19.89	16.22
22	-85.79	42.88	54.89	66.90	78.91	90.92	61.62	74.08	86.54	99.00	111.46	123.92	136.38	25.99	22.88	19.77	16.67	13.56
23	-64.62	42.40	54.32	66.24	78.16	90.08	61.02	73.37	85.72	98.07	110.42	122.77	135.12	18.63	16.39	14.15	11.91	9.67
24	-42.41	41.88	53.75	65.62	77.49	89.36	60.36	72.64	84.92	97.20	109.48	121.76	134.04	9.59	8.43	7.27	6.11	4.95
25	-19.97	41.40	53.15	64.90	76.65	88.40	59.64	71.80	83.96	96.12	108.28	120.44	132.60	-0.18	-0.16	-0.14	-0.81	-0.09
26	1.68	40.92	52.67	64.42	76.17	87.92	59.04	71.18	83.32	95.46	107.60	119.74	131.88	-9.71	-8.53	-7.36	-6.16	-4.97
27	21.59	40.52	52.07	63.62	75.17	86.72	58.50	70.43	82.36	94.29	106.22	118.15	130.08	-18.09	-15.87	-13.66	-11.44	-9.22
28	39.08	40.08	51.54	63.00	74.46	85.92	57.90	69.73	81.56	93.39	105.22	117.05	128.88	-24.55	-21.51	-18.47	-15.44	-12.40
29	53.48	39.68	51.03	62.38	73.73	85.08	57.30	69.02	80.74	92.46	104.18	115.90	127.62	-28.52	-24.96	-21.41	-17.85	-14.30
30	64.20	39.24	50.49	61.74	72.99	84.24	56.70	68.31	79.92	91.53	103.14	114.75	126.36	-29.56	-25.85	-22.14	-18.43	-14.72
31	71.13	38.80	49.90	61.00	72.10	83.20	56.22	67.65	79.08	90.51	101.94	113.37	124.80	-27.76	-24.27	-20.78	-17.29	-13.80
32	73.96	38.48	49.46	60.44	71.42	82.40	55.80	67.10	78.40	89.70	101.00	112.30	123.60	-23.34	-20.38	-17.43	-14.48	-11.52
33	72.47	38.12	48.96	59.80	70.64	81.48	55.20	66.37	77.54	88.71	99.88	111.05	122.22	-16.66	-14.54	-12.42	-10.31	-8.19
34	67.18	37.80	48.51	59.22	69.93	80.64	54.72	65.76	76.80	87.84	98.88	109.92	120.96	-8.58	-7.48	-6.38	-5.28	-4.17
35	58.25	37.48	48.07	58.66	69.25	79.84	54.12	65.06	76.00	86.94	97.88	108.82	119.76	0.22	0.20	0.17	0.14	0.11
36	46.36	37.20	47.64	58.08	68.52	78.96	53.70	64.49	75.28	86.07	96.86	107.65	118.44	8.80	7.66	6.52	5.38	4.24
37	31.69	36.88	47.16	57.44	67.72	78.00	53.16	63.80	74.44	85.08	95.72	106.36	117.00	16.39	14.25	12.11	9.97	7.83
38	15.09	36.48	46.66	56.84	67.02	77.20	52.68	63.20	73.72	84.24	94.76	105.28	115.80	22.14	19.25	16.34	13.44	10.53
39	-3.07	36.12	46.19	56.26	66.33	76.40	52.26	62.65	73.04	83.43	93.82	104.21	114.60	25.71	22.32	18.92	15.53	12.13
40	-21.95	35.80	45.75	55.70	65.65	75.60	51.84	62.10	72.36	82.62	92.88	103.14	113.40	26.60	23.08	19.56	16.04	12.52
41	-40.53	35.56	45.44	55.32	65.20	75.08	51.42	61.62	71.82	82.02	92.22	102.42	112.62	24.99	21.66	18.33	14.99	11.66
42	-58.82	35.28	44.98	54.68	64.38	74.08	50.88	60.92	70.96	81.00	91.04	101.08	111.12	20.89	18.09	15.30	12.50	9.70
43	-75.78	35.08	44.63	54.18	63.73	73.28	50.40	60.32	70.24	80.16	90.08	100.00	109.92	14.96	12.94	10.92	8.91	6.89
44	-91.40	34.80	44.23	53.66	63.09	72.52	49.98	59.78	69.58	79.38	89.18	98.98	108.78	7.64	6.61	5.58	4.54	3.51
45	-104.11	34.56	43.88	53.20	62.52	71.84	49.62	59.31	69.00	78.69	88.38	98.07	107.76	-0.26	-0.22	-0.19	-0.15	-0.12
46	-114.87	34.40	43.57	52.74	61.91	71.08	49.20	58.77	68.34	77.91	87.48	97.05	106.62	-7.99	-6.89	-5.80	-4.70	-3.60
47	-122.17	34.08	43.16	52.24	61.32	70.40	48.78	58.25	67.72	77.19	86.66	96.13	105.60	-14.78	-12.74	-10.69	-8.65	-6.61
48	-127.26	33.88	42.84	51.80	60.76	69.72	48.36	57.73	67.10	76.47	85.84	95.21	104.58	-19.99	-17.22	-14.45	-11.68	-8.90
49	-128.86	33.56	42.44	51.32	60.20	69.08	48.00	57.27	66.54	75.81	85.08	94.35	103.62	-23.17	-19.94	-16.70	-13.47	-10.23
50	-127.78	33.36	42.12	50.88	59.64	68.40	47.58	56.75	65.92	75.09	84.26	93.43	102.60	-23.96	-20.60	-17.25	-13.89	-10.54
51	-124.11	33.12	41.80	50.46	59.16	67.84	47.16	56.26	65.36	74.46	83.56	92.66	101.76	-22.43	-19.28	-16.12	-12.97	-9.82
52	-117.95	32.92	41.49	50.06	58.63	67.20	46.68	55.70	64.72	73.74	82.76	91.78	100.80	-18.83	-16.16	-13.50	-10.83	-8.16
53	-109.75	32.68	41.19	49.70	58.21	66.72	46.32	55.28	64.24	73.20	82.16	91.12	100.08	-13.41	-11.50	-9.60	-7.70	-5.79
54	-99.60	32.40	40.80	49.20	57.60	66.00	46.02	54.85	63.68	72.51	81.34	90.17	99.00	-6.84	-5.86	-4.88	-3.90	-2.93
55	-88.11	32.12	40.45	48.78	57.11	65.44	45.60	54.36	63.12	71.88	80.64	89.40	98.16	0.29	0.25	0.20	0.16	0.12
56	-75.58	31.92	40.14	48.36	56.58	64.80	45.24	53.90	62.56	71.22	79.88	88.54	97.20	7.25	6.20	5.16	4.11	3.07
57	-62.44	31.68	39.81	47.94	56.07	64.20	44.88	53.45	62.02	70.59	79.16	87.73	96.30	13.35	11.42	9.49	7.56	5.62
58	-49.07	31.36	39.41	47.46	55.51	63.56	44.40	52.89	61.38	69.87	78.36	86.85	95.34	18.00	15.38	12.77	10.15	7.53
59	-35.71	31.20	39.13	47.06	54.99	62.92	43.92	52.33	60.74	69.15	77.56	85.97	94.38	20.82	17.78	14.75	11.71	8.67
60	-23.18	31.00	38.87	46.74	54.61	62.48	43.50	51.87	60.24	68.61	76.98	85.35	93.72	21.60	18.43	15.26	12.09	8.92
61	-11.24	30.72	38.54	46.36	54.18	62.00	43.08	51.40	59.72	68.04	76.36	84.68	93.00	20.22	17.24	14.26	11.27	8.29
62	-0.11	30.68	38.15	45.94	53.73	61.52	42.60	50.88	59.16	67.44	75.72	84.00	92.28	16.92	14.41	11.91	9.40	6.89
63	9.85	30.16	37.85	45.54	53.23	60.92	42.18	50.38	58.58	66.78	74.98	83.18	91.38	12.06	10.27	8.47	6.68	4.89
64	18.39	30.00	37.62	45.24	52.86	60.48	41.88	50.02	58.16	66.30	74.44	82.58	90.72	6.10	5.19	4.28	3.37	2.46
65	25.59	29.76	37.31	44.86	52.41	59.96	41.40	49.49	57.58	65.67	73.76	81.85	89.94	-0.30	-0.26	-0.21	-0.17	-0.12
66	31.61	29.56	37.05	44.54	52.03	59.52	40.98	49.03	57.08	65.13	73.18	81.23	89.28	-5.55	-4.71	-4.57	-3.58	-2.60
67	36.29	29.32	36.72	44.12	51.52	58.92	40.68	48.63	56.58	64.53	72.48	80.43	88.38	-12.00	-10.18	-8.37	-6.55	-4.73
68	39.87	29.12	36.46	43.80	51.14	58.48	40.32	48.22	56.12	64.02	71.92	79.82	87.72	-16.21	-13.74	-11.27	-8.80	-6.33
69	42.29	28.88	36.17	43.46	50.75	58.04	39.90	47.76	55.62	63.48	71.34	79.20	87.06	-18.73	-15.87	-13.01	-10.15	-7.28
70	43.80	28.60	35.85	43.10	50.35	57.60	39.42	47.25	55.08	62.91	70.74	78.57	86.40	-19.40	-16.42	-13.45	-10.47	-7.50
71	44.41	28.36	35.54	42.72	49.90	57.08	39.06	46.82	54.58	62.34	70.10	77.86	85.62	-18.20	-15.40	-12.60	-9.80	-7.00
72	44.35	28.12	35.26	42.40	49.54	56.68	38.64	46.37	54.10	61.83	69.56	77.29	85.02	-15.23	-12.88	-10.53	-8.17	-5.82
73	43.79	27.92	35.00	42.08	49.16	56.24	38.28	45.96	53.64	61.32	69.00	76.68	84.36	-10.83	-9.18	-7.47	-5.79	-4.11
74	42.78	27.68	34.72	41.76	48.80	55.84	37.92	45.56	53.20	60.84	68.48	76.12	83.76	-5.47	-4.62	-3.77	-2.92	-2.07
75	41.41	27.48	34.46	41.44	48.42	55.40	37.68	45.25	52.82	60.39	67.96	75.53	83.10	0.32	0.27	0.22	0.17	0.12
76	40.10	27.28	34.20	41.12	48.04	54.96	37.26	44.79	52.32	59.85	67.38	74.91	82.44	5.95	5.02	4.09	3.16	2.23
77	38.44	27.04	33.88	40.72	47.56	54.40	36.84	44.30	51.76	59.22	66.68	74.14	81.60	10.93	9.21	7.48	5.76	4.03
78	36.76	26.80	33.60	40.40	47.20	54.00	36.60	44.00	51.40	58.80	66.20	73.60	81.00	14.78	12.44	10.10	7.76	5.42
79	35.02	26.56	33.32	40.08	46.84	53.60	36.00	43.40	50.80	58.20	65.60	73.00	80.40	17.06	14.35	11.64	8.93	6.22
80	33.30	26.40	33.10	39.80	46.50	53.20	35.70	43.05	50.40	57.75	65.10	72.45	79.80	17.68	14.85	12.03	9.20	6.38
81	31.51	26.12	32.79	39.46	46.13	52.80	35.40	42.70	50.00	57.30	64.60	71.90	79.20	16.60	13.93	11.27	8.60	5.94
82	29.67	25.96	32.57	39.18	45.79	52.40	34.98	42.25	49.52	56.79	64.06	71.33	78.60	13.85	11.62	9.38	7.15	4.91
83	27.83	25.68	32.28	38.88	45.48	52.08	34.68	41.92	49.16	56340	63.64	70.88	78.12	9.87	8.26	6.66	5.06	3.46
84	25.82	25.48	32.01	38.54	45.07	51.60	34.32	41.50	48.68	55.86	63.04	70.22	77.40	4.97	4.16	3.35	2.54	1.73
85	23.90	25.20	31.70	38.20	44.70	51.20	33.84	41.00	48.16	55.32	62.48	69.64	76.80	-0.33	-0.28	-0.22	-0.17	-0.11
86	21.59	25.00	31.47	37.94	44.41	50.88	33.48	40.62	47.76	54.90	62.04	69.18	76.32	-5.52	-4.61	-3.69	-2.78	-1.87
87	19.58	24.80	31.23	37.66	44.09	50.52	33.12	40.23	47.34	54.45	61.56	68.67	75.78	-10.12	-8.44	-6.76	-5.08	-3.41
88	17.21	24.68	31.07	37.46	43.85	50.24	32.76	39.86	46.96	54.06	61.16	68.26	75.36	-13.67	-11.40	-9.12	-6.84	-4.56
89	14.76	24.40	30.80	37.20	43.60	50.00	32.40	39.50	46.60	53.70	60.80	67.90	75.00	-15.83	-13.18	-10.54	-7.89	-5.25
90	12.18	24.16	30.52	36.88	43.24	49.60	32.10	39.15	46.20	53.25	60.30	67.35	74.40	-16.44	-13.67	-10.90	-8.13	-5.36

Table 3. *Z_s Atomic coordinates perpendicular to the layers and lattice constants of clay minerals*

	Mica[a][b] (Å)	Montmorillonite[c] (Å)	Kaolinite[d] Dioctahedral (Å)	Kaolinite[d] Trioctahedral (Å)	Chlorite[e] (Å)
Octahedral	0·00	0·00	3·27		0·00
O, OH	1·12	1·09	4·37		1·05
Tetrahedral	2·70	2·70	0·60		2·71
O	3·28	3·24	0·00		3·26
Interlayer	5·00	7·70			
OH					6·00
Mg					7·05

	Mica (Å)	Mica (°)	Montmorillonite (Å)	Montmorillonite (°)	Dioctahedral (Å)	Dioctahedral (°)	Trioctahedral (Å)	Trioctahedral (°)	Chlorite (Å)	Chlorite (°)
a	5·189		5·21		5·14		5·55		5·33	
b	8·995		9·02		8·93		9·61		9·24	
c sin *β*	20·014		14·40		7·13		7·20		14·10	
α		90		90		91·6		90		90
β		95·18		97		104·8		90		97
γ		90		90		89·9		90		90

(*a*) Atomic parameters from Jackson & West (1933).
(*b*) Lattice parameters from Radoslovich (1960).
(*c*) From MacEwan, Ruiz Amil & Brown (1961).
(*d*) From Brindley (1961*a*).
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Th_3N_4 crystal structure and comparison with that of Th_2N_2O.*

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The existence of Th_3N_4 has been reported (Matignon & Delépine, 1907) and later substantiated (Neumann, Kroeger & Haebler, 1932) by a different method of chemical analysis. The results reported in what follows were obtained with Th_3N_4 prepared by equilibrating ThN powder contained in an induction-heated tungsten crucible with 0·13 atm. nitrogen at 1320°. The composition of the product was determined both by weight gain as well as by ignition to ThO_2. The N:Th ratio was thus found to be $1·33 \pm 0·03$. Thorium sesquioxynitride, Th_2N_2O, was prepared by equilibration of the compacted mixture $3ThN + ThO_2$ with 2 atm. nitrogen at 1700°C. The Th content of this product was determined by ignition to ThO_2; the O:Th ratio was taken to be the same as that of the initial mixture, and nitrogen was computed by difference. The final composition thus obtained was $Th_2N_{2·04\pm0·06}O$. An X-ray diffraction powder pattern of a sample was found to be indistinguishable from that reported earlier (Zachariasen, 1949) for Th_2N_3 with the hexagonal lattice parameters $a_0 = 3·8833 \pm 0·0002$, $c_0 = 6·1870 \pm 0·0003$ Å. We did not succeed in obtaining N:Th ratios in excess of $1·33 \pm 0·03$ by reacting thorium or ThN with nitrogen at pressures up to 2 atm.; therefore, the Th_2N_3 phase was not obtained. Although we did not investigate sufficiently high nitrogen pressures to confirm or exclude the existence of the Th_2N_3 phase, all the experimental results suggest the material previously described as Th_2N_3 was the same as the Th_2N_2O phase described above.

The X-ray diffraction data obtained from a powder pattern of Th_3N_4 are shown in Table 1. The observed intensities are given for two samples I and II. In sample I, the intensities are modified by an appreciable preferential orientation.

The observed values of $\sin^2\theta$ correspond to a rhombohedral lattice with $a_0 = 9·398 \pm 0·002$ Å, $\alpha = 23·78 \pm 0·01°$. The dimensions of the corresponding hexagonal cell are $a_0 = 3·871 \pm 0·001$, $c_0 = 27·385 \pm 0·005$ Å.

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