

pressed by

$$R_v = (I_0/I)_v = \exp(\mu t \sec v), \quad (1)$$

where I_0 and I are the intensities of the incident and transmitted beams, μt is the sum of the separate products of the linear absorption coefficients with the thickness of emulsion, film base and any interleaving paper, and v is the angle the incident X-rays make with the normal to the film. Rossmann (1956) improved the agreement between the experimental and calculated values of R using the relationship

$$R_v = [1/(1-C)] \exp(\mu t \sec v), \quad (2)$$

where C is a factor to allow for the absorption of energy by the photochemical effect (Cox & Shaw, 1930).

Recently we used Co $K\alpha$ radiation and the multiple-film technique (Robertson, 1943) to record intensity data on equi-inclination Weissenberg photographs, but were unable to find the relevant film-factor data in the literature. Owing to the much stronger absorption of Co radiation and the limited range of linearity of response of X-ray film, it was not possible to determine the film factors with sufficient accuracy by comparing reflexion intensities on successive films of the multiple-film pack, and the following procedure was therefore adopted.

For each equi-inclination angle, v , a 60° Weissenberg exposure was recorded twice, on different portions of a twin-pack of Ilford Industrial G film (each film wrapped in its black paper folder as supplied by the manufacturers). The exposure times, t_1 and t_2 , were chosen so that t_2/t_1 was approximately equal to the film factor at the equi-inclination angle under consideration. Then, if the intensity of a reflexion of the shorter (time t_1) exposure on the first (nearer to crystal) film is S_1 , and that of the same reflexion of the longer (time t_2) exposure on the second film is S_2 , the film absorption factor is given by

$$R = t_2 S_1 / t_1 S_2.$$

S_1 and S_2 are approximately equal and errors due to non-linearity are avoided.

The film factors, R (exp), derived in this way are listed in Table 1, together with those calculated according to equation (1), the value of μt ($= 1.951$) being determined by least squares. Application of equation (2) gives virtually identical results ($\mu t = 1.950$, $C = 0.001$).

Table 1. Experimental and calculated R values

v	$\sec v$	R (calc)	
		R (exp)	$\mu t = 1.951$
0.0°	1.000	7.02	7.04
4.7	1.003	7.21	7.08
9.5	1.014	7.26	7.23
15.9	1.040	7.40	7.60
22.6	1.083	8.47	8.27
29.6	1.150	8.99	9.43
33.2	1.195	10.62	10.29

The average discrepancy between experimental and calculated values is 2.35% and the root-mean-square deviation is 0.24. The standard deviation in μt is 0.010 and the standard deviations in the calculated film factors range from 0.07 at $v = 0$ to 0.12 at $v = 33.2^\circ$.

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Absorption corrections for neutron diffraction. By K.D.ROUSE and M.J.COOPER, *Materials Physics Division, A.E.R.E., Harwell, Berkshire, England*, and E.J.YORK and A.CHAKERA, *Computer Analysts and Programmers Ltd., Reading, Berkshire, England*

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Absorption corrections for cylindrical and spherical crystals have been evaluated by numerical integration for values of μR in the range 0 to 1.0, where μ is the mean linear absorption coefficient and R is the radius of the crystal. For this range of μR , which is that normally required for neutron diffraction data, interpolation from existing tables is unsatisfactory. The transmission factor A_{hkl} is tabulated as a function of μR and $\sin^2 \theta$, accurate to four decimal places. The intervals chosen for the tabulation are such that linear interpolation may be used for intermediate values. Analytical expressions, which may be used for calculating the transmission factor when a lower accuracy is acceptable, are also given.

In passing through a crystal a neutron or X-ray beam is attenuated by normal absorption processes, resulting in a reduction in the observed intensity of a given Bragg reflexion. The exact reduction depends on the paths through the crystal and the magnitude of the mean absorption coefficient of the crystal, the transmission factor being

$$A_{hkl} = \frac{1}{V} \int \exp\{-\mu(p+q)\} dV \quad (1)$$

(*International Tables for X-ray Crystallography*, 1959), where μ is the mean linear absorption coefficient, p and q are the lengths of the paths of the incident and reflected beams in the crystal for radiation reflected in an element of volume dV , and V is the volume of the crystal.

This integral can be evaluated rigorously only for certain crystal shapes, two of the most convenient of which are a cylinder and a sphere. For these the integral over all path lengths can be computed to give an absorption factor A^*

Table 1. *Transmission factors for a cylindrical crystal*

μR	(a) A_{hkl} for $\sin^2 \theta$ from 0 to 0.70 $\sin^2 \theta$							
	0.0	0.10	0.20	0.30	0.40	0.50	0.60	0.70
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.9832	0.9832	0.9832	0.9832	0.9832	0.9832	0.9832	0.9832
	0.9667	0.9667	0.9667	0.9668	0.9668	0.9668	0.9668	0.9668
	0.9504	0.9504	0.9505	0.9506	0.9506	0.9506	0.9507	0.9507
	0.9345	0.9345	0.9346	0.9347	0.9348	0.9349	0.9349	0.9349
0.05	0.9188	0.9189	0.9189	0.9190	0.9192	0.9193	0.9194	0.9195
	0.9034	0.9035	0.9036	0.9037	0.9039	0.9041	0.9043	0.9044
	0.8883	0.8884	0.8885	0.8887	0.8890	0.8892	0.8894	0.8896
	0.8734	0.8736	0.8737	0.8740	0.8743	0.8746	0.8749	0.8751
	0.8588	0.8590	0.8592	0.8596	0.8599	0.8602	0.8607	0.8610
0.10	0.8444	0.8447	0.8450	0.8454	0.8458	0.8462	0.8467	0.8471
	0.8303	0.8307	0.8310	0.8315	0.8320	0.8325	0.8330	0.8335
	0.8164	0.8169	0.8173	0.8178	0.8184	0.8190	0.8196	0.8202
	0.8028	0.8033	0.8038	0.8045	0.8051	0.8058	0.8065	0.8072
	0.7894	0.7901	0.7906	0.7913	0.7920	0.7928	0.7936	0.7944
0.15	0.7763	0.7770	0.7776	0.7784	0.7792	0.7801	0.7810	0.7819
	0.7634	0.7642	0.7648	0.7657	0.7666	0.7676	0.7686	0.7696
	0.7507	0.7515	0.7523	0.7533	0.7543	0.7554	0.7565	0.7576
	0.7383	0.7391	0.7400	0.7411	0.7421	0.7433	0.7446	0.7458
	0.7260	0.7270	0.7280	0.7291	0.7303	0.7316	0.7329	0.7343
0.20	0.7140	0.7150	0.7161	0.7173	0.7186	0.7200	0.7215	0.7230
	0.7021	0.7033	0.7045	0.7058	0.7072	0.7087	0.7103	0.7119
	0.6905	0.6917	0.6930	0.6945	0.6960	0.6976	0.6993	0.7011
	0.6790	0.6804	0.6818	0.6834	0.6850	0.6867	0.6886	0.6905
	0.6678	0.6692	0.6708	0.6725	0.6742	0.6761	0.6780	0.6801
0.25	0.6567	0.6583	0.6600	0.6618	0.6636	0.6656	0.6677	0.6699
	0.6458	0.6475	0.6494	0.6513	0.6532	0.6553	0.6576	0.6599
	0.6352	0.6370	0.6389	0.6410	0.6430	0.6453	0.6476	0.6500
	0.6247	0.6266	0.6287	0.6308	0.6330	0.6354	0.6379	0.6404
	0.6144	0.6164	0.6186	0.6209	0.6232	0.6257	0.6283	0.6310
0.30	0.6043	0.6064	0.6087	0.6111	0.6136	0.6162	0.6189	0.6217
	0.5944	0.5966	0.5990	0.6015	0.6041	0.6069	0.6097	0.6126
	0.5846	0.5869	0.5895	0.5921	0.5949	0.5977	0.6007	0.6037
	0.5750	0.5775	0.5801	0.5829	0.5857	0.5887	0.5918	0.5950
	0.5656	0.5681	0.5709	0.5738	0.5768	0.5799	0.5831	0.5865
0.35	0.5563	0.5590	0.5619	0.5649	0.5680	0.5712	0.5746	0.5781
	0.5472	0.5500	0.5530	0.5561	0.5594	0.5627	0.5662	0.5699
	0.5382	0.5412	0.5443	0.5476	0.5509	0.5544	0.5581	0.5618
	0.5294	0.5325	0.5358	0.5391	0.5426	0.5463	0.5500	0.5539
	0.5208	0.5240	0.5274	0.5308	0.5344	0.5383	0.5421	0.5462
0.40	0.5123	0.5156	0.5191	0.5227	0.5264	0.5304	0.5344	0.5386
	0.5040	0.5074	0.5110	0.5147	0.5186	0.5227	0.5268	0.5311
	0.4958	0.4993	0.5030	0.5069	0.5109	0.5151	0.5193	0.5238
	0.4877	0.4913	0.4952	0.4992	0.5033	0.5076	0.5120	0.5167
	0.4798	0.4835	0.4875	0.4916	0.4959	0.5003	0.5048	0.5096
0.45	0.4720	0.4758	0.4799	0.4842	0.4886	0.4931	0.4978	0.5027
	0.4643	0.4683	0.4725	0.4769	0.4814	0.4861	0.4909	0.4959
	0.4568	0.4609	0.4652	0.4697	0.4744	0.4792	0.4841	0.4893
	0.4494	0.4536	0.4580	0.4627	0.4675	0.4724	0.4774	0.4827
	0.4421	0.4464	0.4510	0.4558	0.4607	0.4657	0.4709	0.4763
0.50	0.4349	0.4394	0.4441	0.4490	0.4540	0.4592	0.4645	0.4700

Table 1 (cont.)

(a) A_{hkl} for $\sin^2 \theta$ from 0 to 0.70

μR	0.0	0.10	0.20	0.30	0.40	0.50	0.60	0.70
	$\sin^2 \theta$							
0.50	0.4349	0.4394	0.4441	0.4490	0.4540	0.4592	0.4645	0.4700
	0.4279	0.4325	0.4373	0.4423	0.4474	0.4528	0.4582	0.4638
	0.4210	0.4257	0.4306	0.4358	0.4410	0.4465	0.4520	0.4577
	0.4142	0.4190	0.4241	0.4293	0.4347	0.4403	0.4459	0.4518
	0.4075	0.4124	0.4176	0.4230	0.4285	0.4342	0.4400	0.4459
0.55	0.4010	0.4060	0.4113	0.4168	0.4224	0.4282	0.4341	0.4402
	0.3945	0.3997	0.4051	0.4107	0.4164	0.4223	0.4284	0.4346
	0.3882	0.3934	0.3990	0.4047	0.4106	0.4166	0.4227	0.4291
	0.3820	0.3873	0.3930	0.3988	0.4048	0.4109	0.4172	0.4236
	0.3758	0.3813	0.3871	0.3931	0.3992	0.4054	0.4117	0.4183
0.60	0.3698	0.3754	0.3813	0.3874	0.3936	0.3999	0.4064	0.4131
	0.3639	0.3696	0.3756	0.3818	0.3881	0.3945	0.4012	0.4080
	0.3581	0.3639	0.3700	0.3763	0.3828	0.3893	0.3960	0.4029
	0.3523	0.3583	0.3645	0.3709	0.3775	0.3841	0.3910	0.3980
	0.3467	0.3528	0.3591	0.3656	0.3723	0.3790	0.3860	0.3931
0.65	0.3412	0.3474	0.3538	0.3604	0.3672	0.3740	0.3811	0.3883
	0.3358	0.3421	0.3486	0.3553	0.3622	0.3691	0.3763	0.3836
	0.3305	0.3369	0.3435	0.3503	0.3573	0.3643	0.3716	0.3790
	0.3252	0.3317	0.3384	0.3453	0.3524	0.3595	0.3669	0.3744
	0.3201	0.3267	0.3335	0.3405	0.3477	0.3549	0.3624	0.3700
0.70	0.3150	0.3217	0.3286	0.3357	0.3430	0.3503	0.3579	0.3656
	0.3100	0.3168	0.3238	0.3310	0.3384	0.3458	0.3535	0.3613
	0.3051	0.3120	0.3191	0.3264	0.3339	0.3414	0.3492	0.3571
	0.3002	0.3073	0.3145	0.3219	0.3294	0.3371	0.3449	0.3529
	0.2955	0.3027	0.3100	0.3175	0.3251	0.3328	0.3407	0.3488
0.75	0.2908	0.2981	0.3055	0.3131	0.3208	0.3286	0.3366	0.3448
	0.2862	0.2936	0.3011	0.3088	0.3166	0.3245	0.3326	0.3409
	0.2817	0.2892	0.2968	0.3046	0.3125	0.3204	0.3286	0.3370
	0.2773	0.2849	0.2926	0.3005	0.3084	0.3165	0.3247	0.3331
	0.2730	0.2806	0.2884	0.2964	0.3044	0.3125	0.3209	0.3294
0.80	0.2687	0.2764	0.2843	0.2924	0.3005	0.3087	0.3171	0.3257
	0.2645	0.2723	0.2803	0.2885	0.2966	0.3049	0.3134	0.3221
	0.2603	0.2682	0.2763	0.2846	0.2928	0.3012	0.3098	0.3185
	0.2563	0.2643	0.2725	0.2807	0.2891	0.2975	0.3062	0.3150
	0.2522	0.2603	0.2687	0.2770	0.2854	0.2939	0.3027	0.3115
0.85	0.2483	0.2565	0.2649	0.2733	0.2818	0.2904	0.2992	0.3081
	0.2444	0.2527	0.2612	0.2697	0.2783	0.2869	0.2958	0.3048
	0.2406	0.2490	0.2576	0.2661	0.2748	0.2835	0.2924	0.3015
	0.2369	0.2453	0.2540	0.2626	0.2714	0.2802	0.2891	0.2982
	0.2332	0.2417	0.2505	0.2592	0.2680	0.2768	0.2859	0.2950
0.90	0.2296	0.2382	0.2470	0.2558	0.2647	0.2736	0.2827	0.2919
	0.2260	0.2347	0.2436	0.2525	0.2614	0.2704	0.2796	0.2888
	0.2226	0.2313	0.2403	0.2492	0.2582	0.2672	0.2765	0.2858
	0.2191	0.2279	0.2370	0.2460	0.2551	0.2641	0.2734	0.2828
	0.2157	0.2246	0.2338	0.2428	0.2520	0.2611	0.2704	0.2799
0.95	0.2124	0.2214	0.2306	0.2397	0.2489	0.2581	0.2675	0.2770
	0.2091	0.2182	0.2275	0.2366	0.2459	0.2552	0.2646	0.2742
	0.2059	0.2151	0.2244	0.2336	0.2429	0.2523	0.2618	0.2714
	0.2027	0.2120	0.2214	0.2307	0.2400	0.2494	0.2590	0.2686
	0.1996	0.2090	0.2184	0.2278	0.2372	0.2466	0.2562	0.2659
1.00	0.1965	0.2060	0.2154	0.2249	0.2344	0.2439	0.2535	0.2633

Table 1 (cont.)

(b) A_{hkl} for $\sin^2 \theta$ from 0.65 to 1.0
 $\sin^2 \theta$

μR	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.9832	0.9832	0.9832	0.9832	0.9832	0.9832	0.9833	0.9832
	0.9668	0.9668	0.9668	0.9668	0.9668	0.9668	0.9669	0.9668
	0.9507	0.9507	0.9507	0.9507	0.9508	0.9508	0.9509	0.9508
	0.9349	0.9349	0.9350	0.9350	0.9351	0.9351	0.9352	0.9352
0.05	0.9195	0.9195	0.9196	0.9196	0.9197	0.9198	0.9199	0.9199
	0.9044	0.9044	0.9045	0.9046	0.9047	0.9048	0.9049	0.9050
	0.8896	0.8896	0.8897	0.8899	0.8900	0.8902	0.8903	0.8904
	0.8750	0.8751	0.8753	0.8755	0.8756	0.8758	0.8760	0.8761
	0.8608	0.8610	0.8611	0.8614	0.8616	0.8618	0.8620	0.8622
0.10	0.8469	0.8471	0.8473	0.8476	0.8478	0.8481	0.8483	0.8486
	0.8333	0.8335	0.8338	0.8341	0.8344	0.8347	0.8349	0.8353
	0.8199	0.8202	0.8205	0.8209	0.8212	0.8216	0.8219	0.8223
	0.8068	0.8072	0.8075	0.8080	0.8083	0.8087	0.8091	0.8095
	0.7940	0.7944	0.7948	0.7953	0.7957	0.7962	0.7966	0.7971
0.15	0.7814	0.7819	0.7824	0.7829	0.7834	0.7839	0.7844	0.7849
	0.7691	0.7696	0.7702	0.7707	0.7713	0.7719	0.7724	0.7730
	0.7570	0.7576	0.7582	0.7588	0.7595	0.7601	0.7607	0.7613
	0.7452	0.7458	0.7465	0.7472	0.7479	0.7486	0.7492	0.7499
	0.7336	0.7343	0.7350	0.7358	0.7365	0.7373	0.7380	0.7388
0.20	0.7223	0.7230	0.7238	0.7246	0.7254	0.7263	0.7270	0.7279
	0.7112	0.7119	0.7128	0.7137	0.7145	0.7155	0.7163	0.7172
	0.7003	0.7011	0.7020	0.7029	0.7039	0.7049	0.7058	0.7068
	0.6896	0.6905	0.6915	0.6924	0.6934	0.6945	0.6955	0.6966
	0.6791	0.6801	0.6811	0.6822	0.6832	0.6843	0.6854	0.6866
0.25	0.6688	0.6699	0.6710	0.6721	0.6732	0.6744	0.6756	0.6768
	0.6587	0.6599	0.6610	0.6622	0.6634	0.6647	0.6660	0.6672
	0.6488	0.6500	0.6513	0.6525	0.6538	0.6551	0.6565	0.6578
	0.6391	0.6404	0.6417	0.6430	0.6444	0.6458	0.6472	0.6487
	0.6296	0.6310	0.6323	0.6337	0.6351	0.6367	0.6382	0.6397
0.30	0.6203	0.6217	0.6231	0.6246	0.6261	0.6277	0.6293	0.6309
	0.6111	0.6126	0.6141	0.6157	0.6172	0.6189	0.6206	0.6223
	0.6022	0.6037	0.6053	0.6069	0.6086	0.6103	0.6121	0.6139
	0.5934	0.5950	0.5967	0.5983	0.6001	0.6019	0.6037	0.6056
	0.5848	0.5865	0.5882	0.5899	0.5918	0.5937	0.5955	0.5975
0.35	0.5763	0.5781	0.5799	0.5817	0.5836	0.5856	0.5875	0.5896
	0.5680	0.5699	0.5717	0.5736	0.5756	0.5777	0.5796	0.5818
	0.5599	0.5618	0.5638	0.5657	0.5678	0.5699	0.5720	0.5742
	0.5520	0.5539	0.5559	0.5580	0.5601	0.5623	0.5644	0.5668
	0.5442	0.5462	0.5482	0.5504	0.5526	0.5548	0.5570	0.5595
0.40	0.5365	0.5386	0.5407	0.5429	0.5452	0.5475	0.5498	0.5523
	0.5290	0.5311	0.5333	0.5356	0.5379	0.5403	0.5427	0.5453
	0.5216	0.5238	0.5261	0.5284	0.5308	0.5333	0.5358	0.5384
	0.5143	0.5167	0.5190	0.5214	0.5239	0.5264	0.5289	0.5317
	0.5072	0.5096	0.5120	0.5145	0.5170	0.5196	0.5223	0.5251
0.45	0.5002	0.5027	0.5052	0.5077	0.5103	0.5130	0.5157	0.5186
	0.4933	0.4959	0.4985	0.5011	0.5037	0.5065	0.5093	0.5122
	0.4866	0.4893	0.4919	0.4945	0.4973	0.5001	0.5030	0.5060
	0.4800	0.4827	0.4854	0.4881	0.4909	0.4939	0.4968	0.4999
	0.4736	0.4763	0.4790	0.4819	0.4847	0.4877	0.4907	0.4939
0.50	0.4672	0.4700	0.4728	0.4757	0.4786	0.4817	0.4848	0.4880

Table 1 (cont.)

(b) A_{hkl} for $\sin^2 \theta$ from 0.65 to 1.0

μR	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.50	0.4672	0.4700	0.4728	0.4757	0.4786	0.4817	0.4848	0.4880
	0.4610	0.4638	0.4667	0.4697	0.4726	0.4758	0.4789	0.4822
	0.4549	0.4577	0.4607	0.4637	0.4667	0.4700	0.4732	0.4766
	0.4489	0.4518	0.4548	0.4579	0.4610	0.4643	0.4676	0.4710
	0.4430	0.4459	0.4491	0.4522	0.4553	0.4587	0.4620	0.4655
0.55	0.4372	0.4402	0.4434	0.4466	0.4498	0.4532	0.4566	0.4602
	0.4315	0.4346	0.4378	0.4411	0.4444	0.4478	0.4513	0.4549
	0.4259	0.4291	0.4323	0.4357	0.4390	0.4425	0.4461	0.4498
	0.4204	0.4236	0.4270	0.4304	0.4338	0.4373	0.4410	0.4447
	0.4150	0.4183	0.4217	0.4251	0.4287	0.4322	0.4359	0.4398
0.60	0.4097	0.4131	0.4165	0.4200	0.4236	0.4272	0.4310	0.4349
	0.4045	0.4080	0.4114	0.4150	0.4186	0.4223	0.4262	0.4301
	0.3994	0.4029	0.4064	0.4100	0.4137	0.4175	0.4214	0.4254
	0.3944	0.3980	0.4015	0.4052	0.4089	0.4127	0.4167	0.4208
	0.3894	0.3931	0.3967	0.4004	0.4042	0.4081	0.4121	0.4163
0.65	0.3846	0.3883	0.3920	0.3957	0.3996	0.4035	0.4076	0.4118
	0.3799	0.3836	0.3873	0.3911	0.3950	0.3990	0.4031	0.4074
	0.3752	0.3790	0.3828	0.3866	0.3906	0.3946	0.3988	0.4031
	0.3706	0.3744	0.3783	0.3821	0.3862	0.3903	0.3945	0.3989
	0.3661	0.3700	0.3738	0.3778	0.3818	0.3860	0.3902	0.3948
0.70	0.3617	0.3656	0.3695	0.3735	0.3776	0.3818	0.3861	0.3907
	0.3573	0.3613	0.3652	0.3693	0.3734	0.3777	0.3820	0.3867
	0.3530	0.3571	0.3610	0.3652	0.3693	0.3736	0.3780	0.3827
	0.3488	0.3529	0.3569	0.3611	0.3653	0.3697	0.3741	0.3789
	0.3447	0.3488	0.3529	0.3571	0.3614	0.3657	0.3703	0.3750
0.75	0.3406	0.3448	0.3489	0.3532	0.3575	0.3619	0.3665	0.3713
	0.3366	0.3409	0.3450	0.3493	0.3537	0.3581	0.3628	0.3676
	0.3327	0.3370	0.3411	0.3455	0.3499	0.3544	0.3591	0.3640
	0.3288	0.3331	0.3374	0.3418	0.3462	0.3508	0.3555	0.3604
	0.3250	0.3294	0.3336	0.3381	0.3426	0.3472	0.3520	0.3569
0.80	0.3213	0.3257	0.3300	0.3345	0.3390	0.3437	0.3485	0.3535
	0.3176	0.3221	0.3264	0.3309	0.3355	0.3402	0.3451	0.3501
	0.3140	0.3185	0.3229	0.3274	0.3320	0.3368	0.3417	0.3468
	0.3105	0.3150	0.3194	0.3240	0.3286	0.3335	0.3384	0.3436
	0.3070	0.3115	0.3160	0.3206	0.3253	0.3302	0.3351	0.3404
0.85	0.3036	0.3081	0.3127	0.3173	0.3220	0.3269	0.3319	0.3372
	0.3002	0.3048	0.3094	0.3140	0.3188	0.3237	0.3287	0.3341
	0.2969	0.3015	0.3061	0.3108	0.3156	0.3205	0.3256	0.3310
	0.2937	0.2982	0.3030	0.3077	0.3125	0.3175	0.3226	0.3280
	0.2905	0.2950	0.2998	0.3046	0.3094	0.3144	0.3196	0.3250
0.90	0.2873	0.2919	0.2967	0.3015	0.3064	0.3114	0.3166	0.3221
	0.2842	0.2888	0.2936	0.2985	0.3034	0.3084	0.3137	0.3192
	0.2811	0.2858	0.2906	0.2955	0.3005	0.3055	0.3108	0.3163
	0.2781	0.2828	0.2877	0.2926	0.2976	0.3027	0.3080	0.3135
	0.2751	0.2799	0.2848	0.2897	0.2947	0.2999	0.3052	0.3107
0.95	0.2722	0.2770	0.2819	0.2869	0.2919	0.2971	0.3025	0.3080
	0.2693	0.2742	0.2791	0.2841	0.2891	0.2944	0.2998	0.3053
	0.2665	0.2714	0.2763	0.2814	0.2864	0.2917	0.2972	0.3027
	0.2638	0.2686	0.2736	0.2787	0.2838	0.2891	0.2946	0.3001
	0.2611	0.2659	0.2709	0.2760	0.2812	0.2865	0.2920	0.2976
1.00	0.2584	0.2633	0.2683	0.2734	0.2786	0.2839	0.2895	0.2951

Table 2. Transmission factors for a spherical crystal

μR	(a) A_{hkl} for $\sin^2 \theta$ from 0 to 0.70 $\sin^2 \theta$							
	0.0	0.10	0.20	0.30	0.40	0.50	0.60	0.70
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.9851	0.9851	0.9851	0.9852	0.9852	0.9851	0.9852	0.9851
	0.9704	0.9705	0.9705	0.9706	0.9706	0.9705	0.9706	0.9706
	0.9560	0.9561	0.9561	0.9563	0.9563	0.9562	0.9563	0.9563
	0.9419	0.9419	0.9420	0.9422	0.9422	0.9422	0.9422	0.9423
0.05	0.9279	0.9280	0.9280	0.9281	0.9283	0.9284	0.9284	0.9285
	0.9142	0.9143	0.9143	0.9145	0.9147	0.9148	0.9149	0.9150
	0.9007	0.9008	0.9009	0.9011	0.9013	0.9015	0.9016	0.9017
	0.8874	0.8875	0.8876	0.8879	0.8881	0.8883	0.8886	0.8888
	0.8743	0.8744	0.8746	0.8749	0.8752	0.8754	0.8758	0.8760
0.10	0.8614	0.8616	0.8618	0.8622	0.8625	0.8628	0.8632	0.8635
	0.8487	0.8490	0.8492	0.8497	0.8500	0.8504	0.8509	0.8512
	0.8362	0.8366	0.8368	0.8373	0.8378	0.8382	0.8387	0.8392
	0.8239	0.8243	0.8246	0.8252	0.8258	0.8263	0.8268	0.8274
	0.8118	0.8123	0.8127	0.8133	0.8139	0.8145	0.8152	0.8159
0.15	0.7999	0.8005	0.8009	0.8016	0.8023	0.8030	0.8037	0.8045
	0.7882	0.7888	0.7893	0.7901	0.7909	0.7916	0.7924	0.7933
	0.7767	0.7774	0.7779	0.7788	0.7796	0.7805	0.7814	0.7823
	0.7653	0.7661	0.7667	0.7676	0.7686	0.7695	0.7705	0.7716
	0.7542	0.7549	0.7557	0.7567	0.7577	0.7587	0.7599	0.7610
0.20	0.7432	0.7440	0.7449	0.7459	0.7470	0.7481	0.7494	0.7506
	0.7324	0.7332	0.7342	0.7353	0.7365	0.7377	0.7391	0.7404
	0.7217	0.7227	0.7238	0.7249	0.7262	0.7275	0.7290	0.7304
	0.7111	0.7122	0.7134	0.7147	0.7161	0.7174	0.7191	0.7206
	0.7008	0.7020	0.7033	0.7046	0.7061	0.7076	0.7093	0.7110
0.25	0.6906	0.6919	0.6933	0.6947	0.6963	0.6979	0.6997	0.7015
	0.6806	0.6820	0.6835	0.6850	0.6867	0.6884	0.6903	0.6922
	0.6707	0.6722	0.6738	0.6754	0.6772	0.6790	0.6810	0.6831
	0.6610	0.6626	0.6643	0.6660	0.6679	0.6698	0.6719	0.6741
	0.6515	0.6531	0.6549	0.6568	0.6587	0.6608	0.6630	0.6653
0.30	0.6421	0.6438	0.6457	0.6477	0.6497	0.6519	0.6542	0.6566
	0.6328	0.6346	0.6366	0.6388	0.6409	0.6432	0.6456	0.6481
	0.6237	0.6256	0.6277	0.6300	0.6322	0.6346	0.6371	0.6397
	0.6147	0.6167	0.6189	0.6213	0.6236	0.6261	0.6287	0.6315
	0.6059	0.6080	0.6103	0.6128	0.6153	0.6179	0.6206	0.6234
0.35	0.5972	0.5994	0.6018	0.6044	0.6070	0.6097	0.6125	0.6155
	0.5886	0.5909	0.5935	0.5961	0.5989	0.6017	0.6046	0.6077
	0.5802	0.5826	0.5852	0.5880	0.5908	0.5938	0.5968	0.6001
	0.5719	0.5744	0.5772	0.5800	0.5830	0.5860	0.5892	0.5925
	0.5637	0.5663	0.5692	0.5721	0.5752	0.5784	0.5817	0.5852
0.40	0.5557	0.5584	0.5614	0.5644	0.5676	0.5709	0.5743	0.5779
	0.5478	0.5506	0.5537	0.5568	0.5601	0.5635	0.5670	0.5708
	0.5400	0.5429	0.5461	0.5493	0.5528	0.5563	0.5599	0.5637
	0.5323	0.5354	0.5386	0.5420	0.5455	0.5491	0.5529	0.5568
	0.5247	0.5279	0.5312	0.5347	0.5384	0.5421	0.5460	0.5501
0.45	0.5173	0.5206	0.5240	0.5276	0.5314	0.5352	0.5392	0.5434
	0.5100	0.5134	0.5169	0.5206	0.5245	0.5284	0.5325	0.5369
	0.5028	0.5062	0.5099	0.5137	0.5177	0.5217	0.5260	0.5304
	0.4957	0.4992	0.5030	0.5069	0.5110	0.5152	0.5196	0.5241
	0.4887	0.4923	0.4962	0.5003	0.5045	0.5087	0.5132	0.5179
0.50	0.4818	0.4855	0.4895	0.4937	0.4980	0.5024	0.5070	0.5118

Table 2 (cont.)

(a) A_{hkl} for $\sin^2 \theta$ from 0 to 0.70

μR	0.0	0.10	0.20	0.30	0.40	0.50	0.60	0.70
0.50	0.4818	0.4855	0.4895	0.4937	0.4980	0.5024	0.5070	0.5118
	0.4750	0.4788	0.4829	0.4872	0.4916	0.4962	0.5009	0.5058
	0.4683	0.4723	0.4765	0.4809	0.4854	0.4900	0.4948	0.4998
	0.4618	0.4658	0.4701	0.4746	0.4792	0.4840	0.4889	0.4940
	0.4553	0.4595	0.4639	0.4685	0.4732	0.4780	0.4830	0.4882
0.55	0.4489	0.4532	0.4577	0.4624	0.4672	0.4722	0.4773	0.4826
	0.4426	0.4470	0.4516	0.4564	0.4614	0.4665	0.4717	0.4771
	0.4364	0.4409	0.4457	0.4506	0.4556	0.4608	0.4661	0.4716
	0.4303	0.4349	0.4398	0.4448	0.4499	0.4553	0.4607	0.4663
	0.4243	0.4290	0.4340	0.4391	0.4444	0.4498	0.4553	0.4611
0.60	0.4184	0.4232	0.4283	0.4335	0.4389	0.4444	0.4500	0.4559
	0.4126	0.4175	0.4227	0.4280	0.4335	0.4391	0.4448	0.4508
	0.4069	0.4119	0.4171	0.4226	0.4282	0.4339	0.4397	0.4458
	0.4012	0.4063	0.4117	0.4172	0.4229	0.4287	0.4346	0.4408
	0.3957	0.4009	0.4063	0.4120	0.4178	0.4237	0.4297	0.4360
0.65	0.3902	0.3955	0.4010	0.4068	0.4127	0.4187	0.4248	0.4312
	0.3848	0.3902	0.3958	0.4017	0.4077	0.4138	0.4200	0.4265
	0.3795	0.3850	0.3907	0.3967	0.4028	0.4090	0.4153	0.4219
	0.3742	0.3798	0.3857	0.3917	0.3980	0.4042	0.4107	0.4173
	0.3691	0.3748	0.3808	0.3869	0.3932	0.3995	0.4061	0.4128
0.70	0.3640	0.3698	0.3759	0.3821	0.3885	0.3949	0.4016	0.4084
	0.3590	0.3649	0.3711	0.3774	0.3839	0.3904	0.3972	0.4041
	0.3541	0.3601	0.3664	0.3728	0.3793	0.3859	0.3928	0.3998
	0.3493	0.3554	0.3617	0.3682	0.3749	0.3816	0.3885	0.3956
	0.3445	0.3507	0.3571	0.3637	0.3704	0.3772	0.3843	0.3915
0.75	0.3398	0.3461	0.3526	0.3593	0.3661	0.3730	0.3801	0.3874
	0.3352	0.3416	0.3481	0.3549	0.3618	0.3688	0.3760	0.3834
	0.3306	0.3371	0.3438	0.3506	0.3576	0.3647	0.3720	0.3794
	0.3261	0.3327	0.3394	0.3464	0.3535	0.3606	0.3680	0.3755
	0.3217	0.3284	0.3352	0.3422	0.3494	0.3566	0.3641	0.3717
0.80	0.3173	0.3241	0.3310	0.3381	0.3454	0.3527	0.3602	0.3679
	0.3130	0.3199	0.3269	0.3341	0.3414	0.3488	0.3564	0.3642
	0.3087	0.3157	0.3228	0.3301	0.3375	0.3450	0.3527	0.3605
	0.3046	0.3116	0.3188	0.3262	0.3337	0.3413	0.3490	0.3569
	0.3005	0.3076	0.3149	0.3223	0.3299	0.3375	0.3454	0.3533
0.85	0.2964	0.3036	0.3110	0.3185	0.3262	0.3339	0.3418	0.3498
	0.2924	0.2997	0.3072	0.3148	0.3225	0.3303	0.3383	0.3464
	0.2885	0.2959	0.3034	0.3111	0.3189	0.3267	0.3348	0.3430
	0.2846	0.2921	0.2997	0.3075	0.3154	0.3232	0.3314	0.3396
	0.2808	0.2884	0.2961	0.3039	0.3119	0.3198	0.3280	0.3363
0.90	0.2771	0.2847	0.2925	0.3004	0.3084	0.3164	0.3247	0.3331
	0.2734	0.2811	0.2890	0.2969	0.3050	0.3131	0.3214	0.3299
	0.2697	0.2775	0.2855	0.2935	0.3017	0.3098	0.3182	0.3267
	0.2661	0.2740	0.2820	0.2901	0.2984	0.3065	0.3150	0.3236
	0.2626	0.2705	0.2786	0.2868	0.2951	0.3033	0.3119	0.3205
0.95	0.2591	0.2671	0.2753	0.2835	0.2919	0.3002	0.3088	0.3175
	0.2557	0.2637	0.2720	0.2803	0.2887	0.2971	0.3058	0.3145
	0.2523	0.2604	0.2688	0.2771	0.2856	0.2941	0.3028	0.3116
	0.2489	0.2572	0.2656	0.2740	0.2825	0.2911	0.2998	0.3087
	0.2456	0.2540	0.2624	0.2709	0.2795	0.2881	0.2969	0.3058
1.00	0.2424	0.2508	0.2593	0.2679	0.2765	0.2852	0.2940	0.3030

Table 2 (cont.)

(b) A_{hkl} for $\sin^2 \theta$ from 0.65 to 1.0
 $\sin^2 \theta$

μR	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
	0.9852	0.9852	0.9852	0.9852	0.9852	0.9852	0.9852	0.9851
	0.9706	0.9706	0.9706	0.9706	0.9706	0.9707	0.9707	0.9706
	0.9563	0.9563	0.9563	0.9564	0.9564	0.9564	0.9564	0.9563
	0.9423	0.9423	0.9423	0.9424	0.9424	0.9425	0.9425	0.9424
0.05	0.9285	0.9285	0.9286	0.9286	0.9287	0.9288	0.9288	0.9288
	0.9150	0.9150	0.9151	0.9151	0.9153	0.9154	0.9154	0.9155
	0.9017	0.9017	0.9019	0.9019	0.9021	0.9023	0.9023	0.9024
	0.8887	0.8888	0.8889	0.8890	0.8892	0.8894	0.8894	0.8896
	0.8759	0.8760	0.8762	0.8763	0.8765	0.8768	0.8768	0.8771
0.10	0.8634	0.8635	0.8637	0.8639	0.8641	0.8644	0.8645	0.8648
	0.8511	0.8512	0.8515	0.8517	0.8520	0.8523	0.8524	0.8527
	0.8390	0.8392	0.8395	0.8398	0.8400	0.8404	0.8406	0.8409
	0.8272	0.8274	0.8277	0.8281	0.8284	0.8287	0.8290	0.8294
	0.8155	0.8159	0.8162	0.8166	0.8169	0.8173	0.8176	0.8180
0.15	0.8041	0.8045	0.8049	0.8053	0.8057	0.8061	0.8065	0.8069
	0.7929	0.7933	0.7938	0.7942	0.7947	0.7951	0.7956	0.7960
	0.7819	0.7823	0.7829	0.7833	0.7839	0.7844	0.7848	0.7853
	0.7710	0.7716	0.7721	0.7727	0.7732	0.7738	0.7743	0.7749
	0.7604	0.7610	0.7616	0.7622	0.7628	0.7635	0.7640	0.7646
0.20	0.7500	0.7506	0.7513	0.7519	0.7526	0.7533	0.7539	0.7546
	0.7398	0.7404	0.7412	0.7418	0.7426	0.7433	0.7440	0.7447
	0.7297	0.7304	0.7312	0.7319	0.7327	0.7336	0.7343	0.7351
	0.7198	0.7206	0.7214	0.7222	0.7231	0.7240	0.7247	0.7256
	0.7101	0.7110	0.7118	0.7127	0.7136	0.7145	0.7154	0.7163
0.25	0.7006	0.7015	0.7024	0.7033	0.7043	0.7053	0.7062	0.7072
	0.6912	0.6922	0.6932	0.6941	0.6951	0.6962	0.6972	0.6983
	0.6820	0.6831	0.6841	0.6851	0.6862	0.6873	0.6884	0.6895
	0.6730	0.6741	0.6752	0.6762	0.6773	0.6786	0.6797	0.6809
	0.6641	0.6653	0.6664	0.6675	0.6687	0.6700	0.6712	0.6725
0.30	0.6554	0.6566	0.6578	0.6590	0.6602	0.6616	0.6629	0.6642
	0.6468	0.6481	0.6493	0.6506	0.6519	0.6533	0.6547	0.6561
	0.6384	0.6397	0.6410	0.6424	0.6437	0.6452	0.6467	0.6481
	0.6301	0.6315	0.6329	0.6343	0.6357	0.6373	0.6388	0.6403
	0.6220	0.6234	0.6249	0.6263	0.6278	0.6295	0.6310	0.6326
0.35	0.6140	0.6155	0.6170	0.6185	0.6201	0.6218	0.6234	0.6251
	0.6062	0.6077	0.6093	0.6108	0.6125	0.6143	0.6159	0.6177
	0.5984	0.6001	0.6017	0.6033	0.6051	0.6069	0.6086	0.6105
	0.5909	0.5925	0.5942	0.5959	0.5978	0.5996	0.6014	0.6033
	0.5834	0.5852	0.5869	0.5886	0.5906	0.5925	0.5943	0.5964
0.40	0.5761	0.5779	0.5797	0.5815	0.5835	0.5855	0.5874	0.5895
	0.5689	0.5708	0.5726	0.5745	0.5765	0.5786	0.5806	0.5828
	0.5618	0.5637	0.5657	0.5676	0.5697	0.5718	0.5739	0.5761
	0.5549	0.5568	0.5588	0.5609	0.5630	0.5652	0.5673	0.5696
	0.5480	0.5501	0.5521	0.5542	0.5564	0.5586	0.5608	0.5633
0.45	0.5413	0.5434	0.5455	0.5477	0.5499	0.5522	0.5545	0.5570
	0.5347	0.5369	0.5390	0.5413	0.5435	0.5459	0.5483	0.5508
	0.5282	0.5304	0.5327	0.5349	0.5373	0.5397	0.5422	0.5448
	0.5218	0.5241	0.5264	0.5287	0.5312	0.5336	0.5362	0.5389
	0.5155	0.5179	0.5202	0.5226	0.5251	0.5277	0.5303	0.5330
0.50	0.5093	0.5118	0.5142	0.5166	0.5192	0.5218	0.5245	0.5273

Table 2 (cont.)

(b) A_{hkl} for $\sin^2 \theta$ from 0.65 to 1.0

μR	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.50	0.5093	0.5118	0.5142	0.5166	0.5192	0.5218	0.5245	0.5273
	0.5032	0.5058	0.5082	0.5107	0.5133	0.5160	0.5188	0.5217
	0.4973	0.4998	0.5024	0.5049	0.5076	0.5104	0.5132	0.5161
	0.4914	0.4940	0.4966	0.4992	0.5019	0.5048	0.5077	0.5106
	0.4857	0.4882	0.4910	0.4936	0.4964	0.4993	0.5022	0.5053
0.55	0.4800	0.4826	0.4854	0.4881	0.4909	0.4939	0.4969	0.5000
	0.4744	0.4771	0.4799	0.4827	0.4855	0.4886	0.4916	0.4948
	0.4689	0.4716	0.4745	0.4774	0.4803	0.4834	0.4865	0.4897
	0.4635	0.4663	0.4692	0.4721	0.4751	0.4782	0.4814	0.4847
	0.4581	0.4611	0.4640	0.4670	0.4700	0.4732	0.4764	0.4797
0.60	0.4529	0.4559	0.4589	0.4619	0.4650	0.4682	0.4715	0.4749
	0.4478	0.4508	0.4538	0.4569	0.4601	0.4633	0.4667	0.4701
	0.4427	0.4458	0.4489	0.4520	0.4552	0.4585	0.4619	0.4655
	0.4377	0.4408	0.4440	0.4471	0.4504	0.4538	0.4573	0.4609
	0.4328	0.4360	0.4391	0.4424	0.4457	0.4492	0.4527	0.4564
0.65	0.4280	0.4312	0.4344	0.4377	0.4411	0.4446	0.4482	0.4519
	0.4233	0.4265	0.4298	0.4331	0.4366	0.4401	0.4437	0.4475
	0.4186	0.4219	0.4252	0.4286	0.4321	0.4357	0.4394	0.4432
	0.4140	0.4173	0.4207	0.4241	0.4277	0.4313	0.4350	0.4389
	0.4095	0.4128	0.4163	0.4197	0.4234	0.4270	0.4308	0.4347
0.70	0.4050	0.4084	0.4119	0.4154	0.4191	0.4228	0.4266	0.4306
	0.4006	0.4041	0.4076	0.4111	0.4149	0.4186	0.4225	0.4266
	0.3963	0.3998	0.4033	0.4070	0.4108	0.4145	0.4184	0.4226
	0.3920	0.3956	0.3992	0.4028	0.4067	0.4105	0.4145	0.4187
	0.3878	0.3915	0.3950	0.3988	0.4027	0.4065	0.4106	0.4148
0.75	0.3837	0.3874	0.3910	0.3948	0.3987	0.4026	0.4067	0.4110
	0.3796	0.3834	0.3870	0.3909	0.3948	0.3988	0.4029	0.4072
	0.3756	0.3794	0.3831	0.3870	0.3910	0.3950	0.3992	0.4036
	0.3717	0.3755	0.3793	0.3832	0.3872	0.3913	0.3955	0.3999
	0.3678	0.3717	0.3755	0.3795	0.3835	0.3876	0.3919	0.3963
0.80	0.3640	0.3679	0.3718	0.3758	0.3798	0.3840	0.3883	0.3928
	0.3602	0.3642	0.3681	0.3722	0.3762	0.3805	0.3848	0.3893
	0.3565	0.3605	0.3645	0.3686	0.3727	0.3770	0.3813	0.3859
	0.3529	0.3569	0.3609	0.3650	0.3692	0.3735	0.3779	0.3826
	0.3492	0.3533	0.3574	0.3615	0.3658	0.3701	0.3746	0.3793
0.85	0.3457	0.3498	0.3539	0.3581	0.3624	0.3668	0.3713	0.3760
	0.3422	0.3464	0.3505	0.3547	0.3591	0.3635	0.3680	0.3728
	0.3388	0.3430	0.3471	0.3514	0.3558	0.3602	0.3648	0.3696
	0.3354	0.3396	0.3439	0.3481	0.3525	0.3570	0.3617	0.3665
	0.3321	0.3363	0.3406	0.3449	0.3493	0.3538	0.3586	0.3634
0.90	0.3288	0.3331	0.3374	0.3417	0.3462	0.3507	0.3555	0.3604
	0.3256	0.3299	0.3342	0.3386	0.3431	0.3476	0.3525	0.3574
	0.3224	0.3267	0.3311	0.3355	0.3400	0.3446	0.3495	0.3545
	0.3192	0.3236	0.3280	0.3324	0.3370	0.3416	0.3466	0.3516
	0.3161	0.3205	0.3250	0.3295	0.3340	0.3387	0.3437	0.3487
0.95	0.3131	0.3175	0.3220	0.3265	0.3311	0.3358	0.3408	0.3459
	0.3101	0.3145	0.3190	0.3236	0.3282	0.3330	0.3380	0.3431
	0.3071	0.3116	0.3161	0.3207	0.3254	0.3302	0.3352	0.3404
	0.3042	0.3087	0.3132	0.3179	0.3226	0.3274	0.3325	0.3376
	0.3013	0.3058	0.3104	0.3151	0.3198	0.3247	0.3298	0.3350
1.00	0.2985	0.3030	0.3076	0.3123	0.3171	0.3220	0.3271	0.3323

($=1/A$) for given values of μR and θ , where R is the radius of the crystal and θ is the Bragg angle. Values of the absorption factor for equatorial reflexions from a cylindrical crystal have been tabulated, with an accuracy of better than 10^{-3} , at intervals in θ of 5° and in μR of 0·1 from 0 to 10·0 and of 0·5 from 10·0 to 31·5 (Weber, 1967). A tabulation for a spherical crystal, terminating at $\mu R=10\cdot0$, has been given by Bond in *International Tables for X-ray Crystallography* (1959), based on interpolation of a tabulation at intervals of 1 in μR and 15° in θ . A further tabulation for a spherical crystal, with an accuracy of better than 10^{-3} has recently been given by Weber (1969) at the same intervals as his earlier values for a cylindrical crystal. In both cases further interpolation is necessary for values of μR and θ between those for which A^* is given. For neutron diffraction the value of μR is normally within the range 0 to 1·0, for which interpolation from existing tables is unsatisfactory if accurate corrections are required. We have therefore evaluated the transmission factor [equation (1)] for these two crystal shapes at intervals of 0·01 in μR within this range.

The integral for equatorial reflexions from a cylinder was evaluated using Simpson's rule and the accuracy of the integration was determined from the difference between evaluations using two intervals, one twice the other. The integral for a sphere was obtained by appropriate further integration of the results for a cylinder, the required integrand values being obtained by Aitken interpolation. In both cases the results obtained are accurate to four places of decimals.

Although absorption corrections have previously been tabulated as a function of θ , we find that interpolation can be carried out much more conveniently if they are tabulated as a function of $\sin^2\theta$. The intervals of $\sin^2\theta$ used in the present tables are such that linear interpolation is acceptable. Table 1(a) and (b) list the values of A_{hkl} for equatorial reflexions from a cylindrical crystal at intervals of 0·1 in $\sin^2\theta$ from 0 to 0·7 and intervals of 0·05 in $\sin^2\theta$ from 0·65

to 1·00 respectively. Table 2(a) and (b) gives the corresponding values for a spherical crystal. In all cases the interval in μR is 0·01.

If the high accuracy of the tabulated values is not required it may be more convenient to use an analytical expression for the transmission factor. In this case one of the following approximations may be used.

(a) Error not exceeding 0·004:

$$A_{hkl} = \exp \{ -(a_1 + b_1 \sin^2\theta)\mu R - (a_2 + b_2 \sin^2\theta)(\mu R)^2\}, \quad (2)$$

with the following values for the coefficients.

	Cylinder	Sphere
a_1	1·7133	1·5108
b_1	-0·0368	-0·0315
a_2	-0·0927	-0·0951
b_2	-0·0375	-0·2898
Max error	0·0035	0·0024

(b) Error not exceeding 0·04:

$$A_{hkl} = \exp \{ -(a_1 + b_1 \sin^2\theta)\mu R\}, \quad (3)$$

with the following values for the coefficients.

	Cylinder	Sphere
a_1	1·6598	1·4523
b_1	-0·2832	-0·2252

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The R -factor ratio test in crystallography; an approximation. By G.S. PAWLEY,* *Kemisk Institut, Aarhus Universitet, DK-8000 Aarhus, Denmark*

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The range of validity of an approximation for the F distribution is investigated. The R factor ratio as used by crystallographers is calculated and compared with tabulated values. This is done for the range of degrees of freedom generally encountered in crystallographic problems.

Familiarity with the R -factor ratio test as developed by Hamilton (1964, 1965) is assumed. If we have a crystallographic problem with n observations, we usually fit to them an unconstrained model of the structure involving m parameters. Typically $n \sim 1000$, $m \sim 100$. If we now perform a refinement where we constrain the range of the m parameters so that they are determined by a smaller set of $m-b$ different parameters, we say we are applying b constraints. When all refinements are complete we then need to test for any significance in the resulting difference.

* On leave from Department of Physics, Edinburgh University, Edinburgh, Scotland (now returned).

Let the unconstrained refinement yield an R -factor R_0 and the constrained refinement R_Q [for definitions of R see Hamilton (1964) or (1965)]. We then calculate

$$\mathcal{R} = R_Q/R_0$$

for our significance test. Hamilton shows that \mathcal{R} is distributed as

$$\left[\frac{b}{n-m} \cdot F + 1 \right]^{1/2}$$

where F is F -distributed with b and $n-m$ degrees of freedom. We therefore require the significance points of this distribution.