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A Simple and Accurate Technique for the Correction of X-ray Intensities for Angle Factors in the Equi-Inclination Method

By Tor Löfgren

Institute of Chemistry, University of Uppsala, Uppsala, Sweden

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An improved method for converting Weissenberg intensities to a relative $|F|^2$ scale is presented together with the relevant table of factors. The method is based on a simple change of variable and increases the accuracy.

Development

The factors influencing the X-ray intensity which depend only upon the reflexion direction combine to form

$$\left.\begin{aligned}\alpha &= \cos^2\mu.\sin \Upsilon/(1+\cos^2 2\theta)\\ &= \xi \cos\theta/(1+\cos^2 2\theta)\,,\\ \text{where}\quad \sin^2\theta &= \tfrac{1}{4}(\xi^2+\zeta^2)\,.\end{aligned}\right\}\quad (1)$$

(Compare Chia-Si Lu (1943) and his references. Our notations generally follow those of Buerger (1942–9).) In order to find α, the factor by which the intensity, I, should be multiplied, the $\alpha(\xi, \zeta)$ contour map given by Chia-Si Lu (1943)—see also Cochran (1948)—has been used extensively at this Institute. A disadvantage of this diagram, and one which is not completely removed even in Chia-Si Lu's $\alpha(\Upsilon, \zeta)$ diagram, is the rapid relative change in α for low and especially for high ξ values at any fixed ζ. For example, there is no contour line between $\alpha=0{\cdot}05$ and $\alpha=0{\cdot}10$ for low ξ values, while the same relative change from $\alpha=0{\cdot}50$ to $\alpha=1{\cdot}00$ contains ten lines. For large ξ values even $\alpha=0{\cdot}05$ is omitted. When this diagram is used, pure interpolation errors may exceed twenty percent for low ξ values and may become even greater for large ξ values.

Warren & Fankuchen (1941) gave a method that, after some minor changes to adapt it to our discussion, implies that $\alpha(\xi, 0)$, once calculated with the required accuracy, is corrected for upper zones by the 'simplified correction factor',

$$A^{-1}=\alpha(\xi, \zeta)/\alpha(\xi, 0)\,. \quad (2)$$

This is, however, hardly a practical correction factor, since for $\zeta \le 1{\cdot}00$, $0{\cdot}72 \le A \le +\infty$, i.e., $0 \le A^{-1} \le 1{\cdot}39$.

The large variation of correction factor (2) is caused primarily by the factor $\sin \Upsilon$ of (1), which may make the numerator of (2) vanish for a non-vanishing denominator. This occurs for

$$\xi=\xi_{\text{max.}}=2\cos\mu\,. \quad (3)$$

When ξ_0 is exchanged for ξ according to

$$\xi_0=\xi/\cos\mu=2\sin \Upsilon/2 \quad (4)$$

(compare Buerger (1942–9) p. 261, formula (10)), $\xi_{0,\,\text{max.}}$ will be independent of μ, i.e., the numerator and denominator of

$$B=\alpha(\xi_0, \zeta)/\alpha(\xi_0, 0) \quad (5)$$

(compare (2)), will vanish for the same $\xi_{0,\,\text{max.}}$ value: in fact, $\sin \Upsilon/2$ (see (4)) and thus $\sin \Upsilon$ will be independent of μ (or ζ) for any ξ_0.

Diagram I gives the correction factor B, formula (5), and should be compared with Warren & Fankuchen's (1941) diagram (notice our extension of the ζ interval).

The deviations of B from unity are not so great as to prevent a mental correction, at least for low ζ values.* However, a Table of $\alpha(\xi_0, \zeta)$ has been calculated for a rather dense series of ξ_0 and ζ values. This Table should be sufficient for most purposes (Table 1). To meet a demand for high accuracy, four significant figures are given. This is motivated for the chosen density even if linear interpolation is used.

Practical directions

To find ξ_0 of the reflexions, the zero-zone measuring device (say, 'triangle', Buerger (1942–9), Fig. 145) is used for all zones. As the zero-zone triangle can be accurately and permanently engraved, better α values will result; the errors caused by reasonable inaccuracy in ink graduation may lead to $|F|^2$ errors of the same order of magnitude as those arising from visual intensity estimations. For more accurate work it is recommended that at least the extreme ξ_0 values be obtained either by calculation or from an accurately drawn net.

When the ξ_0 values of higher zones are plotted the radial scale easily can be changed linearly according to (4), but this is generally quite unnecessary unless one net is used for indexing all zones. Regraduating

* The previously mentioned rapid change of α for low and high ξ values in Chia-Si Lu's (1943) $\alpha(\xi, \zeta)$ diagram is so serious that B, if calculated—just for comparison with Diagram I—from values taken from his diagram, would not deviate clearly from unity for any $\zeta \le 1{\cdot}00$, when ξ is low or high. His $\alpha(\Upsilon, \zeta)$ diagram would give a B, as far as one can ascertain equal to unity for small Υ and would give only an indication of a change with ζ for Υ near 180°.

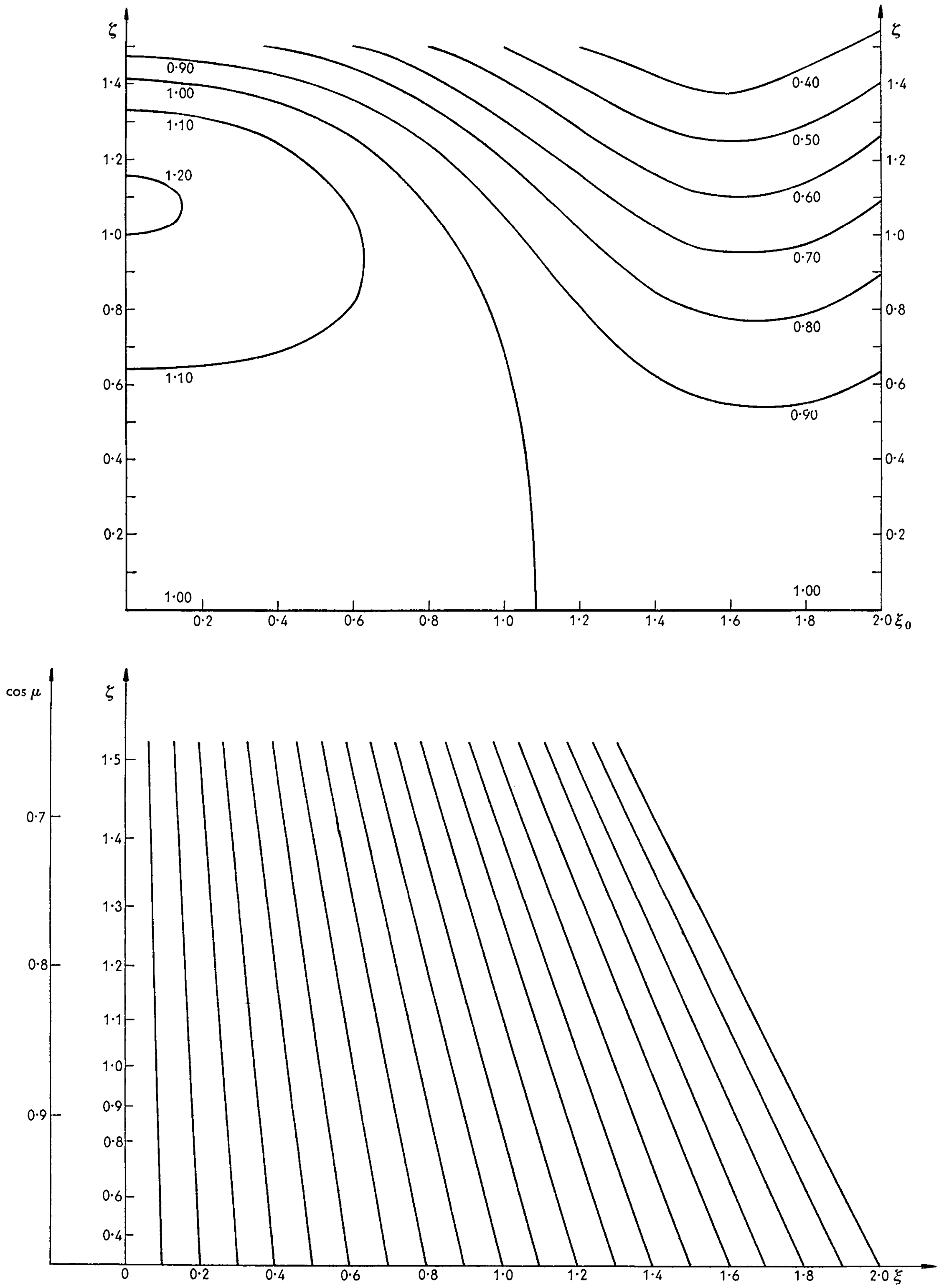

Diagram I and II

the ruler—if such is used—can be performed by means of Diagram II, reproduced in due scale, which gives ξ (as abscissas) for constant ξ_0's (read off as abscissa axis intercepts) and indicated $\cos\mu$ or ζ.

I should like to take the opportunity to thank Mr S. Martinell for computational assistance. My heartfelt thanks are also given to my teacher, Prof. G. Hägg, the Head of this Institute.

Table 1. $\alpha(\xi_0, \zeta)$

$\xi_0 \backslash \zeta$	0.0	0.4	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
0.05	0.02502	0.02602	0.02723	0.02797	0.02874	0.02947	0.03001	0.03018	0.02968	0.02820	0.02548	0.02153
06	03004	03123	03268	03357	03450	03537	03602	03622	03562	03383	03057	02583
07	03506	03646	03815	03918	04026	04127	04204	04226	04155	03947	03566	03013
08	04010	04169	04362	04480	04603	04719	04805	04830	04749	04510	04076	03442
09	04514	04692	04910	05042	05181	05311	05408	05435	05343	05074	04584	03871
10	05019	05218	05459	05606	05759	05903	06011	06040	05937	05638	05092	04300
11	05525	05744	06009	06170	06339	06497	06614	06646	06531	06201	05600	04728
12	06032	06270	06560	06735	06918	07090	07218	07252	07126	06764	06107	05156
13	06541	06800	07112	07303	07501	07686	07823	07859	07721	07327	06615	05583
14	07052	07330	07666	07871	08083	08282	08429	08465	08315	07889	07121	06010
15	07563	07861	08221	08439	08667	08879	09036	09073	08910	08451	07627	06435
16	08077	08395	08778	09011	09253	09478	09643	09681	09505	09014	08132	06860
17	08592	08929	09336	09582	09839	1008	1025	1029	1010	09576	08637	07285
18	09110	09467	09896	1016	1043	1068	1086	1090	1070	1014	09142	07708
19	09629	1000	1046	1073	1102	1128	1147	1151	1129	1070	09645	08131
20	1015	1055	1102	1131	1161	1189	1208	1212	1189	1126	1015	08553
21	1067	1109	1159	1189	1220	1249	1269	1273	1248	1182	1065	08974
22	1120	1163	1216	1247	1280	1310	1331	1334	1308	1238	1115	09394
23	1173	1218	1273	1306	1340	1371	1392	1396	1368	1294	1165	09813
24	1226	1273	1330	1364	1399	1432	1454	1457	1427	1350	1215	1023
25	1279	1329	1388	1423	1460	1493	1516	1519	1487	1406	1265	1065
26	1333	1384	1446	1482	1520	1554	1578	1580	1547	1462	1315	1106
27	1387	1440	1504	1542	1581	1616	1640	1642	1606	1518	1364	1148
28	1442	1496	1562	1601	1642	1678	1702	1703	1666	1574	1414	1189
29	1496	1553	1621	1661	1703	1740	1765	1765	1726	1629	1463	1230
30	1551	1610	1680	1722	1764	1802	1827	1827	1786	1685	1513	1271
31	1607	1667	1739	1782	1826	1866	1890	1889	1845	1740	1562	1312
32	1662	1725	1799	1843	1887	1927	1953	1951	1905	1796	1611	1353
33	1718	1782	1858	1904	1950	1990	2016	2014	1965	1851	1660	1393
34	1775	1841	1919	1965	2012	2053	2079	2076	2025	1907	1709	1433
35	1832	1899	1979	2027	2075	2117	2143	2138	2085	1962	1757	1474
36	1889	1958	2041	2089	2138	2180	2206	2201	2144	2017	1806	1514
37	1947	2018	2102	2152	2201	2244	2270	2263	2204	2072	1854	1554
38	2005	2078	2164	2215	2265	2309	2334	2326	2264	2127	1902	1593
39	2063	2138	2226	2278	2329	2373	2398	2389	2324	2182	1950	1633
40	2123	2199	2289	2341	2393	2438	2463	2451	2384	2237	1998	1672
41	2182	2260	2352	2405	2458	2503	2527	2514	2443	2292	2046	1711
42	2242	2322	2415	2470	2523	2568	2592	2578	2503	2346	2093	1750
43	2303	2384	2479	2534	2588	2633	2657	2641	2563	2400	2140	1788
44	2364	2447	2543	2599	2654	2699	2722	2704	2622	2455	2187	1827
45	2425	2510	2608	2665	2720	2765	2787	2767	2682	2509	2234	1865
46	2488	2574	2674	2731	2787	2832	2853	2830	2741	2563	2280	1903
47	2550	2638	2739	2797	2853	2898	2918	2894	2801	2617	2327	1940
48	2614	2703	2805	2864	2921	2966	2984	2957	2860	2670	2373	1978
49	2677	2768	2872	2931	2988	3033	3050	3021	2920	2724	2419	2015
50	2742	2834	2940	2999	3056	3100	3117	3085	2979	2777	2464	2052
51	2807	2900	3007	3067	3124	3168	3183	3148	3038	2830	2510	2088
52	2873	2967	3075	3136	3193	3236	3250	3212	3098	2883	2555	2125
53	2939	3035	3144	3205	3262	3305	3316	3275	3157	2935	2599	2161
54	3006	3103	3213	3275	3332	3373	3383	3339	3215	2988	2644	2197
55	3074	3172	3283	3345	3402	3442	3450	3403	3274	3040	2688	2232
56	3142	3242	3354	3415	3472	3512	3518	3467	3333	3092	2732	2267
57	3211	3312	3424	3486	3543	3582	3585	3531	3392	3144	2776	2302
58	3281	3383	3496	3558	3614	3651	3653	3595	3450	3195	2819	2336
59	3351	3454	3568	3630	3686	3721	3720	3658	3508	3246	2862	2371
60	3422	3526	3641	3703	3757	3792	3788	3722	3566	3297	2904	2404
61	3494	3599	3714	3776	3829	3863	3856	3786	3624	3347	2946	2438
62	3567	3672	3788	3849	3902	3934	3924	3849	3682	3398	2988	2471
63	3640	3746	3862	3923	3975	4004	3992	3913	3739	3448	3029	2504
64	3715	3821	3937	3998	4048	4076	4060	3976	3796	3497	3071	2536
65	3789	3897	4013	4072	4122	4148	4129	4040	3853	3546	3111	2568
66	3865	3973	4089	4148	4197	4220	4197	4103	3910	3595	3151	2600
67	3942	4050	4165	4224	4271	4292	4266	4166	3966	3643	3191	2631
68	4019	4128	4243	4301	4346	4364	4334	4230	4023	3691	3230	2661
69	4097	4206	4321	4377	4421	4437	4402	4292	4079	3739	3269	2692
70	4177	4285	4399	4455	4497	4509	4471	4355	4134	3786	3308	2722
71	4256	4365	4478	4533	4573	4582	4539	4418	4189	3833	3346	2752
72	4337	4446	4558	4611	4649	4655	4608	4480	4244	3879	3383	2781
73	4418	4527	4638	4690	4726	4728	4676	4542	4298	3925	3420	2809
74	4501	4609	4719	4769	4802	4802	4744	4604	4352	3970	3457	2838
75	4584	4692	4800	4849	4879	4875	4812	4665	4406	4015	3493	2866
76	4669	4775	4881	4929	4957	4948	4881	4726	4459	4059	3528	2893
77	4753	4860	4964	5009	5034	5022	4948	4787	4511	4103	3563	2920
78	4840	4945	5047	5090	5112	5095	5016	4848	4563	4146	3597	2946
79	4926	5031	5130	5171	5190	5168	5083	4908	4615	4189	3631	2972
80	5014	5117	5214	5253	5268	5242	5151	4968	4666	4231	3664	2997
81	5102	5204	5298	5334	5346	5315	5218	5027	4717	4272	3697	3022
82	5192	5293	5383	5417	5425	5389	5285	5085	4767	4313	3729	3047
83	5282	5380	5469	5499	5504	5462	5351	5144	4816	4353	3760	3071
84	5373	5470	5554	5582	5582	5535	5417	5202	4865	4392	3791	3094
85	5464	5560	5640	5665	5661	5608	5483	5259	4913	4431	3821	3117
86	5557	5650	5727	5748	5739	5680	5548	5316	4960	4469	3850	3139
87	5650	5741	5813	5831	5818	5753	5613	5372	5007	4506	3879	3161
88	5745	5833	5901	5915	5896	5825	5678	5427	5052	4542	3907	3182
89	5840	5925	5988	5998	5974	5896	5741	5482	5097	4578	3935	3202
90	5936	6018	6076	6082	6052	5968	5805	5536	5142	4613	3961	3222
91	6032	6111	6163	6165	6130	6039	5867	5589	5185	4647	3987	3242
92	6130	6205	6251	6249	6208	6110	5929	5641	5228	4680	4012	3260
93	6227	6299	6339	6331	6285	6179	5990	5693	5269	4712	4037	3279
94	6326	6393	6428	6415	6363	6249	6051	5744	5310	4744	4061	3296
95	6425	6488	6516	6498	6439	6318	6110	5794	5350	4774	4084	3313
96	6525	6583	6603	6581	6515	6386	6169	5843	5389	4804	4105	3329
97	6625	6678	6692	6663	6590	6453	6227	5890	5427	4833	4127	3345
98	6726	6774	6779	6746	6666	6520	6285	5937	5464	4861	4147	3360
99	6827	6870	6867	6827	6741	6586	6340	5983	5499	4888	4167	3375
1.00	6928	6965	6955	6909	6814	6651	6395	6028	5534	4913	4186	3388
1.01	7030	7061	7041	6989	6887	6714	6449	6071	5567	4938	4204	3402
1.02	7132	7157	7128	7069	6959	6777	6502	6114	5599	4962	4221	3414
1.03	7234	7252	7214	7148	7030	6839	6554	6155	5631	4985	4237	3426
1.04	7336	7348	7299	7227	7101	6900	6604	6194	5661	5007	4252	3437

Table 1 (*cont.*)

ξ/ξ_0 \ ζ	0.0	0.4	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
1.05	0.7439	0.7443	0.7384	0.7304	0.7169	0.6959	0.6653	0.6233	0.5689	0.5027	0.4267	0.3448
1.06	7541	7537	7467	7381	7237	7017	6700	6270	5717	5046	4280	3457
1.07	7643	7631	7551	7456	7304	7074	6746	6305	5743	5065	4293	3467
1.08	7745	7725	7633	7531	7370	7129	6791	6340	5767	5081	4304	3474
1.09	7846	7817	7714	7604	7433	7183	6834	6372	5791	5098	4316	3483
1.10	7947	7909	7794	7676	7496	7235	6876	6403	5813	5112	4325	3489
1.11	8047	8000	7873	7746	7557	7285	6916	6433	5834	5126	4334	3496
1.12	8147	8090	7950	7815	7615	7334	6953	6461	5853	5138	4342	3501
1.13	8245	8179	8025	7883	7674	7381	6990	6487	5870	5149	4349	3506
1.14	8344	8267	8100	7947	7729	7426	7024	6511	5886	5159	4355	3510
1.15	8440	8353	8172	8011	7783	7469	7057	6534	5901	5168	4360	3514
1.16	8535	8438	8243	8073	7834	7511	7087	6555	5913	5175	4364	3516
1.17	8630	8520	8312	8133	7884	7550	7116	6574	5925	5181	4367	3518
1.18	8722	8602	8378	8190	7931	7586	7142	6591	5935	5185	4368	3519
1.19	8813	8681	8443	8245	7976	7621	7166	6606	5943	5189	4370	3519
1.20	8902	8758	8505	8298	8018	7653	7188	6620	5949	5191	4369	3519
1.21	8989	8832	8564	8348	8059	7683	7209	6631	5955	5192	4368	3518
1.22	9074	8904	8621	8396	8096	7710	7226	6641	5958	5191	4366	3516
1.23	9156	8974	8676	8441	8131	7734	7242	6648	5959	5189	4363	3513
1.24	9235	9041	8727	8482	8163	7757	7254	6654	5959	5185	4358	3509
1.25	9312	9105	8775	8522	8192	7776	7265	6656	5957	5181	4353	3505
1.26	9386	9165	8821	8557	8218	7792	7273	6657	5953	5174	4347	3500
1.27	9457	9222	8863	8590	8241	7806	7278	6656	5948	5167	4339	3495
1.28	9524	9277	8900	8619	8261	7817	7281	6653	5940	5158	4331	3488
1.29	9588	9327	8935	8645	8278	7825	7282	6648	5931	5147	4321	3481
1.30	9648	9373	8967	8667	8291	7830	7279	6640	5920	5136	4310	3472
1.31	9703	9415	8995	8686	8301	7832	7274	6630	5908	5123	4299	3464
1.32	9755	9454	9018	8701	8308	7830	7267	6618	5892	5108	4286	3454
1.33	9802	9488	9037	8713	8311	7826	7256	6603	5877	5092	4272	3444
1.34	9845	9517	9052	8719	8310	7819	7243	6586	5858	5074	4257	3432
1.35	9883	9543	9063	8723	8306	7809	7228	6567	5838	5056	4241	3420
1.36	9915	9563	9070	8722	8298	7794	7208	6546	5816	5035	4224	3407
1.37	9943	9578	9073	8718	8287	7777	7188	6523	5793	5014	4206	3393
1.38	9966	9589	9070	8708	8271	7756	7163	6496	5767	4990	4187	3379
1.39	9983	9594	9063	8695	8253	7732	7136	6469	5740	4966	4166	3364
1.40	9994	9594	9051	8678	8230	7705	7106	6438	5711	4940	4145	3347
1.41	1.0000	9589	9036	8656	8203	7675	7074	6405	5679	4912	4122	3331
1.42	0.9999	9578	9014	8630	8172	7641	7038	6370	5646	4884	4099	3313
1.43	9993	9562	8988	8599	8138	7604	7000	6333	5612	4853	4074	3295
1.44	9979	9539	8957	8563	8099	7563	6958	6293	5576	4821	4048	3275
1.45	9961	9512	8922	8525	8057	7520	6915	6251	5537	4789	4022	3256
1.46	9936	9478	8881	8480	8010	7472	6868	6206	5497	4754	3994	3235
1.47	9904	9440	8836	8432	7961	7422	6819	6160	5456	4719	3965	3213
1.48	9865	9394	8785	8380	7906	7368	6767	6112	5412	4681	3935	3190
1.49	9821	9344	8730	8322	7849	7311	6712	6061	5367	4643	3905	3168
1.50	9769	9287	8669	8261	7787	7251	6655	6008	5320	4603	3872	3143
1.51	9711	9225	8604	8195	7722	7187	6595	5953	5272	4562	3840	3119
1.52	9646	9157	8533	8125	7653	7120	6532	5895	5221	4520	3805	3093
1.53	9576	9083	8459	8051	7581	7051	6468	5837	5169	4476	3771	3067
1.54	9498	9003	8379	7972	7504	6978	6399	5775	5116	4431	3734	3039
1.55	9414	8918	8295	7889	7425	6902	6329	5712	5060	4385	3697	3011
1.56	9324	8828	8207	7803	7341	6824	6257	5647	5003	4337	3659	2982
1.57	9228.	8732	8113	7713	7254	6742	6182	5579	4945	4288	3620	2953
1.58	9125	8631	8015	7618	7164	6658	6104	5510	4885	4238	3579	2922
1.59	9017	8525	7914	7520	7071	6570	6025	5439	4823	4186	3538	2891
1.60	8902	8413	7808	7418	6975	6481	5943	5366	4760	4133	3496	2859
1.61	8782	8297	7697	7312	6875	6388	5858	5291	4695	4079	3453	2826
1.62	8656	8177	7584	7204	6773	6293	5772	5215	4629	4024	3408	2792
1.63	8526	8051	7466	7092	6667	6196	5684	5136	4562	3968	3363	2757
1.64	8389	7921	7344	6976	6559	6096	5593	5057	4493	3910	3317	2722
1.65	8248	7787	7220	6857	6448	5994	5501	4974	4422	3851	3270	2685
1.66	8103	7648	7091	6736	6334	5889	5406	4891	4350	3791	3221	2648
1.67	7952	7506	6960	6612	6218	5782	5310	4806	4277	3730	3171	2610
1.68	7797	7359	6824	6484	6099	5674	5212	4719	4202	3667	3121	2571
1.69	7638	7210	6687	6354	5978	5562	5112	4631	4126	3603	3069	2531
1.70	7475	7057	6546	6221	5855	5449	5009	4541	4048	3538	3016	2490
1.71	7309	6900	6402	6086	5729	5334	4906	4449	3969	3472	2963	2449
1.72	7138	6741	6256	5948	5601	5216	4800	4356	3889	3404	2908	2406
1.73	6965	6578	6107	5808	5471	5097	4693	4261	3807	3335	2852	2362
1.74	6787	6413	5955	5665	5338	4976	4584	4165	3724	3266	2795	2317
1.75	6607	6244	5802	5521	5204	4853	4473	4067	3639	3194	2736	2271
1.76	6424	6074	5646	5374	5068	4728	4361	3968	3553	3121	2677	2224
1.77	6239	5900	5488	5225	4930	4602	4247	3867	3465	3047	2616	2176
1.78	6051	5725	5327	5075	4790	4474	4131	3764	3376	2971	2554	2127
1.79	5861	5547	5165	4922	4647	4344	4014	3659	3285	2894	2490	2077
1.80	5667	5367	5000	4767	4503	4211	3894	3553	3193	2816	2425	2025
1.81	5473	5184	4833	4610	4357	4078	3773	3445	3099	2735	2359	1972
1.82	5275	5000	4665	4451	4209	3941	3649	3336	3003	2653	2291	1917
1.83	5075	4813	4493	4290	4059	3803	3524	3224	2905	2570	2221	1861
1.84	4873	4624	4320	4126	3907	3663	3397	3110	2805	2484	2149	1804
1.85	4668	4433	4144	3961	3752	3520	3267	2994	2703	2396	2076	1744
1.86	4461	4238	3966	3792	3595	3375	3135	2875	2598	2306	2000	1683
1.87	4251	4042	3785	3621	3435	3227	3000	2754	2491	2213	1922	1619
1.88	4038	3841	3600	3446	3271	3076	2861	2629	2381	2117	1841	1553
1.89	3821	3638	3412	3268	3104	2921	2719	2501	2267	2019	1758	1485
1.90	3600	3430	3220	3086	2933	2762	2574	2369	2150	1917	1671	1413
1.91	3374	3217	3023	2899	2757	2598	2423	2233	2028	1810	1580	1338
1.92	3142	2998	2820	2705	2575	2428	2267	2091	1902	1699	1485	1259
1.93	2903	2771	2609	2505	2385	2252	2104	1943	1768	1582	1384	1176
1.94	2653	2535	2389	2295	2187	2066	1932	1786	1628	1458	1277	1086
1.95	2391	2286	2157	2073	1977	1869	1750	1619	1477	1324	1162	0990
1.96	2111	2020	1907	1834	1751	1657	1552	1437	1313	1179	1036	0883
1.97	1804	1728	1633	1571	1501	1421	1333	1236	1130	1016	0894	0763
1.98	1453	1393	1318	1269	1213	1150	1079	1002	0917	0825	0727	0622

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