Thus, $\sigma(q_{N/2})$ is simply the root-mean-square (r.m.s.) value of the positional e.s.d.'s.

If the positional e.s.d.'s are roughly the same, we can as a further approximation assume that all σ_j can be replaced by $\sigma = [(1/N)\sum \sigma_j^2]^{1/2}$, *i.e.* replaced by the r.m.s. value σ. Since $\sum \cos^2[2\pi m(j-1)/N] = \sum \sin^2[2\pi m(j-1)/N] = N/2$, it follows from (3)–(5) that for this case

$$\sigma(c_m) = \sigma(s_m) = \sigma(q_m) = \sigma(q_{N/2}) = \sigma \qquad (6)$$

and $\sigma(\varphi_m) = \sigma/q_m$.

For the spherical polar set (Q,θ,Φ) introduced by Cremer & Pople (1975) to describe the puckering of six-membered rings [*viz* $Q = (q_2^2 + q_3^2)^{1/2}$, $\theta = \arctan(q_2/q_3)$ and $\Phi = \varphi_2$], the expressions for the e.s.d.'s of Q and θ are (*cf.* Taylor, 1980) analogous to those for $\sigma(q_m)$ and $\sigma(\varphi_m)$. Thus,

$$\begin{aligned}\sigma^2(Q) &= \sigma^2(q_3)\cos^2\theta + \sigma^2(q_2)\sin^2\theta \\ \sigma^2(\theta) &= [\sigma^2(q_3)\sin^2\theta + \sigma^2(q_2)\cos^2\theta]/Q^2.\end{aligned} \qquad (7)$$

For the case when all σ_j can be replaced by their r.m.s. value, σ, the e.s.d.'s of Q and θ become

$$\sigma(Q) = \sigma \quad \text{and} \quad \sigma(\theta) = \sigma/Q. \qquad (8)$$

Taylor (1980) has given two examples of calculations of puckering-parameter e.s.d.'s, with his expressions for non-isotropic e.s.d.'s of independent atomic positions. For the pyranose rings observed in the crystal structures of β-DL-arabinopyranose (Takagi, Nordenson & Jeffrey, 1979) and β-L-arabinopyranose (Takagi & Jeffrey, 1977) he obtained for the spherical polar set Q,θ,Φ: 0·584 (1) Å, 2·1 (1)°, 140 (3)° and 0·573 (2) Å, 1·5 (2)°, 116 (7)°, respectively. Calculating the e.s.d.'s from individual isotropic positional e.s.d.'s, as suggested in the present paper [formulas (3)–(5) and (7)], yields the same rounded-off e.s.d.'s (*viz* 0·00098 Å, 0·096°, 2·7° and 0·0018 Å, 0·18°, 6·7°, respectively). These e.s.d. values are furthermore obtained even if the individual positional e.s.d.'s are replaced by their r.m.s. value, σ [formulas (6) and (8)]. The two examples thus illustrate the validity of the different approximations utilized in the present study.

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A table of maxima and minima of the Bessel functions $J_n(z)$ for $n = 0$ to $n = 30$.

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Abstract

Maxima and minima are tabulated for the Bessel functions $J_n(x)$ for values of n from 0 to 30 [*i.e.* zeros of $J_n'(x)$]. The first six points are recorded for each function. The table considerably extends the range of earlier tables available in the literature. It should have applications in the interpretation of diffraction patterns from helical or wave-form structures or features, and has been used in connection with some electron microscope images.

Bessel functions of the first kind of order n, where n is a positive integer, have come into the calculations and interpretation of diffraction patterns from helical (or wave-form) structures. Particular applications include the interpretation of X-ray diffraction patterns from large biological molecules based upon helices (Cochran, Crick & Vand, 1952; Klug, Crick & Wyckoff, 1958; Sherwood, 1976). The same principles have been successfully applied to the interpretation of electron microscope images of such molecules and their associated growth forms in biological or bio-medical sections (Misell, 1978). More recently, images of metal structures containing dislocations or other features have been interpreted in the same way (Andrews & Keown, 1981).

Standard tables are available in two volumes of functions (Abramowitz & Stegun, 1965; Jahnke & Emde, 1945). Generally, numerical values of the Bessel functions are given and their zeros. Maxima and minima are also provided in Table 9.5 of Cochran, Crick & Vand (1952) for values of n up to and including 8. Table 1 may be regarded as an extension of this table and also one provided by Spiegel (1974). A formula given by Gray & Matthews (1922) and Gray & Macrobert (1966) does not appear to be entirely reliable and the calculations have been based upon a computer program used in the Medical Research Council Laboratory of Molecular Biology (Cambridge).

For some practical purposes values to one or two decimal places are sufficiently accurate. Graphical interpolation is also accurate for some applications, and reference may also be made to the recurrence relation

$$J_n'(z) = J_{n-1}(z) - J_{n+1}(z)$$

so that the maxima and minima are at values of (z) where J_{n-1} and J_{n+1} intersect. Evidently the present tabulation is more accurate and should be available as an addition to the tables for these functions and for use when required by

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Table 1. *Maxima and minima of* $J_n(z)$; *z values for* $J_n'(z)=0$

n	$s=0$	1	2	3	4	5
0	0·0000	3·8317	7·0156	10·1735	13·3237	16·4706
1	1·8412	5·3314	8·5363	11·7060	14·8636	18·0155
2	3·0542	6·7061	9·9695	13·1704	16·3475	19·5129
3	4·2012	8·0152	11·3459	14·5858	17·7887	20·9725
4	5·3176	9·2824	12·6819	15·9641	19·1960	22·4010
5	6·4156	10·5199	13·9872	17·3128	20·5755	23·8036
6	7·5013	11·7349	15·2682	18·6374	21·9317	25·1839
7	8·5778	12·9324	16·5294	19·9419	23·2681	26·5450
8	9·6474	14·1155	17·7740	21·2291	24·5872	27·8893
9	10·7114	15·2867	19·0046	22·5014	25·8913	29·2186
10	11·7709	16·4479	20·2230	23·7607	27·1820	30·5345
11	12·8265	17·6003	21·4309	25·0085	28·4609	31·8384
12	13·8788	18·7451	22·6293	26·2460	29·7290	33·1314
13	14·9284	19·8832	23·8194	27·4743	30·9874	34·4145
14	15·9754	21·0154	25·0020	28·6943	32·2370	35·6885
15	17·0203	22·1422	26·1778	29·9066	33·4784	36·9542
16	18·0633	23·2643	27·3474	31·1119	34·7125	38·2121
17	19·1045	24·3819	28·5114	32·3109	35·9396	39·4628
18	20·1441	25·4956	29·6701	33·5039	37·1604	40·7068
19	21·1823	26·6055	30·8241	34·6915	38·3752	41·9446
20	22·2191	27·7121	31·9737	35·8739	39·5845	43·1765
21	23·2548	28·8156	32·1192	37·0516	40·7886	44·4030
22	24·2894	29·9161	34·2608	38·2249	41·9879	45·6243
23	25·3229	31·0140	35·3988	39·3940	43·1825	46·8408
24	26·3555	32·1093	36·5334	40·5591	44·3729	48·0526
25	27·3872	33·2023	37·6649	41·7206	45·5592	49·2601
26	28·4181	34·2930	38·7934	42·8786	46·7416	50·4634
27	29·4482	35·3816	39·9191	44·0332	47·9203	51·6629
28	30·4775	36·4683	41·0421	45·1847	49·0956	52·8586
29	31·5062	37·5531	42·1626	46·3333	50·2676	54·0507
30	32·5342	38·6361	43·2807	47·4790	51·4364	55·2395

workers in different fields of diffraction, or in other fields of science and engineering.

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On the application of Hamilton's test: an incorrect formula in *International Tables for X-ray Crystallography*, Vol. IV.

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Abstract

For Hamilton's R-factor ratio test, formula (7) in chapter 4.2 of *International Tables for X-ray Crystallography* (1974), Vol. IV, is incorrect and should be replaced by

$$\mathscr{R}_{b,N_1,\alpha} = 1 + \frac{4000}{N_1}(\mathscr{R}_{b,4000,\alpha} - 1).$$

All relevant information is given in the *Abstract*.

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