Table 2. *Observed and calculated structure factors for* Yb_3Ge_5

hkℓ	$\|F_o\|$	$\|F_c\|$	α, °	hkℓ	$\|F_o\|$	$\|F_c\|$	α, °
010	26·9	19·9	180·00	221	157·8	152·9	233·71
020	25·2	14·0	180·00	231	90·1	86·1	351·04
030	219·4	226·2	0·00	241	54·6	61·9	275·46
040	0·0	7·5	180·00	331	78·2	80·2	343·86
050	64·1	69·1	0·00	002	235·0	289·0	0·00
110	133·4	122·2	122·09	012	19·6	17·6	180·00
120	107·0	98·4	242·88	022	15·7	9·4	180·00
130	64·8	61·6	127·78	032	197·0	198·4	0·00
140	100·8	97·1	98·10	042	0·0	9·9	180·00
150	85·6	77·5	252·15	112	112·9	108·4	120·00
220	152·8	120·3	240·46	122	88·7	83·1	248·20
230	64·2	59·2	7·69	132	58·4	55·9	128·51
240	90·0	89·1	228·53	142	90·2	89·3	94·31
330	130·6	127·3	1·61	222	116·0	116·1	240·63
001	58·8	51·1	0·00	202	53·1	52·2	77·49
011	15·9	16·1	180·00	003	50·4	52·0	0·00
021	100·7	87·6	0·00	013	14·6	10·8	180·00
031	84·2	79·3	0·00	023	69·2	65·6	0·00
041	81·7	71·0	180·00	033	69·2	69·3	180·00
051	73·2	73·5	0·00	113	170·9	168·7	120·51
113	212·2	203·6	119·26	123	39·8	35·9	338·43
121	56·3	48·6	5·75	133	44·1	46·3	126·42
131	57·9	56·4	127·88	223	126·5	127·4	235·43
141	152·5	147·0	138·58	004	185·1	202·0	0·00

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Table 3. *Interatomic distances* Å *for* Yb_3Ge_5

The e.s.d.'s include only the uncertainties in the positional parameters.

Yb – 4 Ge(2)	3·015 ± 0·006 Å
– 4 Ge(1)	3·016 ± 0·002
– 2 Ge(2)	3·356 ± 0·021
– 4 Yb	3·778 ± 0·005
– 2 Yb	4·166
Ge(1) – 3 Ge(2)	2·585 ± 0·017
– 6 Yb	3·016 ± 0·002
– 3 Ge(1)	3·928
Ge(2) – 2 Ge(1)	2·585 ± 0·017
– 2 Ge(2)	2·979 ± 0·044
– 4 Yb	3·015 ± 0·006
– 2 Yb	3·356 ± 0·021

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The rate of refinement of coordinates for the minimum residual method in three dimensions.

By E. STANLEY, *Department of Physics, University of Saskatchewan, Regina Campus, Regina, Saskatchewan, Canada*

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Bhuiya & Stanley (1963) proposed a method of refinement in which each parameter, u_j, is varied in turn from $u_j - n\Delta u_j$ to $u_j + n\Delta u_j$ in $2n$ increments of Δu_j. The lowest value of the residual, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, within the range of variation is noted and the corresponding value of u_j is taken as the best value of the parameter within the permitted range of variation. This method has worked very well in two-dimensional studies and the rate of refinement in two dimensions has been studied in detail by Stanley (1964) who showed that, for small errors, the rate of refinement could be related to the average error in the coordinates on the basis of the figures given by Luzzati (1952) for the residual as a function of error in coordinates and sin θ.

Tables 1 and 2 give values of the residual R for centrosymmetric and non-centrosymmetric space groups, for three-dimensional data, as a function of the standard devi-

Table 1. *Values of* $(\bar{1})R$ *as a function of* $\sigma(r)$ *and* B

$\sigma(r)$ \ B	0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02	0.114	0.109	0.105	0.100	0.096	0.092	0.088	0.084	0.080	0.077	0.074
0.04	0.219	0.211	0.202	0.194	0.186	0.177	0.170	0.162	0.166	0.149	0.143
0.06	0.314	0.302	0.291	0.279	0.268	0.256	0.246	0.235	0.226	0.217	0.209
0.08	0.398	0.384	0.370	0.356	0.342	0.328	0.315	0.302	0.291	0.280	0.270
0.10	0.471	0.456	0.439	0.424	0.408	0.393	0.378	0.363	0.350	0.337	0.326
0.12	0.534	0.518	0.501	0.484	0.466	0.450	0.433	0.418	0.403	0.390	0.377
0.14	0.587	0.570	0.553	0.535	0.517	0.500	0.483	0.467	0.451	0.437	0.423
0.16	0.630	0.614	0.597	0.579	0.561	0.544	0.526	0.510	0.494	0.479	0.465
0.18	0.667	0.651	0.634	0.616	0.599	0.582	0.564	0.548	0.532	0.517	0.503
0.20	0.696	0.681	0.665	0.648	0.631	0.614	0.597	0.581	0.565	0.551	0.536
0.22	0.720	0.705	0.690	0.674	0.658	0.642	0.626	0.610	0.595	0.580	0.566
0.24	0.738	0.725	0.711	0.696	0.681	0.665	0.650	0.635	0.620	0.606	0.592
0.26	0.752	0.740	0.727	0.714	0.700	0.685	0.671	0.657	0.643	0.629	0.616
0.28	0.764	0.753	0.741	0.729	0.716	0.702	0.689	0.676	0.663	0.650	0.637
0.30	0.772	0.763	0.752	0.741	0.729	0.717	0.704	0.692	0.679	0.667	0.656
0.32	0.780	0.771	0.762	0.751	0.740	0.729	0.717	0.706	0.694	0.683	0.672
0.34	0.786	0.778	0.769	0.760	0.750	0.739	0.729	0.718	0.707	0.696	0.686
0.36	0.791	0.784	0.776	0.767	0.758	0.749	0.739	0.729	0.719	0.709	0.699
0.38	0.795	0.788	0.781	0.773	0.765	0.756	0.747	0.738	0.729	0.720	0.711
0.40	0.798	0.793	0.786	0.779	0.771	0.763	0.755	0.746	0.738	0.729	0.721
0.42	0.801	0.796	0.790	0.786	0.777	0.769	0.761	0.754	0.746	0.738	0.730
0.44	0.804	0.799	0.794	0.788	0.781	0.775	0.767	0.760	0.753	0.745	0.738
0.46	0.807	0.802	0.797	0.791	0.785	0.779	0.773	0.766	0.759	0.752	0.745
0.48	0.809	0.805	0.800	0.795	0.789	0.783	0.777	0.771	0.764	0.758	0.752
0.50	0.817	0.807	0.802	0.798	0.792	0.787	0.781	0.775	0.770	0.763	0.757

Table 2. *Values of* $(1)R$ *as a function of* $\sigma(r)$ *and* B

$\sigma(r)$ \ B	0.0	1.0	2.0	3.0	4.0	5.0	6.0	7.0	8.0	9.0	10.0
0.00	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.02	0.073	0.070	0.068	0.065	0.062	0.059	0.056	0.054	0.051	0.049	0.047
0.04	0.144	0.138	0.132	0.127	0.121	0.116	0.110	0.106	0.101	0.097	0.093
0.06	0.211	0.203	0.195	0.187	0.179	0.171	0.163	0.156	0.149	0.143	0.137
0.08	0.272	0.262	0.252	0.242	0.232	0.222	0.213	0.204	0.195	0.187	0.180
0.10	0.325	0.314	0.303	0.291	0.280	0.268	0.256	0.247	0.238	0.229	0.220
0.12	0.370	0.359	0.346	0.334	0.322	0.310	0.298	0.287	0.276	0.266	0.257
0.14	0.409	0.397	0.384	0.371	0.359	0.346	0.334	0.322	0.311	0.300	0.290
0.16	0.441	0.429	0.416	0.404	0.391	0.378	0.365	0.353	0.342	0.331	0.321
0.18	0.467	0.456	0.443	0.431	0.418	0.405	0.393	0.381	0.369	0.358	0.348
0.20	0.488	0.477	0.466	0.454	0.441	0.429	0.417	0.405	0.394	0.383	0.372
0.22	0.505	0.495	0.484	0.473	0.461	0.449	0.437	0.426	0.415	0.404	0.394
0.24	0.518	0.509	0.499	0.488	0.477	0.466	0.455	0.444	0.434	0.423	0.413
0.26	0.529	0.520	0.511	0.501	0.491	0.480	0.470	0.460	0.450	0.440	0.431
0.28	0.537	0.529	0.521	0.512	0.502	0.493	0.485	0.473	0.464	0.455	0.446
0.30	0.544	0.536	0.528	0.521	0.512	0.503	0.494	0.485	0.476	0.467	0.459
0.32	0.549	0.543	0.536	0.528	0.520	0.512	0.504	0.495	0.487	0.479	0.471
0.34	0.553	0.547	0.541	0.534	0.527	0.519	0.512	0.504	0.496	0.489	0.481
0.36	0.557	0.552	0.546	0.540	0.533	0.526	0.519	0.512	0.505	0.498	0.491
0.38	0.560	0.555	0.550	0.544	0.538	0.532	0.525	0.519	0.512	0.505	0.498
0.40	0.563	0.558	0.553	0.548	0.543	0.537	0.531	0.525	0.518	0.512	0.506
0.42	0.565	0.561	0.557	0.552	0.547	0.541	0.536	0.530	0.524	0.518	0.513
0.44	0.567	0.563	0.559	0.555	0.550	0.545	0.540	0.535	0.529	0.524	0.519
0.46	0.569	0.565	0.562	0.558	0.553	0.549	0.544	0.539	0.534	0.529	0.524
0.48	0.570	0.567	0.564	0.560	0.556	0.552	0.547	0.542	0.538	0.533	0.528
0.50	0.572	0.569	0.566	0.562	0.558	0.554	0.550	0.546	0.541	0.537	0.533

ation of the coordinates, $\sigma(r)$, and the general temperature coefficient, B, calculated from the relationship

$$R=\frac{\int_0^{S_{\max}} 4\pi s^2 R(\sigma,s) f(s) \exp(-Bs^2/4)ds}{\int_0^{S_{\max}} 4\pi s^2 f(s) \exp(-Bs^2/4)ds}$$

where the integrals are taken over the range of $s=2\sin\theta/\lambda$ limited by the sphere of reflection of Cu $K\alpha$ radiation and $f(s)$ is the scattering factor for carbon atoms of the type proposed by Vand, Eiland & Pepinsky (1957).

Using the expression $\delta\sigma=\frac{|\Delta r_N|^2}{2N\sigma}$ given by Stanley (1964) and the values of σ and $dR/d\sigma$ from the tables corresponding to the observed values of R a comparison can be made between the theoretical reduction in R as the refinement progresses and that observed in practice. The example used is that of a problem with six atoms in the asymmetric unit (space group $P2_1/c$) whose structure has been determined and refined by Dr G. Germain (private communication). Table 3 gives the details of the progress in refinement in one typical cycle. The agreement, for a six-atom problem, is reasonably good.

Table 3. *Progress of refinement in a typical cycle*

Initial value of $R=24{\cdot}705\,\%$

Atom No.	$\lvert\Delta r_N\rvert$	R	ΔR obs.	ΔR calc.
1	0·10 Å	24·007 %	0·698 %	0·686 %
2	0·15	22·109	1·898	1·711
3	0·05	21·973	0·136	0·191
4	0·16	18·013	3·960	2·311
5	0·07	17·895	0·118	0·462
6	0·05	17·692	0·203	0·232

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Acta Cryst. (1965). **18**, 1087

The Fourier transform of the coiled-coil model for *a*-keratin. A correction.

By R. D. B. FRASER, T. P. MACRAE and A. MILLER. *Division of Protein Chemistry, C.S.I.R.O., Wool Research Laboratories, Parkville N. 2, Victoria, Australia*

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In a recent communication (Fraser, MacRae & Miller, 1964) atomic coordinates were given for the asymmetric unit of the coiled-coil model for α-keratin. An error has since been discovered in a computer routine used to list these coordinates, and Table 2 in the original communication should be replaced by the following. The routine was not used in the Fourier-transform calculations.

References

FRASER, R. D. B., MACRAE, T. P. & MILLER, A. (1964). *Acta Cryst.* **17**, 813.

Table 2

(*a*) Atomic coordinates of asymmetric unit in a coiled-coil with $r_0=5{\cdot}2$ Å (Oz = major helix axis).

	x	y	z		x	y	z
β–C(1)	8·400	0·000	0·000	C(4)	6·487	0·182	4·180
α–C(1)	7·350	0·887	−0·697	O(4)	6·466	0·683	3·040
N(1)	6·242	1·151	0·233	β–C(5)	7·541	0·990	6·338
C(1)	5·090	1·658	−0·155	α–C(5)	6·282	1·040	5·456
O(1)	4·804	1·974	−1·315	N(5)	5·135	0·511	6·202
β–C(2)	4·636	2·845	2·016	C(5)	3·992	0·191	5·633
α–C(2)	4·082	1·843	0·998	O(5)	3·742	0·301	4·437
N(2)	3·855	0·547	1·636	β–C(6)	2·583	0·753	7·621
C(2)	3·634	−0·563	0·966	α–C(6)	2·939	−0·342	6·618
O(2)	3·577	−0·647	−0·256	N(6)	3·487	−1·509	7·305
β–C(3)	2·169	−1·591	2·712	C(6)	4·114	−2·488	6·691
α–C(3)	3·424	−1·795	1·864	O(6)	4·302	−2·547	5·473
N(3)	4·598	−1·960	2·721	β–C(7)	3·383	−4·259	8·317
C(3)	5·835	−1·893	2·275	α–C(7)	4·595	−3·602	7·647
O(3)	6·149	−1·693	1·089	N(7)	5·469	−3·009	8·666
β–C(4)	6·748	−3·509	3·996	C(7)	6·438	−2·164	8·376
α–C(4)	6·892	−2·101	3·392	O(7)	6·727	−1·778	7·225
N(4)	6·679	−1·095	4·444				

(*b*) Bond lengths and angles in a coiled-coil compared with values in an undistorted α-helix.

Bond	Maximum	Undistorted	Minimum	Angle	Maximum	Undistorted	Minimum
βC–αC	1·541	1·535	1·527	βC–αC–N	110·57	109·91	109·31
αC–N	1·471	1·465	1·461	αC–N–C*	123·65	123·16	122·71
N–C*	1·318	1·317	1·315	N–C*–O*	125·27	125·00	124·66
C–O	1·248	1·237	1·226	O–C–αC	122·44	121·79	121·08
C–αC	1·555	1·546	1·537	C–αC–βC	110·27	109·75	109·21
N · · · O†	2·864	2·841	2·812	N–C*–αC*	113·71	113·21	112·70
				C–αC–N	108·94	108·86	108·74
				C*–N · · · O†	116·00	115·44	114·88

† Hydrogen-bonded atoms. * Indicates next residue.