Libration corrections for Compound 9.

ATOM 1	ATOM 2		DIST	DIST	CORRNS	CORRN	CORRN	CORRN
GP	CORRN	GP	CORRN	GP CORRN				
O1	C1	, 1	1.1881	1.191	0.0029	0.0029	0.0000	0.0000
O2	C8	, 1	1.1936	1.196	0.0028	0.0028	0.0000	0.0000
O3	C1	, 1	1.4002	1.403	0.0031	0.0031	0.0000	0.0000
O3	C8	, 1	1.3865	1.390	0.0032	0.0032	0.0000	0.0000
C1	C2	, 1	1.4978	1.500	0.0027	0.0027	0.0000	0.0000
C2	C3	, 1	1.5690	1.572	0.0029	0.0029	0.0000	0.0000
C2	C7	, 1	1.5301	1.534	0.0038	0.0038	0.0000	0.0000
C3	C4	, 1	1.5205	1.524	0.0031	0.0031	0.0000	0.0000
C3	C9	, 1	1.5428	1.546	0.0034	0.0034	0.0000	0.0000
C4	C5	, 1	1.3232	1.326	0.0033	0.0033	0.0000	0.0000
C5	C6	, 1	1.5178	1.521	0.0033	0.0033	0.0000	0.0000
C6	C7	, 1	1.5704	1.573	0.0029	0.0029	0.0000	0.0000
C6	C9	, 1	1.5400	1.543	0.0032	0.0032	0.0000	0.0000
C7	C8	, 1	1.4991	1.502	0.0026	0.0026	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

1	10,	-0.615
2	8,	0.603
4	7,	-0.634
13	21,	-0.599
17	21,	-0.602

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O1	0.0371	0.0308	0.0214	-0.0018	0.0032	0.0027	OBSERVED
	0.0364	0.0306	0.0209	-0.0006	0.0047	0.0039	CALCULATED
	0.0007	0.0002	0.0005	-0.0012	-0.0015	-0.0012	DIFFERENCE
O2	0.0206	0.0282	0.0403	0.0046	-0.0018	-0.0051	OBSERVED
	0.0208	0.0283	0.0401	0.0058	-0.0010	-0.0052	CALCULATED
	-0.0003	-0.0001	0.0002	-0.0011	-0.0008	0.0000	DIFFERENCE
O3	0.0196	0.0253	0.0256	-0.0019	0.0063	-0.0023	OBSERVED
	0.0204	0.0223	0.0245	-0.0032	0.0056	-0.0059	CALCULATED
	-0.0008	0.0030	0.0011	0.0013	0.0008	0.0036	DIFFERENCE
C1	0.0224	0.0205	0.0201	-0.0013	0.0023	-0.0035	OBSERVED
	0.0236	0.0219	0.0194	-0.0016	0.0035	-0.0007	CALCULATED
	-0.0012	-0.0014	0.0007	0.0003	-0.0012	-0.0028	DIFFERENCE
C2	0.0169	0.0209	0.0191	-0.0006	0.0009	-0.0007	OBSERVED
	0.0175	0.0202	0.0193	-0.0002	0.0010	0.0001	CALCULATED
	-0.0006	0.0008	-0.0001	-0.0004	-0.0001	-0.0008	DIFFERENCE
C3	0.0215	0.0222	0.0211	0.0060	0.0032	0.0002	OBSERVED
	0.0219	0.0216	0.0232	0.0032	0.0039	-0.0005	CALCULATED
	-0.0004	0.0006	-0.0021	0.0028	-0.0007	0.0007	DIFFERENCE

C4	0.0301	0.0200	0.0266	-0.0026	0.0102	-0.0060	OBSERVED
	0.0281	0.0193	0.0271	-0.0018	0.0068	-0.0051	CALCULATED
	0.0021	0.0007	-0.0005	-0.0007	0.0034	-0.0009	DIFFERENCE
C5	0.0213	0.0288	0.0264	-0.0037	0.0040	-0.0096	OBSERVED
	0.0229	0.0264	0.0242	-0.0042	0.0025	-0.0077	CALCULATED
	-0.0016	0.0025	0.0022	0.0005	0.0016	-0.0019	DIFFERENCE
C6	0.0210	0.0261	0.0188	-0.0001	-0.0013	-0.0002	OBSERVED
	0.0208	0.0264	0.0195	-0.0010	0.0000	-0.0006	CALCULATED
	0.0002	-0.0003	-0.0007	0.0009	-0.0013	0.0004	DIFFERENCE
C7	0.0181	0.0167	0.0218	0.0005	0.0013	0.0003	OBSERVED
	0.0176	0.0185	0.0216	-0.0009	0.0002	0.0004	CALCULATED
	0.0006	-0.0018	0.0002	0.0014	0.0011	0.0000	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C8	0.0210	0.0173	0.0264	-0.0013	0.0004	-0.0045	OBSERVED
	0.0176	0.0204	0.0277	0.0005	0.0010	-0.0040	CALCULATED
	0.0034	-0.0031	-0.0013	-0.0018	-0.0006	-0.0004	DIFFERENCE
C9	0.0206	0.0277	0.0200	-0.0013	0.0059	-0.0005	OBSERVED
	0.0214	0.0285	0.0209	0.0000	0.0046	-0.0013	CALCULATED
	-0.0007	-0.0008	-0.0008	-0.0013	0.0013	0.0008	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.088; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.057
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0016
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0014
(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit = 2.31, defined as square root of [sum of squares of delta(U)/esd(u) divided by (number of independent observations - number of parameters)]

Libration corrections for Compound 10.

ATOM 1 GP	CORRN	ATOM 2 GP	CORRN	DIST	DIST CORRNS	CORRN	CORRN	CORRN
O1		C1 , 1		1.1921	1.195	0.0029	0.0029	0.0000	0.0000
O2		C8 , 1		1.1944	1.197	0.0029	0.0029	0.0000	0.0000
O3		C1 , 1		1.3931	1.396	0.0032	0.0032	0.0000	0.0000
O3		C8 , 1		1.3907	1.394	0.0033	0.0033	0.0000	0.0000
C1		C2 , 1		1.5039	1.507	0.0031	0.0031	0.0000	0.0000
C2		C3 , 1		1.5492	1.553	0.0033	0.0033	0.0000	0.0000
C2		C7 , 1		1.5336	1.537	0.0038	0.0038	0.0000	0.0000
C3		C4 , 1		1.5068	1.511	0.0039	0.0039	0.0000	0.0000
C3		C9 , 1		1.5463	1.550	0.0033	0.0033	0.0000	0.0000
C4		C5 , 1		1.3292	1.333	0.0033	0.0033	0.0000	0.0000
C5		C6 , 1		1.5075	1.511	0.0040	0.0040	0.0000	0.0000
C6		C7 , 1		1.5498	1.553	0.0033	0.0033	0.0000	0.0000
C6		C10 , 1		1.5460	1.549	0.0033	0.0033	0.0000	0.0000
C7		C8 , 1		1.5031	1.506	0.0031	0.0031	0.0000	0.0000
C9		C10 , 1		1.5475	1.551	0.0039	0.0039	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

1	12, -0.505
5	6, -0.513
13	17, -0.574

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O1	0.0186	0.0366	0.0359	-0.0021	0.0049	0.0029	OBSERVED
	0.0194	0.0354	0.0321	-0.0016	0.0065	0.0036	CALCULATED
	-0.0007	0.0012	0.0038	-0.0005	-0.0017	-0.0007	DIFFERENCE
O2	0.0321	0.0216	0.0333	0.0072	0.0012	0.0061	OBSERVED
	0.0317	0.0211	0.0310	0.0077	0.0014	0.0074	CALCULATED
	0.0004	0.0005	0.0023	-0.0005	-0.0002	-0.0013	DIFFERENCE
O3	0.0234	0.0203	0.0247	-0.0020	0.0027	0.0041	OBSERVED
	0.0240	0.0206	0.0211	-0.0029	0.0011	0.0042	CALCULATED
	-0.0006	-0.0003	0.0036	0.0009	0.0016	-0.0001	DIFFERENCE
C1	0.0213	0.0221	0.0167	-0.0007	-0.0002	-0.0006	OBSERVED
	0.0182	0.0231	0.0204	-0.0015	0.0023	0.0009	CALCULATED
	0.0031	-0.0011	-0.0038	0.0008	-0.0025	-0.0016	DIFFERENCE
C2	0.0177	0.0164	0.0163	0.0003	0.0008	-0.0024	OBSERVED
	0.0174	0.0167	0.0170	0.0003	0.0004	-0.0025	CALCULATED
	0.0003	-0.0003	-0.0007	0.0000	0.0004	0.0001	DIFFERENCE
C3	0.0188	0.0163	0.0212	0.0031	0.0001	0.0012	OBSERVED
	0.0194	0.0165	0.0215	0.0024	-0.0014	0.0006	CALCULATED
	-0.0007	-0.0002	-0.0004	0.0008	0.0014	0.0006	DIFFERENCE

C4	0.0245	0.0194	0.0170	-0.0026	-0.0037	0.0024	OBSERVED
	0.0245	0.0203	0.0179	-0.0013	-0.0053	0.0006	CALCULATED
	0.0000	-0.0009	-0.0008	-0.0013	0.0016	0.0018	DIFFERENCE
C5	0.0287	0.0156	0.0148	-0.0005	0.0013	-0.0002	OBSERVED
	0.0289	0.0174	0.0155	-0.0001	0.0004	-0.0018	CALCULATED
	-0.0002	-0.0017	-0.0006	-0.0004	0.0009	0.0016	DIFFERENCE
C6	0.0187	0.0173	0.0193	0.0023	0.0032	0.0013	OBSERVED
	0.0194	0.0174	0.0193	0.0012	0.0033	0.0004	CALCULATED
	-0.0008	0.0000	-0.0001	0.0010	-0.0001	0.0009	DIFFERENCE
C7	0.0162	0.0173	0.0170	-0.0002	-0.0015	-0.0001	OBSERVED
	0.0160	0.0174	0.0170	0.0000	-0.0012	-0.0002	CALCULATED
	0.0002	-0.0001	0.0000	-0.0001	-0.0004	0.0001	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C8	0.0217	0.0209	0.0157	0.0006	-0.0014	0.0023	OBSERVED
	0.0222	0.0180	0.0201	0.0019	-0.0004	0.0034	CALCULATED
	-0.0004	0.0028	-0.0044	-0.0012	-0.0010	-0.0011	DIFFERENCE
C9	0.0277	0.0143	0.0257	0.0004	0.0014	0.0019	OBSERVED
	0.0276	0.0143	0.0265	0.0002	0.0012	0.0018	CALCULATED
	0.0001	0.0000	-0.0008	0.0003	0.0001	0.0001	DIFFERENCE
C10	0.0231	0.0193	0.0254	-0.0033	0.0036	0.0029	OBSERVED
	0.0232	0.0190	0.0256	-0.0032	0.0040	0.0024	CALCULATED
	-0.0001	0.0003	-0.0002	-0.0001	-0.0004	0.0005	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.094; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.073
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0015
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0013

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(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit =  3.19, defined as square root of [sum of squares of delta(U)/esd(u)
 divided by (number of independent observations  -  number of parameters)]
```

Libration correction for Compound 11.

ATOM 1 GP	CORRN	ATOM 2 GP	CORRN	DIST	DIST	CORRNS	CORRN	CORRN	CORRN
N1		C1 , 1		1.3824	1.385	0.0030	0.0030	0.0000	0.0000
N1		C8 , 1		1.3909	1.395	0.0037	0.0037	0.0000	0.0000
N1		C10 , 1		1.4553	1.458	0.0030	0.0030	0.0000	0.0000
O1		C1 , 1		1.2154	1.219	0.0033	0.0033	0.0000	0.0000
O2		C8 , 1		1.2099	1.213	0.0028	0.0028	0.0000	0.0000
C1		C2 , 1		1.5067	1.510	0.0034	0.0034	0.0000	0.0000
C2		C3 , 1		1.5706	1.574	0.0035	0.0035	0.0000	0.0000
C2		C7 , 1		1.5370	1.541	0.0039	0.0039	0.0000	0.0000
C3		C4 , 1		1.5147	1.518	0.0035	0.0035	0.0000	0.0000
C3		C9 , 1		1.5385	1.543	0.0040	0.0040	0.0000	0.0000
C4		C5 , 1		1.3267	1.330	0.0034	0.0034	0.0000	0.0000
C5		C6 , 1		1.5168	1.521	0.0039	0.0039	0.0000	0.0000
C6		C7 , 1		1.5700	1.574	0.0037	0.0037	0.0000	0.0000
C6		C9 , 1		1.5395	1.543	0.0031	0.0031	0.0000	0.0000
C7		C8 , 1		1.5019	1.505	0.0029	0.0029	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

4 7, -0.505
17 21, -0.531

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
N1	0.0200	0.0205	0.0198	0.0007	-0.0010	0.0002	OBSERVED
	0.0194	0.0213	0.0190	0.0009	0.0002	-0.0011	CALCULATED
	0.0006	-0.0008	0.0008	-0.0002	-0.0011	0.0013	DIFFERENCE
O1	0.0234	0.0251	0.0409	-0.0043	0.0018	-0.0004	OBSERVED
	0.0233	0.0254	0.0385	-0.0048	0.0017	-0.0001	CALCULATED
	0.0001	-0.0003	0.0025	0.0005	0.0001	-0.0003	DIFFERENCE
O2	0.0240	0.0326	0.0258	-0.0065	-0.0053	-0.0010	OBSERVED
	0.0247	0.0315	0.0243	-0.0065	-0.0060	-0.0014	CALCULATED
	-0.0007	0.0011	0.0014	0.0000	0.0007	0.0004	DIFFERENCE
C1	0.0182	0.0236	0.0203	0.0005	0.0030	-0.0033	OBSERVED
	0.0181	0.0219	0.0228	-0.0004	0.0018	-0.0019	CALCULATED
	0.0000	0.0018	-0.0025	0.0009	0.0012	-0.0014	DIFFERENCE
C2	0.0182	0.0251	0.0183	0.0025	0.0011	-0.0023	OBSERVED
	0.0182	0.0247	0.0187	0.0027	0.0011	-0.0024	CALCULATED
	0.0001	0.0004	-0.0004	-0.0001	0.0000	0.0001	DIFFERENCE
C3	0.0194	0.0382	0.0196	0.0020	-0.0037	-0.0041	OBSERVED
	0.0208	0.0365	0.0204	0.0032	-0.0035	-0.0038	CALCULATED
	-0.0014	0.0016	-0.0007	-0.0012	-0.0002	-0.0002	DIFFERENCE

C4	0.0254	0.0390	0.0182	0.0026	-0.0013	-0.0083	OBSERVED
	0.0243	0.0409	0.0179	0.0027	-0.0020	-0.0093	CALCULATED
	0.0011	-0.0019	0.0002	-0.0001	0.0008	0.0010	DIFFERENCE
C5	0.0236	0.0413	0.0161	0.0017	0.0009	-0.0013	OBSERVED
	0.0238	0.0422	0.0159	0.0013	0.0024	-0.0020	CALCULATED
	-0.0001	-0.0009	0.0001	0.0004	-0.0015	0.0006	DIFFERENCE
C6	0.0281	0.0297	0.0199	-0.0021	-0.0005	0.0053	OBSERVED
	0.0279	0.0318	0.0197	-0.0012	0.0003	0.0046	CALCULATED
	0.0002	-0.0021	0.0002	-0.0010	-0.0008	0.0007	DIFFERENCE
C7	0.0247	0.0207	0.0176	-0.0003	-0.0006	-0.0018	OBSERVED
	0.0242	0.0209	0.0173	0.0003	-0.0003	-0.0013	CALCULATED
	0.0005	-0.0003	0.0003	-0.0006	-0.0004	-0.0005	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C8	0.0227	0.0233	0.0146	-0.0012	0.0006	-0.0026	OBSERVED
	0.0210	0.0228	0.0169	-0.0020	-0.0017	-0.0021	CALCULATED
	0.0017	0.0005	-0.0024	0.0008	0.0023	-0.0005	DIFFERENCE
C9	0.0306	0.0403	0.0214	0.0066	-0.0028	0.0053	OBSERVED
	0.0312	0.0388	0.0216	0.0060	-0.0029	0.0053	CALCULATED
	-0.0006	0.0015	-0.0002	0.0006	0.0001	0.0000	DIFFERENCE
C10	0.0248	0.0254	0.0290	0.0043	-0.0038	0.0020	OBSERVED
	0.0262	0.0265	0.0294	0.0046	-0.0020	0.0033	CALCULATED
	-0.0013	-0.0011	-0.0003	-0.0003	-0.0018	-0.0013	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.063; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.046
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0011
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0010

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(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit =  2.15, defined as square root of [sum of squares of delta(U)/esd(u)
 divided by (number of independent observations  -  number of parameters)]
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Libration corrections for Compound 13.

ATOM 1	ATOM 2	DIST	DIST	CORRNS	CORRN	CORRN	CORRN
GP	CORRN	GP	CORRN	GP	CORRN		
O1	C1 , 1	1.2176	1.222	0.0046	0.0046	0.0000	0.0000
O2	C8 , 1	1.2169	1.222	0.0047	0.0047	0.0000	0.0000
C1	C2 , 1	1.5062	1.510	0.0043	0.0043	0.0000	0.0000
C1	C10 , 1	1.4760	1.481	0.0049	0.0049	0.0000	0.0000
C2	C3 , 1	1.5664	1.571	0.0050	0.0050	0.0000	0.0000
C2	C7 , 1	1.5364	1.542	0.0058	0.0058	0.0000	0.0000
C3	C4 , 1	1.4989	1.504	0.0050	0.0050	0.0000	0.0000
C3	C11 , 1	1.5365	1.541	0.0044	0.0044	0.0000	0.0000
C4	C5 , 1	1.3230	1.328	0.0050	0.0050	0.0000	0.0000
C5	C6 , 1	1.4953	1.500	0.0050	0.0050	0.0000	0.0000
C6	C7 , 1	1.5654	1.570	0.0047	0.0047	0.0000	0.0000
C6	C12 , 1	1.5491	1.554	0.0047	0.0047	0.0000	0.0000
C7	C8 , 1	1.5124	1.517	0.0048	0.0048	0.0000	0.0000
C8	C9 , 1	1.4638	1.468	0.0043	0.0043	0.0000	0.0000
C9	C10 , 1	1.3270	1.332	0.0050	0.0050	0.0000	0.0000
C11	C12 , 1	1.5300	1.536	0.0058	0.0058	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

13 17, -0.513 21, -0.525

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O1	0.0284	0.0368	0.0490	-0.0080	-0.0021	0.0124	OBSERVED
	0.0301	0.0394	0.0449	-0.0090	0.0011	0.0117	CALCULATED
	-0.0017	-0.0026	0.0041	0.0010	-0.0032	0.0007	DIFFERENCE
O2	0.0358	0.0315	0.0650	-0.0108	0.0021	-0.0132	OBSERVED
	0.0365	0.0313	0.0608	-0.0130	0.0029	-0.0144	CALCULATED
	-0.0007	0.0002	0.0042	0.0022	-0.0008	0.0012	DIFFERENCE
C1	0.0249	0.0257	0.0259	-0.0035	-0.0055	0.0069	OBSERVED
	0.0248	0.0248	0.0290	-0.0018	-0.0016	0.0064	CALCULATED
	0.0001	0.0009	-0.0031	-0.0018	-0.0039	0.0005	DIFFERENCE
C2	0.0303	0.0164	0.0235	-0.0016	-0.0051	0.0027	OBSERVED
	0.0276	0.0166	0.0255	-0.0004	-0.0063	0.0014	CALCULATED
	0.0027	-0.0002	-0.0020	-0.0012	0.0012	0.0014	DIFFERENCE
C3	0.0382	0.0253	0.0318	-0.0091	-0.0055	-0.0042	OBSERVED
	0.0383	0.0221	0.0314	-0.0027	-0.0111	-0.0038	CALCULATED
	-0.0001	0.0032	0.0004	-0.0063	0.0056	-0.0004	DIFFERENCE
C4	0.0351	0.0369	0.0239	0.0053	-0.0057	-0.0028	OBSERVED
	0.0392	0.0338	0.0251	0.0022	-0.0094	-0.0010	CALCULATED
	-0.0041	0.0030	-0.0012	0.0030	0.0037	-0.0018	DIFFERENCE

C5	0.0439	0.0275	0.0259	0.0067	0.0035	0.0028	OBSERVED
	0.0401	0.0328	0.0254	0.0045	0.0025	0.0026	CALCULATED
	0.0037	-0.0053	0.0005	0.0022	0.0010	0.0002	DIFFERENCE
C6	0.0286	0.0298	0.0338	-0.0012	0.0057	-0.0077	OBSERVED
	0.0296	0.0299	0.0326	0.0028	0.0040	-0.0041	CALCULATED
	-0.0010	-0.0001	0.0012	-0.0039	0.0017	-0.0037	DIFFERENCE
C7	0.0231	0.0205	0.0278	0.0005	-0.0045	-0.0035	OBSERVED
	0.0229	0.0206	0.0284	0.0012	-0.0037	-0.0044	CALCULATED
	0.0001	-0.0001	-0.0006	-0.0007	-0.0008	0.0008	DIFFERENCE
C8	0.0286	0.0206	0.0298	-0.0031	0.0010	-0.0043	OBSERVED
	0.0283	0.0204	0.0374	-0.0037	0.0008	-0.0067	CALCULATED
	0.0004	0.0002	-0.0076	0.0006	0.0002	0.0024	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C9	0.0375	0.0195	0.0390	0.0035	0.0038	-0.0029	OBSERVED
	0.0350	0.0184	0.0361	0.0029	0.0041	-0.0024	CALCULATED
	0.0025	0.0011	0.0029	0.0005	-0.0003	-0.0005	DIFFERENCE
C10	0.0284	0.0261	0.0360	0.0069	0.0051	0.0016	OBSERVED
	0.0280	0.0258	0.0311	0.0060	0.0034	0.0039	CALCULATED
	0.0004	0.0003	0.0049	0.0009	0.0017	-0.0023	DIFFERENCE
C11	0.0623	0.0230	0.0366	0.0083	-0.0087	-0.0080	OBSERVED
	0.0545	0.0249	0.0385	0.0073	-0.0098	-0.0119	CALCULATED
	0.0078	-0.0019	-0.0019	0.0010	0.0011	0.0039	DIFFERENCE
C12	0.0385	0.0417	0.0396	0.0162	-0.0061	-0.0159	OBSERVED
	0.0423	0.0370	0.0378	0.0132	0.0000	-0.0116	CALCULATED
	-0.0038	0.0047	0.0017	0.0030	-0.0061	-0.0043	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.112; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.081
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0029
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))

NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0025
(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit = 3.41, defined as square root of [sum of squares of delta(U)/esd(u) divided by (number of independent observations - number of parameters)]

Libration corrections for Compound 13.Q.

ATOM 1 GP	CORRN	ATOM 2 GP	CORRN	DIST	DIST CORRNS	CORRN	CORRN	CORRN
O1		C1 , 1		1.2219	1.226	0.0036	0.0036	0.0000	0.0000
O2		C8 , 1		1.2225	1.226	0.0035	0.0035	0.0000	0.0000
C1		C2 , 1		1.5081	1.512	0.0039	0.0039	0.0000	0.0000
C1		C10 , 1		1.4752	1.479	0.0034	0.0034	0.0000	0.0000
C2		C3 , 1		1.5632	1.567	0.0040	0.0040	0.0000	0.0000
C2		C7 , 1		1.5522	1.557	0.0046	0.0046	0.0000	0.0000
C3		C4 , 1		1.5040	1.508	0.0041	0.0041	0.0000	0.0000
C3		C11 , 1		1.5397	1.544	0.0039	0.0039	0.0000	0.0000
C4		C5 , 1		1.3281	1.332	0.0039	0.0039	0.0000	0.0000
C12		C11 , 1		1.5428	1.547	0.0046	0.0046	0.0000	0.0000
C12		C6 , 1		1.5442	1.548	0.0035	0.0035	0.0000	0.0000
C5		C6 , 1		1.5030	1.507	0.0045	0.0045	0.0000	0.0000
C6		C7 , 1		1.5581	1.562	0.0039	0.0039	0.0000	0.0000
C7		C8 , 1		1.5173	1.521	0.0034	0.0034	0.0000	0.0000
C8		C9 , 1		1.4678	1.472	0.0039	0.0039	0.0000	0.0000
C9		C10 , 1		1.3308	1.335	0.0039	0.0039	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

1 10, -0.552
2 8, 0.535
13 21, -0.644

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O1	0.0346	0.0491	0.0283	0.0058	-0.0110	-0.0055	OBSERVED
	0.0354	0.0448	0.0284	0.0051	-0.0118	-0.0071	CALCULATED
	-0.0008	0.0042	-0.0001	0.0007	0.0008	0.0016	DIFFERENCE
O2	0.0209	0.0384	0.0399	0.0029	-0.0030	0.0018	OBSERVED
	0.0215	0.0372	0.0414	0.0051	-0.0028	0.0017	CALCULATED
	-0.0005	0.0012	-0.0015	-0.0021	-0.0003	0.0000	DIFFERENCE
C1	0.0265	0.0213	0.0250	-0.0006	-0.0037	-0.0034	OBSERVED
	0.0270	0.0269	0.0225	0.0010	-0.0040	-0.0041	CALCULATED
	-0.0005	-0.0056	0.0025	-0.0017	0.0002	0.0007	DIFFERENCE
C2	0.0182	0.0223	0.0235	-0.0015	-0.0008	-0.0030	OBSERVED
	0.0187	0.0225	0.0228	-0.0012	-0.0013	-0.0032	CALCULATED
	-0.0005	-0.0002	0.0007	-0.0003	0.0005	0.0001	DIFFERENCE
C3	0.0231	0.0257	0.0290	0.0050	-0.0032	-0.0061	OBSERVED
	0.0240	0.0262	0.0294	0.0044	-0.0011	-0.0059	CALCULATED
	-0.0009	-0.0005	-0.0003	0.0006	-0.0020	-0.0002	DIFFERENCE
C4	0.0359	0.0211	0.0309	0.0004	0.0006	-0.0050	OBSERVED
	0.0337	0.0194	0.0347	0.0009	0.0018	-0.0049	CALCULATED
	0.0023	0.0017	-0.0038	-0.0005	-0.0011	-0.0001	DIFFERENCE

C12	0.0325	0.0437	0.0229	-0.0032	0.0027	-0.0093	OBSERVED
	0.0310	0.0448	0.0234	-0.0033	0.0020	-0.0093	CALCULATED
	0.0015	-0.0011	-0.0005	0.0001	0.0006	0.0000	DIFFERENCE
C5	0.0270	0.0270	0.0325	-0.0054	0.0023	-0.0102	OBSERVED
	0.0282	0.0249	0.0334	-0.0062	0.0009	-0.0089	CALCULATED
	-0.0013	0.0021	-0.0009	0.0008	0.0013	-0.0013	DIFFERENCE
C11	0.0254	0.0383	0.0340	0.0006	0.0046	-0.0138	OBSERVED
	0.0262	0.0393	0.0323	0.0019	0.0044	-0.0121	CALCULATED
	-0.0008	-0.0011	0.0017	-0.0013	0.0002	-0.0017	DIFFERENCE
C6	0.0224	0.0326	0.0233	-0.0013	-0.0039	-0.0057	OBSERVED
	0.0233	0.0329	0.0233	-0.0037	-0.0026	-0.0052	CALCULATED
	-0.0009	-0.0003	0.0000	0.0024	-0.0012	-0.0005	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C7	0.0204	0.0227	0.0214	-0.0014	-0.0004	0.0008	OBSERVED
	0.0194	0.0222	0.0219	-0.0018	-0.0006	0.0007	CALCULATED
	0.0010	0.0006	-0.0005	0.0004	0.0002	0.0001	DIFFERENCE
C8	0.0206	0.0192	0.0306	-0.0006	-0.0001	0.0004	OBSERVED
	0.0198	0.0230	0.0292	0.0007	0.0008	0.0005	CALCULATED
	0.0009	-0.0038	0.0014	-0.0014	-0.0009	-0.0001	DIFFERENCE
C9	0.0268	0.0261	0.0312	0.0032	0.0072	-0.0026	OBSERVED
	0.0262	0.0232	0.0292	0.0004	0.0065	-0.0028	CALCULATED
	0.0006	0.0029	0.0021	0.0028	0.0008	0.0003	DIFFERENCE
C10	0.0349	0.0265	0.0221	0.0008	0.0036	-0.0037	OBSERVED
	0.0332	0.0263	0.0224	0.0003	0.0028	-0.0038	CALCULATED
	0.0017	0.0002	-0.0003	0.0005	0.0008	0.0001	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.078; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.064
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0016
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))

NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0014
(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit = 2.67, defined as square root of [sum of squares of delta(U)/esd(u) divided by (number of independent observations - number of parameters)]

Libration corrections for Compound 14.

ATOM 1 GP	CORRN	ATOM 2 GP	CORRN	DIST	DIST	CORRNS	CORRN	CORRN	CORRN
SI		O3 , 1		1.6566	1.659	0.0027	0.0027	0.0000	0.0000
SI		C13 , 1		1.8526	1.857	0.0041	0.0041	0.0000	0.0000
SI		C14 , 1		1.8493	1.854	0.0049	0.0049	0.0000	0.0000
SI		C15 , 1		1.8438	1.848	0.0043	0.0043	0.0000	0.0000
O1		C1 , 1		1.2211	1.224	0.0031	0.0031	0.0000	0.0000
O2		C8 , 1		1.2211	1.224	0.0027	0.0027	0.0000	0.0000
O3		C3 , 1		1.4099	1.413	0.0034	0.0034	0.0000	0.0000
C1		C2 , 1		1.5086	1.512	0.0037	0.0037	0.0000	0.0000
C1		C10 , 1		1.4717	1.474	0.0019	0.0019	0.0000	0.0000
C2		C3 , 1		1.5812	1.585	0.0042	0.0042	0.0000	0.0000
C2		C7 , 1		1.5496	1.553	0.0036	0.0036	0.0000	0.0000
C3		C4 , 1		1.4994	1.502	0.0028	0.0028	0.0000	0.0000
C3		C11 , 1		1.5445	1.548	0.0032	0.0032	0.0000	0.0000
C4		C5 , 1		1.3244	1.328	0.0032	0.0032	0.0000	0.0000
C5		C6 , 1		1.5031	1.506	0.0034	0.0034	0.0000	0.0000
C6		C7 , 1		1.5586	1.563	0.0046	0.0046	0.0000	0.0000
C6		C12 , 1		1.5415	1.544	0.0021	0.0021	0.0000	0.0000
C7		C8 , 1		1.5107	1.513	0.0021	0.0021	0.0000	0.0000
C8		C9 , 1		1.4724	1.476	0.0034	0.0034	0.0000	0.0000
C9		C10 , 1		1.3277	1.331	0.0030	0.0030	0.0000	0.0000
C11		C12 , 1		1.5381	1.542	0.0036	0.0036	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then,
in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then
those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4,
ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I
AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

4	12, -0.690			
5	11, 0.716			
6	10, -0.682			
13	17, -0.770	21, -0.749		

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
SI	0.0218	0.0432	0.0210	-0.0059	0.0019	-0.0088	OBSERVED
	0.0223	0.0462	0.0229	-0.0052	0.0006	-0.0091	CALCULATED
	-0.0005	-0.0031	-0.0019	-0.0007	0.0013	0.0003	DIFFERENCE
O1	0.0311	0.0359	0.0336	0.0040	-0.0063	0.0107	OBSERVED
	0.0312	0.0312	0.0302	0.0054	-0.0027	0.0117	CALCULATED
	-0.0001	0.0047	0.0035	-0.0014	-0.0036	-0.0010	DIFFERENCE
O2	0.0228	0.0702	0.0308	-0.0047	-0.0041	-0.0015	OBSERVED
	0.0233	0.0620	0.0296	-0.0072	-0.0047	-0.0068	CALCULATED
	-0.0005	0.0082	0.0012	0.0025	0.0006	0.0053	DIFFERENCE
O3	0.0226	0.0309	0.0184	-0.0038	-0.0017	-0.0034	OBSERVED
	0.0238	0.0293	0.0165	-0.0056	0.0011	-0.0064	CALCULATED
	-0.0012	0.0015	0.0019	0.0019	-0.0028	0.0030	DIFFERENCE
C1	0.0263	0.0206	0.0223	-0.0046	-0.0059	0.0002	OBSERVED
	0.0255	0.0229	0.0211	-0.0003	-0.0024	0.0055	CALCULATED
	0.0008	-0.0023	0.0012	-0.0042	-0.0034	-0.0053	DIFFERENCE
C2	0.0206	0.0212	0.0161	0.0016	-0.0003	-0.0026	OBSERVED
	0.0223	0.0180	0.0157	-0.0006	-0.0025	-0.0009	CALCULATED
	-0.0017	0.0032	0.0004	0.0022	0.0022	-0.0017	DIFFERENCE

C3	0.0226	0.0223	0.0170	-0.0014	-0.0018	0.0005	OBSERVED
	0.0250	0.0181	0.0145	-0.0013	0.0013	-0.0021	CALCULATED
	-0.0025	0.0042	0.0025	0.0000	-0.0031	0.0026	DIFFERENCE
C4	0.0350	0.0200	0.0189	0.0001	0.0023	-0.0011	OBSERVED
	0.0311	0.0197	0.0209	0.0008	0.0054	-0.0028	CALCULATED
	0.0039	0.0003	-0.0020	-0.0007	-0.0031	0.0018	DIFFERENCE
C5	0.0352	0.0253	0.0219	0.0089	0.0032	0.0030	OBSERVED
	0.0337	0.0261	0.0252	0.0096	0.0042	0.0034	CALCULATED
	0.0016	-0.0008	-0.0033	-0.0007	-0.0010	-0.0004	DIFFERENCE
C6	0.0254	0.0350	0.0192	0.0079	-0.0038	0.0032	OBSERVED
	0.0298	0.0368	0.0185	0.0090	-0.0025	0.0054	CALCULATED
	-0.0044	-0.0018	0.0007	-0.0010	-0.0013	-0.0021	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C7	0.0229	0.0289	0.0152	0.0000	-0.0030	-0.0029	OBSERVED
	0.0233	0.0297	0.0168	-0.0008	-0.0041	-0.0022	CALCULATED
	-0.0003	-0.0008	-0.0016	0.0009	0.0011	-0.0007	DIFFERENCE
C8	0.0231	0.0318	0.0236	-0.0006	-0.0017	-0.0025	OBSERVED
	0.0226	0.0381	0.0227	-0.0047	-0.0031	-0.0025	CALCULATED
	0.0005	-0.0063	0.0010	0.0041	0.0015	0.0000	DIFFERENCE
C9	0.0284	0.0336	0.0221	-0.0041	0.0043	0.0016	OBSERVED
	0.0247	0.0347	0.0229	-0.0067	0.0000	0.0027	CALCULATED
	0.0037	-0.0010	-0.0008	0.0027	0.0043	-0.0011	DIFFERENCE
C10	0.0342	0.0285	0.0181	-0.0056	-0.0020	0.0034	OBSERVED
	0.0272	0.0313	0.0210	-0.0042	-0.0008	0.0078	CALCULATED
	0.0070	-0.0028	-0.0030	-0.0014	-0.0012	-0.0044	DIFFERENCE
C11	0.0318	0.0288	0.0208	0.0002	0.0031	0.0037	OBSERVED
	0.0339	0.0219	0.0173	0.0003	0.0046	0.0016	CALCULATED
	-0.0021	0.0069	0.0035	0.0000	-0.0015	0.0021	DIFFERENCE
C12	0.0358	0.0326	0.0169	0.0045	-0.0002	0.0048	OBSERVED
	0.0379	0.0371	0.0177	0.0080	0.0006	0.0083	CALCULATED
	-0.0021	-0.0046	-0.0008	-0.0035	-0.0008	-0.0035	DIFFERENCE

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 C13       0.0321   0.0367   0.0360   0.0079  -0.0034  -0.0097    OBSERVED
           0.0247   0.0389   0.0299   0.0036   0.0021  -0.0084    CALCULATED
           0.0074  -0.0021   0.0061   0.0043  -0.0054  -0.0013    DIFFERENCE

 C14       0.0275   0.1404   0.0290   0.0222  -0.0032  -0.0041    OBSERVED
           0.0231   0.0874   0.0299   0.0017  -0.0072  -0.0031    CALCULATED
           0.0044   0.0530  -0.0009   0.0205   0.0041  -0.0009    DIFFERENCE

 C15       0.0556   0.0620   0.0812  -0.0316   0.0366  -0.0303    OBSERVED
           0.0337   0.0584   0.0346  -0.0221   0.0121  -0.0207    CALCULATED
           0.0218   0.0035   0.0466  -0.0095   0.0245  -0.0096    DIFFERENCE

           Cartesian Crystal Frame

  WEIGHTED R FOR ALL U'S =  0.183;  FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.150
KEYR
 [R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

 A SORT OF ESD OF WEIGHTED DELTA(U)    0.0036
 SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
  NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES);   NINPAR IS THE NUMBER OF
INDEPENDENT PARAMETERS DETERMINED

 R.M.S. OF THE WEIGHTED DELTA(U) =    0.0033
 (SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

 Goodness of fit =  6.47, defined as square root of [sum of squares of delta(U)/esd(u)
  divided by (number of independent observations  -  number of parameters)]
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Libration Corrections for Compound 15

ATOM 1 GP	CORRN	ATOM 2 GP	CORRN	DIST	DIST	CORRNS	CORRN	CORRN	CORRN
O3		C13 , 1		1.4277	1.430	0.0021	0.0021	0.0000	0.0000
O3		C3 , 1		1.4203	1.423	0.0025	0.0025	0.0000	0.0000
O1		C1 , 1		1.2180	1.220	0.0020	0.0020	0.0000	0.0000
O2		C8 , 1		1.2223	1.224	0.0020	0.0020	0.0000	0.0000
C4		C5 , 1		1.3286	1.331	0.0023	0.0023	0.0000	0.0000
C4		C3 , 1		1.5085	1.511	0.0024	0.0024	0.0000	0.0000
C8		C7 , 1		1.5187	1.521	0.0019	0.0019	0.0000	0.0000
C8		C9 , 1		1.4720	1.475	0.0026	0.0026	0.0000	0.0000
C7		C2 , 1		1.5514	1.554	0.0025	0.0025	0.0000	0.0000
C7		C6 , 1		1.5537	1.556	0.0022	0.0022	0.0000	0.0000
C10		C1 , 1		1.4748	1.477	0.0019	0.0019	0.0000	0.0000
C10		C9 , 1		1.3313	1.333	0.0022	0.0022	0.0000	0.0000
C12		C11 , 1		1.5455	1.548	0.0026	0.0026	0.0000	0.0000
C12		C6 , 1		1.5445	1.546	0.0019	0.0019	0.0000	0.0000
C2		C1 , 1		1.5098	1.512	0.0024	0.0024	0.0000	0.0000
C2		C3 , 1		1.5848	1.587	0.0019	0.0019	0.0000	0.0000
C11		C3 , 1		1.5433	1.546	0.0024	0.0024	0.0000	0.0000
C5		C6 , 1		1.5066	1.509	0.0026	0.0026	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then, in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then those of PHIwith overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4, ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

1	11,	0.572	12,	-0.697
4	5,	0.515	12,	-0.693
5	11,	0.606		
6	19,	-0.509		
11	12,	-0.539		

13 17, -0.664

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O3	0.0234	0.0156	0.0168	0.0005	-0.0004	-0.0010	OBSERVED
	0.0228	0.0160	0.0175	-0.0001	-0.0005	-0.0006	CALCULATED
	0.0005	-0.0004	-0.0007	0.0006	0.0001	-0.0004	DIFFERENCE
O1	0.0195	0.0269	0.0298	0.0009	0.0042	-0.0049	OBSERVED
	0.0195	0.0268	0.0295	0.0015	0.0045	-0.0048	CALCULATED
	0.0000	0.0000	0.0004	-0.0006	-0.0003	-0.0001	DIFFERENCE
O2	0.0319	0.0283	0.0343	-0.0007	0.0002	-0.0136	OBSERVED
	0.0319	0.0237	0.0324	-0.0038	0.0015	-0.0112	CALCULATED
	0.0000	0.0046	0.0018	0.0031	-0.0014	-0.0024	DIFFERENCE
C4	0.0155	0.0223	0.0168	-0.0033	0.0002	0.0026	OBSERVED
	0.0203	0.0203	0.0123	-0.0030	-0.0001	0.0007	CALCULATED
	-0.0048	0.0020	0.0045	-0.0004	0.0003	0.0020	DIFFERENCE
C8	0.0227	0.0187	0.0228	-0.0044	0.0032	-0.0023	OBSERVED
	0.0243	0.0194	0.0240	-0.0030	0.0004	-0.0045	CALCULATED
	-0.0016	-0.0007	-0.0011	-0.0014	0.0029	0.0022	DIFFERENCE
C7	0.0200	0.0151	0.0207	0.0002	0.0016	0.0009	OBSERVED
	0.0218	0.0154	0.0214	0.0003	0.0008	-0.0001	CALCULATED
	-0.0018	-0.0003	-0.0007	0.0000	0.0008	0.0009	DIFFERENCE

C10	0.0185	0.0235	0.0251	-0.0016	-0.0019	0.0031	OBSERVED
	0.0189	0.0240	0.0263	-0.0011	-0.0033	-0.0008	CALCULATED
	-0.0004	-0.0005	-0.0012	-0.0004	0.0013	0.0039	DIFFERENCE
C12	0.0188	0.0243	0.0226	0.0037	-0.0012	0.0022	OBSERVED
	0.0213	0.0229	0.0245	0.0047	-0.0024	0.0015	CALCULATED
	-0.0025	0.0014	-0.0019	-0.0009	0.0011	0.0007	DIFFERENCE
C2	0.0168	0.0165	0.0155	-0.0015	0.0011	0.0007	OBSERVED
	0.0187	0.0161	0.0158	-0.0002	0.0015	0.0013	CALCULATED
	-0.0019	0.0004	-0.0002	-0.0013	-0.0003	-0.0006	DIFFERENCE
C1	0.0163	0.0160	0.0233	-0.0028	0.0024	0.0015	OBSERVED
	0.0178	0.0201	0.0222	0.0002	0.0013	-0.0009	CALCULATED
	-0.0015	-0.0041	0.0011	-0.0030	0.0011	0.0024	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C13	0.0253	0.0228	0.0186	0.0002	0.0013	-0.0043	OBSERVED
	0.0275	0.0222	0.0199	-0.0009	0.0026	-0.0057	CALCULATED
	-0.0021	0.0005	-0.0014	0.0011	-0.0013	0.0014	DIFFERENCE
C11	0.0173	0.0246	0.0177	0.0005	-0.0015	0.0005	OBSERVED
	0.0195	0.0216	0.0142	0.0002	-0.0013	0.0019	CALCULATED
	-0.0022	0.0030	0.0035	0.0004	-0.0002	-0.0014	DIFFERENCE
C5	0.0168	0.0265	0.0165	-0.0018	0.0013	-0.0006	OBSERVED
	0.0205	0.0252	0.0161	-0.0019	0.0025	-0.0040	CALCULATED
	-0.0037	0.0013	0.0004	0.0001	-0.0012	0.0034	DIFFERENCE
C9	0.0231	0.0259	0.0224	-0.0050	-0.0038	-0.0011	OBSERVED
	0.0225	0.0247	0.0239	-0.0047	-0.0031	-0.0028	CALCULATED
	0.0006	0.0013	-0.0015	-0.0003	-0.0007	0.0017	DIFFERENCE
C3	0.0152	0.0153	0.0172	-0.0006	0.0001	0.0001	OBSERVED
	0.0183	0.0161	0.0126	-0.0002	0.0001	0.0010	CALCULATED
	-0.0031	-0.0008	0.0046	-0.0003	0.0000	-0.0008	DIFFERENCE
C6	0.0179	0.0193	0.0225	0.0023	0.0022	-0.0013	OBSERVED
	0.0212	0.0200	0.0238	0.0032	0.0010	-0.0032	CALCULATED
	-0.0032	-0.0007	-0.0014	-0.0009	0.0011	0.0019	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.067; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.051
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUMSQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0011
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0009
(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit = 0.37, defined as square root of [sum of squares of delta(U)/esd(u) divided by (number of independent observations - number of parameters)]

Libration Corrections for Compound 11s

UNIQUE ATOM 1 GP CORRN	ATOM 2 GP CORRN		UNCORR DIST GP CORRN	CORRD DIST	SUM OF CORRNS	BODY CORRN	ANHARM CORRN	B&L CORRN
O2	C8	, 1	1.2150	1.219	0.0039	0.0039	0.0000	0.0000
O1	C1	, 1	1.2141	1.218	0.0035	0.0035	0.0000	0.0000
N1	C8	, 1	1.3865	1.390	0.0038	0.0038	0.0000	0.0000
N1	C1	, 1	1.3884	1.393	0.0044	0.0044	0.0000	0.0000
N1	C10	, 1	1.4546	1.458	0.0039	0.0039	0.0000	0.0000
C8	C7	, 1	1.5061	1.510	0.0042	0.0042	0.0000	0.0000
C1	C2	, 1	1.5063	1.510	0.0039	0.0039	0.0000	0.0000
C7	C6	, 1	1.5465	1.551	0.0043	0.0043	0.0000	0.0000
C7	C2	, 1	1.5436	1.548	0.0048	0.0048	0.0000	0.0000
C4	C3	, 1	1.5376	1.543	0.0050	0.0050	0.0000	0.0000
C4	C5	, 1	1.5563	1.561	0.0048	0.0048	0.0000	0.0000
C3	C2	, 1	1.5485	1.553	0.0041	0.0041	0.0000	0.0000
C3	C9	, 1	1.5427	1.547	0.0041	0.0041	0.0000	0.0000
C6	C5	, 1	1.5371	1.542	0.0044	0.0044	0.0000	0.0000
C6	C9	, 1	1.5335	1.538	0.0048	0.0048	0.0000	0.0000

CORRELATION MATRIX

THE PARAMETER NUMBERS ARE:

1	L11	7	T11	13	S11 (IF PRESENT) OR PHI1 SQUARED		
2	L12	8	T12	14	S12 (OR SEE BELOW)		
3	L13	9	T13	15	S13	19	S31
4	L22	10	T22	16	S21	20	S32
5	L23	11	T23	17	S22	21	S33
6	L33	12	T33	18	S23		

IF S IS ABSENT, PARAMETER NUMBERS FOR RIGID GROUPS START AT 13; WITH S, THEY START AT 22.

If ICORL.GE.0, seven parameters for each ARG are given: FIRST, <PHI squared> + 2<PHI Lambda-parallel>, then, in order, correlations of PHI with LAMBDA, the overall rotation, about each of the three CCS axes, and then those of PHI with overall TRANSL along each of the three CCS axes.

ONLY CORRELATION COEFFICIENTS = 0.500 OR LARGER ARE PRINTED; IF IEXU IS NON-ZERO, or NS = -2 OR -4, ONLY VALUES = 0.900 OR LARGER ARE PRINTED. EACH LINE BEGINS AT THE LEFT WITH THE VALUE OF I AND EACH VALUE ON A LINE IS PRECEDED BY THE CORRESPONDING VALUE OF J

1	10,	-0.531
4	7,	-0.544
13	21,	-0.548
17	21,	-0.528

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
O2	0.0225	0.0313	0.0366	0.0062	-0.0017	-0.0049	OBSERVED
	0.0218	0.0311	0.0351	0.0069	-0.0014	-0.0043	CALCULATED
	0.0007	0.0002	0.0015	-0.0008	-0.0003	-0.0006	DIFFERENCE
O1	0.0265	0.0348	0.0361	0.0099	-0.0081	0.0042	OBSERVED
	0.0264	0.0337	0.0351	0.0101	-0.0085	0.0048	CALCULATED
	0.0000	0.0012	0.0011	-0.0002	0.0004	-0.0005	DIFFERENCE
N1	0.0170	0.0234	0.0214	0.0001	-0.0048	0.0003	OBSERVED
	0.0175	0.0235	0.0209	0.0000	-0.0036	0.0009	CALCULATED
	-0.0004	-0.0001	0.0005	0.0002	-0.0012	-0.0006	DIFFERENCE
C8	0.0152	0.0261	0.0213	0.0002	-0.0001	0.0028	OBSERVED
	0.0160	0.0244	0.0231	0.0007	-0.0015	0.0004	CALCULATED
	-0.0008	0.0016	-0.0018	-0.0005	0.0015	0.0024	DIFFERENCE
C1	0.0222	0.0235	0.0212	0.0022	-0.0024	0.0048	OBSERVED
	0.0209	0.0226	0.0246	0.0027	-0.0043	0.0042	CALCULATED
	0.0012	0.0009	-0.0035	-0.0006	0.0018	0.0006	DIFFERENCE
C7	0.0172	0.0261	0.0235	-0.0043	-0.0013	0.0015	OBSERVED
	0.0167	0.0269	0.0241	-0.0048	-0.0013	0.0014	CALCULATED
	0.0005	-0.0008	-0.0006	0.0005	0.0000	0.0002	DIFFERENCE

C4	0.0219	0.0344	0.0230	-0.0027	0.0000	-0.0023	OBSERVED
	0.0223	0.0360	0.0221	-0.0030	0.0010	-0.0016	CALCULATED
	-0.0004	-0.0016	0.0009	0.0004	-0.0010	-0.0007	DIFFERENCE
C3	0.0277	0.0262	0.0312	-0.0024	-0.0003	-0.0083	OBSERVED
	0.0280	0.0275	0.0305	-0.0025	-0.0002	-0.0070	CALCULATED
	-0.0003	-0.0013	0.0007	0.0001	0.0000	-0.0014	DIFFERENCE
C6	0.0188	0.0387	0.0243	-0.0036	-0.0063	0.0007	OBSERVED
	0.0188	0.0382	0.0248	-0.0043	-0.0060	0.0001	CALCULATED
	0.0000	0.0006	-0.0005	0.0006	-0.0003	0.0006	DIFFERENCE
C2	0.0244	0.0196	0.0281	-0.0016	-0.0019	0.0021	OBSERVED
	0.0251	0.0194	0.0280	-0.0027	-0.0013	0.0021	CALCULATED
	-0.0007	0.0002	0.0000	0.0011	-0.0006	0.0000	DIFFERENCE

VIBRATION TENSORS IN THE CARTESIAN CRYSTAL SYSTEM

	U11	U22	U33	U12	U13	U23	
C5	0.0240	0.0361	0.0223	-0.0018	-0.0045	0.0062	OBSERVED
	0.0238	0.0364	0.0215	-0.0023	-0.0048	0.0067	CALCULATED
	0.0003	-0.0003	0.0009	0.0005	0.0002	-0.0005	DIFFERENCE
C9	0.0305	0.0426	0.0321	-0.0122	-0.0034	-0.0103	OBSERVED
	0.0303	0.0417	0.0315	-0.0110	-0.0037	-0.0101	CALCULATED
	0.0002	0.0009	0.0005	-0.0011	0.0004	-0.0002	DIFFERENCE
C10	0.0235	0.0313	0.0295	-0.0026	-0.0072	-0.0054	OBSERVED
	0.0240	0.0340	0.0286	-0.0028	-0.0065	-0.0065	CALCULATED
	-0.0005	-0.0027	0.0009	0.0002	-0.0007	0.0011	DIFFERENCE

Cartesian Crystal Frame

WEIGHTED R FOR ALL U'S = 0.056; FOR DIAGONAL U'S ONLY, WEIGHTED R = 0.040
KEYR
[R HERE IS SQRT(SUM SQUARES WEIGHTED DELTA U DIVIDED BY SUM SQUARES WEIGHTED UOBS).]

A SORT OF ESD OF WEIGHTED DELTA(U) 0.0011
SQRT(SUM((WT(UOBS-UCALC))**2)/((NINOBS-NINPAR)*(AVE. of (WT**2)))
NINOBS IS THE NUMBER OF INDEPENDENT OBSERVATIONS (U VALUES); NINPAR IS THE NUMBER OF INDEPENDENT PARAMETERS DETERMINED

R.M.S. OF THE WEIGHTED DELTA(U) = 0.0009

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(SQRT(SUM(WT(UOBS-UCALC))**2/SUM(WT**2)))

Goodness of fit =  2.14, defined as square root of [sum of squares of delta(U)/esd(u)
 divided by (number of independent observations  -  number of parameters)]
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