

Ms. 7965. On the correct calculation of amphibole/melt and amphibole/clinopyroxene DTi and their use in petrogenetic studies. Roberta Oberti, Riccardo Vannucci, Alberto Zanetti, Massimo Tiepolo, and Richard C. Brumm

Table 3. Final atomic coordinates and anisotropic displacement-parameters

SAMPLE 1

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10708	.08782	.21726	.0021	.0009	.0071	-.0001	.0009	-.0001
O 2	.11924	.17301	.73050	.0020	.0007	.0086	.0001	.0007	.0004
O 3	.10801	.00000	.71381	.0020	.0010	.0111	.0000	.0009	.0000
O 4	.36788	.24991	.78633	.0040	.0007	.0107	-.0004	.0014	.0005
O 5	.35003	.13995	.10990	.0024	.0011	.0106	.0000	.0008	.0013
O 6	.34473	.11608	.60886	.0026	.0013	.0117	.0003	.0010	-.0013
O 7	.34069	.00000	.27728	.0033	.0009	.0179	.0000	.0015	.0000
T 1	.28174	.08544	.30209	.0015	.0004	.0054	-.0001	.0006	-.0001
T 2	.29147	.17257	.81084	.0015	.0005	.0048	-.0001	.0005	.0002
M 1	.00000	.08696	.50000	.0024	.0011	.0059	.0000	.0016	.0000
M 2	.00000	.17751	.00000	.0018	.0005	.0057	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0022	.0003	.0051	.0000	.0002	.0000
M 4	.00000	.27960	.50000	.0026	.0005	.0084	.0000	.0031	.0000
A	.00000	.50000	.00000	.0154	.0015	.0312	.0000	.0214	.0000
AM	.04691	.50000	.10192	.0166	.0017	.0361	.0000	.0177	.0000
A2	.00000	.47138	.00000	.0077	.0014	.0414	.0000	.0154	.0000
H	.18906	.00000	.76299	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.26270	.50000	1.6965	.0000	.0000	.0000	.0000	.0000

SAMPLE 2

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10687	.08869	.21674	.0019	.0011	.0095	-.0003	.0006	-.0001
O 2	.11912	.17327	.73099	.0023	.0008	.0093	.0001	.0004	.0005
O 3	.10844	.00000	.71159	.0024	.0013	.0111	.0000	.0005	.0000
O 4	.36749	.25016	.78758	.0040	.0007	.0118	-.0003	.0018	.0003
O 5	.35022	.13943	.10833	.0025	.0010	.0100	.0000	.0009	.0010
O 6	.34489	.11727	.60653	.0027	.0012	.0125	.0002	.0010	-.0014
O 7	.33947	.00000	.28155	.0036	.0009	.0184	.0000	.0018	.0000
T 1	.28183	.08569	.30211	.0015	.0004	.0057	-.0002	.0004	-.0001
T 2	.29141	.17270	.81088	.0016	.0005	.0053	-.0001	.0006	.0001
M 1	.00000	.08636	.50000	.0024	.0012	.0060	.0000	.0016	.0000
M 2	.00000	.17799	.00000	.0017	.0004	.0062	.0000	.0008	.0000

M 3	.00000	.00000	.00000	.0024	.0004	.0055	.0000	.0004	.0000
M 4	.00000	.27898	.50000	.0030	.0006	.0097	.0000	.0031	.0000
A	.00000	.50000	.00000	.0101	.0011	.0448	.0000	.0205	.0000
AM	.05191	.50000	.09947	.0126	.0017	.0389	.0000	.0155	.0000
A2	.00000	.47320	.00000	.0089	.0017	.0490	.0000	.0154	.0000
H	.19476	.00000	.76271	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25883	.50000	1.5183	.0000	.0000	.0000	.0000	.0000
SAMPLE 3									
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.10668	.08854	.21645	.0018	.0010	.0078	-.0003	.0005	-.0003
O 2	.11938	.17320	.73225	.0020	.0007	.0099	.0001	.0007	.0005
O 3	.10816	.00000	.71216	.0027	.0010	.0134	.0000	.0010	.0000
O 4	.36794	.25004	.78770	.0039	.0008	.0105	-.0004	.0018	.0004
O 5	.35059	.13968	.10886	.0023	.0011	.0097	.0000	.0006	.0015
O 6	.34497	.11659	.60822	.0023	.0012	.0106	.0003	.0006	-.0012
O 7	.33991	.00000	.27811	.0034	.0009	.0185	.0000	.0015	.0000
T 1	.28183	.08560	.30176	.0015	.0004	.0052	-.0001	.0008	-.0001
T 2	.29160	.17263	.81118	.0015	.0004	.0053	-.0001	.0006	.0002
M 1	.00000	.08701	.50000	.0023	.0011	.0060	.0000	.0015	.0000
M 2	.00000	.17797	.00000	.0016	.0004	.0053	.0000	.0007	.0000
M 3	.00000	.00000	.00000	.0023	.0003	.0048	.0000	.0001	.0000
M 4	.00000	.27964	.50000	.0025	.0005	.0085	.0000	.0031	.0000
A	.00000	.50000	.00000	.0112	.0007	.0546	.0000	.0218	.0000
AM	.05745	.50000	.10702	.0087	.0008	.0322	.0000	.0109	.0000
A2	.00000	.47313	.00000	.0134	.0009	.0681	.0000	.0271	.0000
H	.18953	.00000	.76031	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.26301	.50000	1.5581	.0000	.0000	.0000	.0000	.0000

SAMPLE 4

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.10725	.08809	.21688	.0019	.0010	.0082	-.0002	.0008	-.0001
O 2	.11931	.17291	.73103	.0020	.0008	.0093	.0000	.0009	.0003
O 3	.10846	.00000	.71251	.0023	.0010	.0116	.0000	.0011	.0000
O 4	.36779	.24994	.78632	.0039	.0007	.0113	-.0004	.0014	.0005
O 5	.35049	.13988	.10922	.0023	.0011	.0110	.0000	.0008	.0013
O 6	.34497	.11614	.60771	.0027	.0013	.0127	.0002	.0011	-.0015

O 7	.34124	.00000	.27543	.0031	.0009	.0165	.0000	.0017	.0000
T 1	.28228	.08544	.30173	.0015	.0004	.0053	-.0001	.0004	-.0001
T 2	.29176	.17251	.81053	.0015	.0005	.0057	-.0001	.0008	.0001
M 1	.00000	.08694	.50000	.0023	.0011	.0062	.0000	.0018	.0000
M 2	.00000	.17793	.00000	.0018	.0005	.0062	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0023	.0004	.0059	.0000	.0003	.0000
M 4	.00000	.27935	.50000	.0029	.0006	.0097	.0000	.0033	.0000
A	.00000	.50000	.00000	.0203	.0010	.0529	.0000	.0304	.0000
AM	.05291	.50000	.11146	.0120	.0016	.0301	.0000	.0144	.0000
A2	.00000	.47208	.00000	.0081	.0012	.0468	.0000	.0171	.0000
H	.19227	.00000	.76236	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.26163	.50000	1.2726	.0000	.0000	.0000	.0000	.0000

SAMPLE 5

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10756	.08769	.21629	.0025	.0009	.0089	-.0001	.0017	.0001
O 2	.11961	.17287	.73048	.0016	.0009	.0099	-.0001	.0006	.0005
O 3	.10908	.00000	.71249	.0021	.0010	.0127	.0000	.0003	.0000
O 4	.36794	.25011	.78365	.0042	.0008	.0098	-.0005	.0004	.0006
O 5	.35154	.14012	.10885	.0029	.0011	.0122	.0000	.0014	.0015
O 6	.34593	.11587	.60694	.0026	.0014	.0111	.0003	.0009	-.0016
O 7	.34293	.00000	.27231	.0030	.0011	.0185	.0000	.0038	.0000
T 1	.28356	.08535	.30044	.0014	.0004	.0052	-.0001	.0005	-.0002
T 2	.29250	.17227	.80958	.0015	.0005	.0053	-.0001	.0007	.0002
M 1	.00000	.08641	.50000	.0024	.0012	.0056	.0000	.0022	.0000
M 2	.00000	.17782	.00000	.0018	.0005	.0047	.0000	.0009	.0000
M 3	.00000	.00000	.00000	.0019	.0004	.0062	.0000	-.0001	.0000
M 4	.00000	.27844	.50000	.0029	.0007	.0090	.0000	.0038	.0000
A	.00000	.50000	.00000	.0296	.0013	.0792	.0000	.0449	.0000
AM	.06031	.50000	.12244	.0056	.0027	.0151	.0000	.0055	.0000
A2	.00000	.47223	.00000	.0067	.0013	.0393	.0000	.0148	.0000
H	.18755	.00000	.76700	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25955	.50000	1.6837	.0000	.0000	.0000	.0000	.0000

SAMPLE 6

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10617	.08922	.21595	.0022	.0012	.0100	-.0003	.0009	-.0003
O 2	.11972	.17393	.73130	.0021	.0009	.0117	.0000	.0005	.0005

O 3	.10834	.00000	.71176	.0025	.0013	.0130	.0000	.0008	.0000
O 4	.36821	.24976	.78791	.0043	.0008	.0127	-.0003	.0018	.0004
O 5	.34998	.13919	.10798	.0025	.0012	.0116	.0001	.0008	.0013
O 6	.34436	.11723	.60696	.0028	.0014	.0123	.0002	.0011	-.0012
O 7	.33837	.00000	.28153	.0037	.0010	.0194	.0000	.0014	.0000
T 1	.28114	.08571	.30215	.0017	.0005	.0061	-.0001	.0004	-.0001
T 2	.29150	.17263	.81119	.0017	.0006	.0062	-.0001	.0006	.0002
M 1	.00000	.08753	.50000	.0030	.0013	.0083	.0000	.0017	.0000
M 2	.00000	.17832	.00000	.0019	.0005	.0069	.0000	.0009	.0000
M 3	.00000	.00000	.00000	.0023	.0005	.0063	.0000	.0001	.0000
M 4	.00000	.27902	.50000	.0029	.0007	.0101	.0000	.0030	.0000
A	.00000	.50000	.00000	.0116	.0031	.0302	.0000	.0160	.0000
AM	.04354	.50000	.08824	.0161	.0015	.0474	.0000	.0231	.0000
A2	.00000	.47101	.00000	.0081	.0031	.0619	.0000	.0214	.0000
H	.18857	.00000	.75610	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25756	.50000	1.1765	.0000	.0000	.0000	.0000	.0000
SAMPLE 7									
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.10721	.08694	.21866	.0019	.0007	.0079	-.0002	.0006	-.0001
O 2	.11911	.17231	.72949	.0017	.0008	.0079	-.0001	.0008	.0002
O 3	.10767	.00000	.71436	.0021	.0008	.0112	.0000	.0013	.0000
O 4	.36662	.24995	.78654	.0034	.0007	.0112	-.0004	.0016	.0003
O 5	.34949	.13969	.11029	.0021	.0011	.0096	.0000	.0003	.0012
O 6	.34483	.11572	.60960	.0024	.0011	.0125	.0001	.0016	-.0015
O 7	.34104	.00000	.27706	.0032	.0009	.0165	.0000	.0015	.0000
T 1	.28137	.08530	.30263	.0015	.0004	.0049	-.0001	.0004	-.0001
T 2	.29070	.17274	.81107	.0014	.0005	.0050	-.0001	.0007	.0001
M 1	.00000	.08664	.50000	.0020	.0011	.0054	.0000	.0014	.0000
M 2	.00000	.17702	.00000	.0018	.0005	.0058	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0022	.0004	.0056	.0000	.0002	.0000
M 4	.00000	.27873	.50000	.0027	.0006	.0083	.0000	.0028	.0000
A	.00000	.50000	.00000	.0048	.0024	.0220	.0000	.0091	.0000
AM	.04732	.50000	.09659	.0071	.0021	.0215	.0000	.0082	.0000
A2	.00000	.46954	.00000	.0068	.0011	.0348	.0000	.0083	.0000
H	.21780	.00000	.77457	.5757	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25434	.50000	.9489	.0000	.0000	.0000	.0000	.0000

SAMPLE 8												
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23												
O 1	.10689	.08862	.21697	.0022	.0010	.0082	-.0002	.0009	-.0002			
O 2	.11962	.17324	.73142	.0018	.0008	.0097	.0001	.0003	.0005			
O 3	.10880	.00000	.71210	.0022	.0011	.0119	.0000	.0004	.0000			
O 4	.36755	.25002	.78775	.0040	.0007	.0102	-.0003	.0015	.0003			
O 5	.35031	.13919	.10787	.0023	.0011	.0106	-.0001	.0006	.0012			
O 6	.34491	.11703	.60693	.0026	.0012	.0113	.0002	.0009	-.0013			
O 7	.34012	.00000	.27921	.0034	.0009	.0171	.0000	.0010	.0000			
T 1	.28177	.08558	.30185	.0014	.0004	.0055	-.0001	.0003	-.0001			
T 2	.29146	.17254	.81068	.0015	.0005	.0054	-.0001	.0005	.0001			
M 1	.00000	.08687	.50000	.0022	.0011	.0061	.0000	.0013	.0000			
M 2	.00000	.17816	.00000	.0017	.0004	.0058	.0000	.0007	.0000			
M 3	.00000	.00000	.00000	.0023	.0004	.0054	.0000	.0001	.0000			
M 4	.00000	.27929	.50000	.0029	.0006	.0099	.0000	.0031	.0000			
A	.00000	.50000	.00000	.0095	.0005	.0391	.0000	.0192	.0000			
AM	.05351	.50000	.10405	.0131	.0015	.0360	.0000	.0141	.0000			
A2	.00000	.47348	.00000	.0118	.0019	.0594	.0000	.0204	.0000			
H	.20647	.00000	.75928	1.0000	.0000	.0000	.0000	.0000	.0000			
M42	.00000	.26032	.50000	1.1776	.0000	.0000	.0000	.0000	.0000			

SAMPLE 9												
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23												
O 1	.10666	.08844	.21720	.0020	.0009	.0094	-.0002	.0010	-.0002			
O 2	.11876	.17293	.73091	.0019	.0008	.0094	.0000	.0003	.0005			
O 3	.10793	.00000	.71244	.0021	.0011	.0121	.0000	.0003	.0000			
O 4	.36719	.25015	.78815	.0040	.0007	.0112	-.0003	.0015	.0002			
O 5	.35037	.13923	.10890	.0022	.0011	.0116	.0000	.0007	.0012			
O 6	.34473	.11706	.60763	.0025	.0012	.0125	.0001	.0013	-.0014			
O 7	.34001	.00000	.28010	.0035	.0009	.0174	.0000	.0012	.0000			
T 1	.28161	.08563	.30244	.0015	.0004	.0053	-.0001	.0003	-.0001			
T 2	.29112	.17256	.81135	.0014	.0005	.0052	-.0001	.0004	.0001			
M 1	.00000	.08668	.50000	.0022	.0011	.0059	.0000	.0013	.0000			
M 2	.00000	.17808	.00000	.0018	.0005	.0064	.0000	.0008	.0000			
M 3	.00000	.00000	.00000	.0025	.0004	.0064	.0000	.0000	.0000			
M 4	.00000	.27879	.50000	.0028	.0007	.0098	.0000	.0029	.0000			
A	.00000	.50000	.00000	.0185	.0020	.0456	.0000	.0285	.0000			

AM	.04721	.50000	.10194	.0152	.0013	.0369	.0000	.0171	.0000
A2	.00000	.47344	.00000	.0150	.0022	.0707	.0000	.0270	.0000
H	.14814	.00000	.45519	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25509	.50000	.8573	.0000	.0000	.0000	.0000	.0000
SAMPLE 10									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10707	.08827	.21662	.0020	.0010	.0079	-.0001	.0006	-.0001
O 2	.11946	.17302	.73086	.0021	.0007	.0087	.0001	.0003	.0006
O 3	.10819	.00000	.71252	.0020	.0011	.0134	.0000	.0011	.0000
O 4	.36752	.24969	.78788	.0040	.0007	.0105	-.0003	.0016	.0005
O 5	.35005	.13930	.10825	.0024	.0011	.0093	-.0001	.0005	.0013
O 6	.34471	.11667	.60706	.0024	.0012	.0117	.0002	.0010	-.0012
O 7	.34018	.00000	.27808	.0030	.0009	.0164	.0000	.0006	.0000
T 1	.28158	.08550	.30178	.0015	.0004	.0052	-.0001	.0006	-.0001
T 2	.29123	.17251	.81041	.0015	.0004	.0050	-.0001	.0006	.0001
M 1	.00000	.08707	.50000	.0024	.0010	.0058	.0000	.0017	.0000
M 2	.00000	.17802	.00000	.0017	.0005	.0064	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0022	.0003	.0054	.0000	.0001	.0000
M 4	.00000	.27856	.50000	.0029	.0007	.0097	.0000	.0032	.0000
A	.00000	.50000	.00000	.0109	.0020	.0524	.0000	.0234	.0000
AM	.05402	.50000	.10389	.0103	.0008	.0291	.0000	.0111	.0000
A2	.00000	.47186	.00000	.0137	.0022	.0593	.0000	.0224	.0000
H	.18507	.00000	.75975	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25700	.50000	1.4282	.0000	.0000	.0000	.0000	.0000
SAMPLE 11									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10702	.08822	.21762	.0021	.0010	.0081	-.0002	.0004	-.0002
O 2	.11917	.17288	.73038	.0019	.0008	.0093	.0000	.0005	.0003
O 3	.10848	.00000	.71242	.0026	.0011	.0109	.0000	.0008	.0000
O 4	.36725	.25006	.78720	.0040	.0007	.0117	-.0003	.0017	.0003
O 5	.35022	.13930	.10769	.0022	.0011	.0106	.0000	.0005	.0013
O 6	.34514	.11699	.60686	.0026	.0012	.0114	.0002	.0012	-.0012
O 7	.34044	.00000	.28001	.0033	.0009	.0186	.0000	.0015	.0000
T 1	.28202	.08556	.30204	.0016	.0004	.0055	-.0001	.0004	-.0001
T 2	.29136	.17257	.81061	.0016	.0005	.0052	-.0001	.0006	.0001
M 1	.00000	.08611	.50000	.0023	.0013	.0057	.0000	.0015	.0000

M 2 .00000 .17794 .00000 .0018 .0005 .0060 .0000 .0008 .0000

M 3 .00000 .00000 .00000 .0023 .0004 .0054 .0000 .0001 .0000

M 4 .00000 .27858 .50000 .0029 .0007 .0096 .0000 .0030 .0000

A .00000 .50000 .00000 .0233 .0011 .0495 .0000 .0339 .0000

AM .04893 .50000 .10564 .0148 .0013 .0313 .0000 .0175 .0000

A2 .00000 .47307 .00000 .0117 .0018 .0649 .0000 .0233 .0000

H -.79732 .00000 2.04358 1.0000 .0000 .0000 .0000 .0000 .0000

M42 .00000 .25697 .50000 1.2224 .0000 .0000 .0000 .0000 .0000

SAMPLE 12

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23

O 1 .10656 .08920 .21610 .0024 .0010 .0084 -.0002 .0010 -.0002

O 2 .11960 .17386 .73234 .0019 .0008 .0108 .0001 .0008 .0006

O 3 .10832 .00000 .71187 .0023 .0010 .0129 .0000 .0008 .0000

O 4 .36807 .25002 .78748 .0042 .0007 .0119 -.0003 .0016 .0004

O 5 .35039 .13935 .10800 .0026 .0011 .0102 .0000 .0012 .0014

O 6 .34431 .11663 .60752 .0028 .0013 .0129 .0002 .0011 -.0013

O 7 .33955 .00000 .27843 .0032 .0009 .0182 .0000 .0015 .0000

T 1 .28146 .08569 .30172 .0016 .0004 .0057 -.0001 .0006 -.0001

T 2 .29166 .17262 .81122 .0016 .0005 .0056 -.0001 .0006 .0001

M 1 .00000 .08744 .50000 .0023 .0011 .0054 .0000 .0014 .0000

M 2 .00000 .17822 .00000 .0019 .0005 .0069 .0000 .0011 .0000

M 3 .00000 .00000 .00000 .0022 .0004 .0060 .0000 .0003 .0000

M 4 .00000 .27873 .50000 .0031 .0009 .0100 .0000 .0034 .0000

A .00000 .50000 .00000 .0154 .0020 .0391 .0000 .0229 .0000

AM .04892 .50000 .10030 .0155 .0019 .0440 .0000 .0198 .0000

A2 .00000 .47165 .00000 .0067 .0025 .0465 .0000 .0148 .0000

H .19030 .00000 .76353 1.0000 .0000 .0000 .0000 .0000 .0000

M42 .00000 .25674 .50000 1.3619 .0000 .0000 .0000 .0000 .0000

SAMPLE 13

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23

O 1 .10686 .08881 .21668 .0020 .0011 .0090 -.0003 .0011 .0001

O 2 .11980 .17365 .73258 .0022 .0008 .0104 .0000 .0007 .0005

O 3 .10872 .00000 .71231 .0021 .0011 .0105 .0000 -.0002 .0000

O 4 .36809 .24993 .78650 .0042 .0007 .0102 -.0003 .0019 .0005

O 5 .35042 .13965 .10915 .0022 .0011 .0097 .0000 .0007 .0013

O 6 .34421 .11652 .60824 .0024 .0013 .0125 .0001 .0011 -.0013

O 7	.33924	.00000	.27913	.0037	.0009	.0175	.0000	.0021	.0000
T 1	.28131	.08563	.30234	.0015	.0004	.0053	-.0001	.0005	-.0001
T 2	.29146	.17262	.81103	.0016	.0005	.0056	-.0001	.0008	.0000
M 1	.00000	.08738	.50000	.0022	.0010	.0046	.0000	.0015	.0000
M 2	.00000	.17800	.00000	.0018	.0005	.0071	.0000	.0012	.0000
M 3	.00000	.00000	.00000	.0023	.0004	.0056	.0000	.0003	.0000
M 4	.00000	.27824	.50000	.0029	.0009	.0097	.0000	.0031	.0000
A	.00000	.50000	.00000	.0266	.0011	.0502	.0000	.0363	.0000
AM	.04505	.50000	.10565	.0200	.0019	.0468	.0000	.0238	.0000
A2	.00000	.47198	.00000	.0081	.0022	.0402	.0000	.0142	.0000
H	.18517	.00000	.77373	.0032	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25144	.50000	.9642	.0000	.0000	.0000	.0000	.0000

SAMPLE 14

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10687	.08854	.21707	.0021	.0010	.0090	-.0003	.0009	-.0003
O 2	.11981	.17327	.73009	.0019	.0008	.0106	.0001	.0007	.0004
O 3	.10816	.00000	.71238	.0026	.0011	.0130	.0000	.0007	.0000
O 4	.36690	.24944	.78786	.0040	.0007	.0107	-.0003	.0021	.0001
O 5	.34931	.13872	.10742	.0023	.0010	.0108	.0000	.0011	.0013
O 6	.34475	.11704	.60669	.0026	.0011	.0125	.0002	.0014	-.0012
O 7	.33937	.00000	.28157	.0034	.0008	.0178	.0000	.0014	.0000
T 1	.28114	.08547	.30202	.0016	.0004	.0055	-.0001	.0007	-.0001
T 2	.29095	.17237	.81012	.0016	.0005	.0054	-.0001	.0007	.0001
M 1	.00000	.08724	.50000	.0024	.0010	.0060	.0000	.0016	.0000
M 2	.00000	.17833	.00000	.0018	.0005	.0062	.0000	.0012	.0000
M 3	.00000	.00000	.00000	.0023	.0003	.0058	.0000	.0004	.0000
M 4	.00000	.27896	.50000	.0030	.0006	.0099	.0000	.0033	.0000
A	.00000	.50000	.00000	.0179	.0027	.0614	.0000	.0303	.0000
AM	.04644	.50000	.09553	.0144	.0015	.0384	.0000	.0187	.0000
A2	.00000	.46667	.00000	.0060	.0005	.0454	.0000	.0119	.0000
H	.19431	.00000	.79745	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25860	.50000	1.1868	.0000	.0000	.0000	.0000	.0000

SAMPLE 15

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10709	.08832	.21710	.0019	.0010	.0086	-.0002	.0009	-.0001
O 2	.11949	.17289	.73021	.0021	.0008	.0096	.0000	.0006	.0004

O 3	.10840	.00000	.71185	.0022	.0011	.0125	.0000	.0007	.0000
O 4	.36697	.24995	.78800	.0039	.0007	.0113	-.0004	.0022	.0002
O 5	.34990	.13886	.10732	.0023	.0011	.0104	.0001	.0007	.0013
O 6	.34515	.11732	.60605	.0024	.0011	.0118	.0002	.0008	-.0013
O 7	.33996	.00000	.28132	.0035	.0009	.0172	.0000	.0015	.0000
T 1	.28171	.08554	.30191	.0014	.0004	.0052	-.0001	.0004	-.0001
T 2	.29120	.17249	.81011	.0016	.0005	.0053	-.0001	.0007	.0001
M 1	.00000	.08636	.50000	.0024	.0012	.0062	.0000	.0017	.0000
M 2	.00000	.17807	.00000	.0018	.0005	.0065	.0000	.0009	.0000
M 3	.00000	.00000	.00000	.0023	.0004	.0055	.0000	.0001	.0000
M 4	.00000	.27873	.50000	.0029	.0007	.0096	.0000	.0031	.0000
A	.00000	.50000	.00000	.0170	.0006	.0620	.0000	.0316	.0000
AM	.05435	.50000	.10581	.0140	.0011	.0387	.0000	.0169	.0000
A2	.00000	.47483	.00000	.0162	.0015	.0735	.0000	.0292	.0000
H	.19702	.00000	.76330	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25899	.50000	1.4853	.0000	.0000	.0000	.0000	.0000

SAMPLE 16

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10731	.08762	.21791	.0018	.0008	.0087	-.0001	.0009	-.0003
O 2	.11880	.17228	.73048	.0020	.0007	.0081	.0000	.0006	.0002
O 3	.10772	.00000	.71366	.0022	.0010	.0101	.0000	.0011	.0000
O 4	.36646	.25006	.78859	.0038	.0007	.0083	-.0004	.0010	.0001
O 5	.35002	.13943	.10895	.0023	.0011	.0122	.0000	.0013	.0015
O 6	.34519	.11651	.60970	.0026	.0011	.0124	.0001	.0008	-.0015
O 7	.34053	.00000	.27894	.0029	.0009	.0200	.0000	.0023	.0000
T 1	.28171	.08540	.30318	.0013	.0004	.0051	-.0001	.0004	-.0001
T 2	.29059	.17257	.81130	.0015	.0004	.0058	-.0001	.0008	.0001
M 1	.00000	.08615	.50000	.0022	.0012	.0073	.0000	.0019	.0000
M 2	.00000	.17764	.00000	.0015	.0004	.0052	.0000	.0009	.0000
M 3	.00000	.00000	.00000	.0026	.0004	.0058	.0000	.0003	.0000
M 4	.00000	.27938	.50000	.0027	.0005	.0095	.0000	.0032	.0000
A	.00000	.50000	.00000	.0135	.0005	.0703	.0000	.0291	.0000
AM	.05018	.50000	.09409	.0127	.0014	.0477	.0000	.0177	.0000
A2	.00000	.47293	.00000	.0115	.0014	.0465	.0000	.0188	.0000
H	.21087	.00000	.91256	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.26147	.50000	.9043	.0000	.0000	.0000	.0000	.0000

SAMPLE 17												
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23												
O 1	.10701	.08711	.21878	.0023	.0008	.0068	-.0001	.0008	-.0002			
O 2	.11813	.17201	.73074	.0020	.0007	.0080	.0000	.0005	.0002			
O 3	.10721	.00000	.71450	.0019	.0009	.0111	.0000	.0002	.0000			
O 4	.36603	.25044	.78816	.0037	.0007	.0092	-.0002	.0017	.0002			
O 5	.34991	.13977	.11237	.0026	.0011	.0103	.0000	.0008	.0012			
O 6	.34493	.11601	.61101	.0027	.0011	.0116	.0001	.0010	-.0013			
O 7	.34066	.00000	.27862	.0032	.0008	.0173	.0000	.0014	.0000			
T 1	.28147	.08538	.30404	.0016	.0004	.0052	-.0001	.0005	-.0001			
T 2	.29037	.17270	.81256	.0014	.0004	.0049	-.0001	.0005	.0001			
M 1	.00000	.08631	.50000	.0024	.0012	.0057	.0000	.0016	.0000			
M 2	.00000	.17744	.00000	.0018	.0005	.0056	.0000	.0009	.0000			
M 3	.00000	.00000	.00000	.0025	.0004	.0069	.0000	.0001	.0000			
M 4	.00000	.27931	.50000	.0030	.0006	.0090	.0000	.0028	.0000			
A	.00000	.50000	.00000	.0079	.0022	.0262	.0000	.0120	.0000			
AM	.04618	.50000	.09495	.0092	.0019	.0259	.0000	.0111	.0000			
A2	.00000	.46915	.00000	.0079	.0012	.0411	.0000	.0121	.0000			
H	.19220	.00000	.79000	.5500	.0000	.0000	.0000	.0000	.0000			
M42	.00000	.25436	.50000	1.3263	.0000	.0000	.0000	.0000	.0000			

SAMPLE 18												
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23												
O 1	.10687	.08686	.21900	.0017	.0007	.0074	-.0002	.0007	-.0001			
O 2	.11809	.17208	.73087	.0018	.0007	.0078	.0000	.0010	.0002			
O 3	.10702	.00000	.71606	.0019	.0007	.0101	.0000	.0010	.0000			
O 4	.36601	.25041	.78847	.0033	.0007	.0092	-.0002	.0021	.0000			
O 5	.34956	.14012	.11485	.0023	.0010	.0103	.0000	.0010	.0011			
O 6	.34451	.11543	.61274	.0021	.0011	.0116	.0001	.0008	-.0013			
O 7	.34026	.00000	.27738	.0028	.0008	.0171	.0000	.0014	.0000			
T 1	.28091	.08533	.30487	.0013	.0004	.0054	-.0001	.0006	-.0001			
T 2	.29005	.17273	.81334	.0012	.0004	.0047	-.0001	.0006	.0000			
M 1	.00000	.08684	.50000	.0022	.0010	.0062	.0000	.0016	.0000			
M 2	.00000	.17703	.00000	.0017	.0005	.0059	.0000	.0010	.0000			
M 3	.00000	.00000	.00000	.0023	.0004	.0069	.0000	-.0001	.0000			
M 4	.00000	.27956	.50000	.0027	.0006	.0085	.0000	.0025	.0000			
A	.00000	.50000	.00000	.0046	.0024	.0175	.0000	.0055	.0000			

AM	.04190	.50000	.08869	.0068	.0022	.0216	.0000	.0085	.0000
A2	.00000	.46894	.00000	.0060	.0016	.0343	.0000	.0098	.0000
H	.20378	.00000	.78892	.7037	.0000	.0000	.0000	.0000	.0000
SAMPLE 19									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10755	.08639	.21985	.0018	.0007	.0065	-.0001	.0007	-.0001
O 2	.11847	.17186	.72938	.0018	.0007	.0078	.0000	.0006	.0002
O 3	.10710	.00000	.71630	.0020	.0007	.0106	.0000	.0012	.0000
O 4	.36550	.24993	.78790	.0031	.0007	.0102	-.0002	.0019	.0001
O 5	.34924	.13956	.11223	.0023	.0011	.0099	.0000	.0010	.0010
O 6	.34450	.11559	.61098	.0022	.0011	.0119	.0002	.0010	-.0013
O 7	.34033	.00000	.27764	.0026	.0009	.0172	.0000	.0011	.0000
T 1	.28071	.08517	.30385	.0015	.0004	.0055	-.0001	.0006	-.0001
T 2	.28975	.17255	.81191	.0014	.0004	.0052	-.0001	.0009	-.0001
M 1	.00000	.08687	.50000	.0023	.0010	.0064	.0000	.0020	.0000
M 2	.00000	.17689	.00000	.0018	.0005	.0061	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0021	.0005	.0071	.0000	-.0002	.0000
M 4	.00000	.27912	.50000	.0027	.0006	.0088	.0000	.0028	.0000
A	.00000	.50000	.00000	.0053	.0026	.0163	.0000	.0060	.0000
AM	.04027	.50000	.08619	.0065	.0025	.0193	.0000	.0076	.0000
A2	.00000	.46714	.00000	.0059	.0013	.0319	.0000	.0075	.0000
H	.21016	.00000	.77040	.8272	.0000	.0000	.0000	.0000	.0000
SAMPLE 20									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10718	.08752	.21812	.0020	.0008	.0073	-.0002	.0007	-.0001
O 2	.11968	.17295	.72901	.0019	.0007	.0078	.0000	.0005	.0004
O 3	.10822	.00000	.71412	.0021	.0009	.0108	.0000	.0007	.0000
O 4	.36643	.24930	.78772	.0035	.0007	.0100	-.0004	.0018	.0002
O 5	.34879	.13904	.10970	.0023	.0010	.0093	.0000	.0005	.0011
O 6	.34432	.11611	.60852	.0024	.0011	.0109	.0002	.0010	-.0012
O 7	.33878	.00000	.28034	.0031	.0009	.0166	.0000	.0011	.0000
T 1	.28040	.08531	.30291	.0014	.0004	.0047	-.0001	.0004	-.0001
T 2	.29033	.17242	.81090	.0014	.0004	.0046	-.0001	.0006	.0001
M 1	.00000	.08761	.50000	.0024	.0009	.0058	.0000	.0016	.0000
M 2	.00000	.17773	.00000	.0017	.0004	.0052	.0000	.0009	.0000
M 3	.00000	.00000	.00000	.0021	.0004	.0054	.0000	.0002	.0000

M 4	.00000	.27911	.50000	.0028	.0006	.0085	.0000	.0029	.0000
A	.00000	.50000	.00000	.0062	.0023	.0251	.0000	.0110	.0000
AM	.03490	.50000	.07303	.0182	.0018	.0556	.0000	.0257	.0000
A2	.00000	.46921	.00000	.0057	.0012	.0391	.0000	.0118	.0000
H	.19581	.00000	.76144	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25656	.50000	1.1665	.0000	.0000	.0000	.0000	.0000

SAMPLE 21

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10738	.08778	.21719	.0020	.0009	.0078	-.0002	.0012	-.0001
O 2	.11942	.17272	.73024	.0022	.0008	.0083	.0000	.0005	.0005
O 3	.10794	.00000	.71318	.0022	.0010	.0122	.0000	.0007	.0000
O 4	.36678	.24982	.78738	.0039	.0007	.0105	-.0003	.0021	.0004
O 5	.35008	.13952	.10896	.0023	.0010	.0101	.0000	.0008	.0011
O 6	.34452	.11631	.60791	.0026	.0011	.0125	.0002	.0011	-.0011
O 7	.34076	.00000	.27778	.0035	.0008	.0166	.0000	.0012	.0000
T 1	.28168	.08542	.30222	.0015	.0004	.0051	-.0001	.0005	-.0001
T 2	.29103	.17242	.81084	.0015	.0005	.0046	-.0001	.0007	.0001
M 1	.00000	.08710	.50000	.0023	.0010	.0055	.0000	.0016	.0000
M 2	.00000	.17793	.00000	.0019	.0005	.0063	.0000	.0011	.0000
M 3	.00000	.00000	.00000	.0023	.0004	.0054	.0000	.0002	.0000
M 4	.00000	.27915	.50000	.0029	.0006	.0091	.0000	.0030	.0000
A	.00000	.50000	.00000	.0080	.0049	.0486	.0000	.0185	.0000
AM	.04659	.50000	.08963	.0171	.0023	.0608	.0000	.0245	.0000
A2	.00000	.46818	.00000	.0080	.0012	.0527	.0000	.0128	.0000
H 2	.19202	.00000	4.74648	1.0000	.0000	.0000	.0000	.0000	.0000
M42	.00000	.25869	.50000	.8093	.0000	.0000	.0000	.0000	.0000

SAMPLE 22

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11010	.08673	.21867	.0015	.0004	.0042	-.0001	.0006	-.0001
O 2	.11827	.17075	.72568	.0020	.0006	.0034	-.0001	.0007	-.0003
O 3	.10632	.00000	.71530	.0020	.0006	.0057	.0000	.0012	.0000
O 4	.36244	.24766	.79739	.0038	.0006	.0063	-.0006	.0017	-.0005
O 5	.34302	.13060	.09776	.0023	.0008	.0099	.0000	.0018	.0009
O 6	.33931	.11654	.59360	.0021	.0009	.0063	.0002	.0004	-.0012
O 7	.33118	.00000	.29933	.0027	.0003	.0112	.0000	.0017	.0000
T 1	.27466	.08516	.30046	.0016	.0003	.0042	.0000	.0007	-.0001

T 2	.28480	.17170	.80593	.0016	.0003	.0041	-.0001	.0006	.0000
M 1	.00000	.08837	.50000	.0020	.0006	.0043	.0000	.0012	.0000
M 2	.00000	.17962	.00000	.0021	.0004	.0058	.0000	.0013	.0000
M 3	.00000	.00000	.00000	.0023	.0003	.0049	.0000	.0012	.0000
M 4	.00000	.27775	.50000	.0035	.0005	.0105	.0000	.0038	.0000
A	.00000	.50000	.00000	.0010	.0021	.0127	.0000	.0035	.0000
AM	.02267	.50000	.05059	.0086	.0013	.0281	.0000	.0095	.0000
H	.19780	.00000	.75713	1.0000	.0000	.0000	.0000	.0000	.0000

SAMPLE 23

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11004	.08688	.21935	.0014	.0005	.0051	.0000	.0005	.0000
O 2	.11788	.17027	.72497	.0017	.0006	.0058	-.0001	.0011	-.0001
O 3	.10583	.00000	.71327	.0016	.0008	.0062	.0000	.0011	.0000
O 4	.36186	.24795	.79738	.0033	.0007	.0088	-.0006	.0008	-.0003
O 5	.34340	.12995	.09544	.0019	.0009	.0101	.0001	.0018	.0011
O 6	.34034	.11736	.59297	.0021	.0010	.0072	.0001	.0003	-.0011
O 7	.33186	.00000	.30172	.0018	.0004	.0127	.0000	.0014	.0000
T 1	.27561	.08515	.30029	.0011	.0003	.0047	-.0001	.0006	-.0001
T 2	.28493	.17164	.80593	.0012	.0004	.0047	-.0002	.0003	.0000
M 1	.00000	.08677	.50000	.0017	.0010	.0047	.0000	.0010	.0000
M 2	.00000	.17993	.00000	.0016	.0005	.0060	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0017	.0004	.0036	.0000	.0004	.0000
M 4	.00000	.27734	.50000	.0034	.0007	.0118	.0000	.0038	.0000
A	.00000	.50000	.00000	.0032	.0020	.0159	.0000	.0036	.0000
AM	.02978	.50000	.06502	.0063	.0011	.0236	.0000	.0097	.0000
H	.19911	.00000	.76177	1.0000	.0000	.0000	.0000	.0000	.0000

SAMPLE 24

ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11043	.08715	.22008	.0016	.0005	.0066	.0000	.0011	-.0001
O 2	.11769	.16946	.72398	.0018	.0007	.0069	.0000	.0015	-.0001
O 3	.10564	.00000	.71239	.0018	.0010	.0071	.0000	.0013	.0000
O 4	.36103	.24809	.79932	.0034	.0008	.0097	-.0006	.0011	-.0002
O 5	.34330	.12924	.09349	.0021	.0009	.0103	.0000	.0018	.0011
O 6	.34074	.11786	.59114	.0022	.0010	.0070	.0001	.0003	-.0011
O 7	.33206	.00000	.30411	.0020	.0005	.0119	.0000	.0010	.0000
T 1	.27632	.08517	.30071	.0012	.0004	.0050	.0000	.0008	.0000

T 2	.28490	.17145	.80547	.0012	.0004	.0050	-.0002	.0003	.0001
M 1	.00000	.08556	.50000	.0017	.0011	.0053	.0000	.0013	.0000
M 2	.00000	.18052	.00000	.0018	.0005	.0067	.0000	.0011	.0000
M 3	.00000	.00000	.00000	.0021	.0004	.0041	.0000	.0006	.0000
M 4	.00000	.27711	.50000	.0038	.0007	.0136	.0000	.0045	.0000
A	.00000	.50000	.00000	.0041	.0015	.0058	.0000	.0023	.0000
AM	.03424	.50000	.07619	.0049	.0011	.0143	.0000	.0060	.0000
SAMPLE 25									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11065	.08676	.22057	.0015	.0005	.0058	-.0001	.0007	.0000
O 2	.11739	.16911	.72330	.0020	.0007	.0075	-.0001	.0012	-.0001
O 3	.10555	.00000	.71168	.0021	.0012	.0076	.0000	.0008	.0000
O 4	.36046	.24851	.79930	.0038	.0008	.0094	-.0007	.0009	-.0004
O 5	.34411	.12955	.09409	.0022	.0009	.0102	.0001	.0015	.0010
O 6	.34210	.11844	.59172	.0022	.0010	.0079	.0001	.0004	-.0010
O 7	.33343	.00000	.30618	.0022	.0004	.0128	.0000	.0015	.0000
T 1	.27727	.08507	.30115	.0014	.0004	.0055	-.0001	.0007	-.0001
T 2	.28525	.17158	.80554	.0014	.0005	.0055	-.0002	.0005	.0001
M 1	.00000	.08334	.50000	.0019	.0015	.0052	.0000	.0012	.0000
M 2	.00000	.17966	.00000	.0019	.0006	.0075	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0020	.0004	.0050	.0000	.0005	.0000
M 4	.00000	.27673	.50000	.0035	.0007	.0129	.0000	.0041	.0000
A	.00000	.50000	.00000	.0056	.0014	.0272	.0000	.0094	.0000
AM	.03707	.50000	.07636	.0061	.0012	.0209	.0000	.0083	.0000
SAMPLE 26									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11035	.08668	.22118	.0015	.0005	.0055	.0001	.0007	.0001
O 2	.11724	.16915	.72312	.0014	.0007	.0069	.0000	.0011	-.0003
O 3	.10549	.00000	.71161	.0015	.0011	.0061	.0000	.0011	.0000
O 4	.36039	.24850	.79902	.0032	.0008	.0088	-.0007	.0005	-.0002
O 5	.34415	.12967	.09448	.0021	.0009	.0102	.0001	.0017	.0010
O 6	.34209	.11847	.59219	.0019	.0010	.0064	.0001	.0007	-.0009
O 7	.33360	.00000	.30581	.0021	.0005	.0135	.0000	.0014	.0000
T 1	.27720	.08511	.30103	.0011	.0003	.0048	-.0001	.0006	-.0001
T 2	.28533	.17156	.80605	.0012	.0004	.0049	-.0002	.0004	.0001
M 1	.00000	.08334	.50000	.0016	.0014	.0045	.0000	.0012	.0000

M 2	.00000	.17970	.00000	.0017	.0005	.0071	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0018	.0004	.0046	.0000	.0007	.0000
M 4	.00000	.27680	.50000	.0034	.0006	.0115	.0000	.0041	.0000
A	.00000	.50000	.00000	.0067	.0013	.0298	.0000	.0124	.0000
AM	.03563	.50000	.07448	.0060	.0012	.0220	.0000	.0081	.0000
SAMPLE 27									
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.11013	.08701	.21932	.0013	.0005	.0056	-.0001	.0007	.0000
O 2	.11784	.17020	.72443	.0016	.0006	.0064	-.0001	.0010	-.0001
O 3	.10595	.00000	.71292	.0019	.0009	.0071	.0000	.0012	.0000
O 4	.36152	.24783	.79785	.0036	.0007	.0095	-.0007	.0008	-.0003
O 5	.34331	.12961	.09509	.0020	.0009	.0108	.0001	.0019	.0012
O 6	.34040	.11743	.59260	.0020	.0011	.0080	.0001	.0004	-.0011
O 7	.33145	.00000	.30302	.0019	.0004	.0131	.0000	.0014	.0000
T 1	.27556	.08516	.30046	.0012	.0004	.0049	.0000	.0007	-.0001
T 2	.28484	.17154	.80578	.0012	.0004	.0050	-.0002	.0004	.0001
M 1	.00000	.08675	.50000	.0018	.0010	.0048	.0000	.0011	.0000
M 2	.00000	.18028	.00000	.0016	.0005	.0065	.0000	.0010	.0000
M 3	.00000	.00000	.00000	.0019	.0004	.0048	.0000	.0006	.0000
M 4	.00000	.27729	.50000	.0034	.0007	.0124	.0000	.0039	.0000
A	.00000	.50000	.00000	.0018	.0017	.0101	.0000	.0025	.0000
AM	.03052	.50000	.06593	.0056	.0012	.0230	.0000	.0080	.0000
H	.20378	.00000	.76121	.5000	.0000	.0000	.0000	.0000	.0000

SAMPLE 28

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.10994	.08693	.21904	.0013	.0005	.0053	-.0001	.0008	.0000
O 2	.11819	.17058	.72519	.0016	.0006	.0059	-.0001	.0012	-.0002
O 3	.10601	.00000	.71362	.0015	.0007	.0068	.0000	.0010	.0000
O 4	.36222	.24771	.79698	.0032	.0007	.0080	-.0006	.0011	-.0003
O 5	.34315	.13003	.09614	.0019	.0009	.0098	.0001	.0019	.0010
O 6	.33993	.11691	.59376	.0019	.0010	.0071	.0001	.0003	-.0011
O 7	.33104	.00000	.30080	.0018	.0004	.0120	.0000	.0013	.0000
T 1	.27505	.08514	.30033	.0011	.0003	.0045	-.0001	.0007	-.0001
T 2	.28478	.17162	.80588	.0012	.0004	.0046	-.0001	.0005	.0000
M 1	.00000	.08773	.50000	.0016	.0008	.0046	.0000	.0012	.0000

M 2 .00000 .17997 .00000 .0016 .0005 .0066 .0000 .0011 .0000

M 3 .00000 .00000 .00000 .0017 .0004 .0044 .0000 .0007 .0000

M 4 .00000 .27764 .50000 .0033 .0006 .0116 .0000 .0038 .0000

A .00000 .50000 .00000 .0023 .0019 .0167 .0000 .0043 .0000

AM .02413 .50000 .05462 .0080 .0014 .0301 .0000 .0124 .0000

H .19755 .00000 .76213 .5100 .0000 .0000 .0000 .0000 .0000

SAMPLE 29

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23

O 1 .10999 .08696 .21937 .0013 .0005 .0041 -.0001 .0003 -.0001

O 2 .11772 .17023 .72475 .0016 .0007 .0068 .0000 .0011 -.0002

O 3 .10602 .00000 .71355 .0018 .0008 .0080 .0000 .0011 .0000

O 4 .36167 .24806 .79769 .0036 .0007 .0081 -.0005 .0014 -.0001

O 5 .34327 .12983 .09611 .0021 .0008 .0095 .0002 .0022 .0011

O 6 .34014 .11726 .59290 .0022 .0010 .0072 .0001 .0002 -.0012

O 7 .33193 .00000 .30365 .0022 .0005 .0118 .0000 .0013 .0000

T 1 .27532 .08519 .30053 .0012 .0004 .0044 -.0001 .0006 -.0001

T 2 .28475 .17173 .80625 .0012 .0004 .0050 -.0002 .0004 .0001

M 1 .00000 .08675 .50000 .0016 .0011 .0045 .0000 .0011 .0000

M 2 .00000 .17994 .00000 .0019 .0004 .0062 .0000 .0011 .0000

M 3 .00000 .00000 .00000 .0018 .0003 .0045 .0000 .0007 .0000

M 4 .00000 .27748 .50000 .0034 .0007 .0113 .0000 .0038 .0000

A .00000 .50000 .00000 .0051 .0030 .0340 .0000 .0084 .0000

AM .02795 .50000 .05721 .0077 .0006 .0311 .0000 .0135 .0000

H .20936 .00000 .76850 1.0000 .0000 .0000 .0000 .0000 .0000

SAMPLE 30

ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23

O 1 .11020 .08753 .21918 .0012 .0006 .0096 -.0002 .0022 .0000

O 2 .11821 .16972 .72407 .0017 .0008 .0041 .0001 .0000 -.0003

O 3 .10568 .00000 .71243 .0024 .0011 .0024 .0000 -.0002 .0000

O 4 .36175 .24737 .79964 .0036 .0008 .0109 -.0005 .0030 -.0003

O 5 .34354 .12883 .09260 .0020 .0008 .0102 .0001 .0017 .0009

O 6 .34110 .11792 .59096 .0025 .0010 .0066 .0000 .0001 -.0011

O 7 .33099 .00000 .30392 .0016 .0004 .0104 .0000 .0007 .0000

T 1 .27612 .08507 .29960 .0013 .0004 .0058 -.0001 .0010 .0000

T 2 .28496 .17119 .80447 .0016 .0004 .0048 -.0001 .0005 .0000

M 1 .00000 .08597 .50000 .0016 .0011 .0047 .0000 .0017 .0000

M 2	.00000	.18074	.00000	.0017	.0005	.0073	.0000	.0007	.0000
M 3	.00000	.00000	.00000	.0021	.0003	.0034	.0000	.0003	.0000
M 4	.00000	.27695	.50000	.0038	.0006	.0137	.0000	.0044	.0000
A	.00000	.50000	.00000	.0010	.0015	.0066	.0000	-.0008	.0000
AM	.03536	.50000	.07673	.0041	.0010	.0137	.0000	.0053	.0000
SAMPLE 31									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.11059	.08683	.22006	.0014	.0006	.0048	-.0001	.0003	.0000
O 2	.11698	.16940	.72483	.0018	.0006	.0079	.0000	.0019	-.0001
O 3	.10510	.00000	.71073	.0016	.0010	.0081	.0000	.0013	.0000
O 4	.36068	.24835	.79884	.0034	.0008	.0106	-.0008	.0011	-.0002
O 5	.34372	.12949	.09511	.0026	.0009	.0105	.0002	.0023	.0011
O 6	.34078	.11789	.59154	.0020	.0011	.0079	.0001	.0006	-.0014
O 7	.33267	.00000	.30603	.0018	.0004	.0138	.0000	.0011	.0000
T 1	.27646	.08518	.30084	.0012	.0004	.0054	.0000	.0007	.0000
T 2	.28494	.17163	.80617	.0015	.0003	.0055	-.0001	.0003	.0002
M 1	.00000	.08513	.50000	.0015	.0012	.0047	.0000	.0012	.0000
M 2	.00000	.18005	.00000	.0017	.0005	.0074	.0000	.0013	.0000
M 3	.00000	.00000	.00000	.0019	.0004	.0040	.0000	.0000	.0000
M 4	.00000	.27711	.50000	.0036	.0008	.0137	.0000	.0042	.0000
A	.00000	.50000	.00000	.0028	.0027	.0189	.0000	.0062	.0000
AM	.03255	.50000	.06909	.0059	.0008	.0272	.0000	.0098	.0000
H	.18553	.00000	.78517	1.0000	.0000	.0000	.0000	.0000	.0000
SAMPLE 32									
ATOM	x/a	y/b	z/c	B11	B22	B33	B12	B13	B23
O 1	.10987	.08706	.21823	.0014	.0005	.0054	.0000	.0002	-.0001
O 2	.11808	.17075	.72505	.0018	.0006	.0061	.0000	.0012	-.0001
O 3	.10557	.00000	.71357	.0013	.0007	.0070	.0000	.0006	.0000
O 4	.36180	.24761	.79684	.0029	.0007	.0077	-.0006	.0006	-.0002
O 5	.34271	.12982	.09479	.0018	.0008	.0088	.0001	.0014	.0009
O 6	.33996	.11682	.59328	.0018	.0009	.0077	.0000	.0000	-.0010
O 7	.33076	.00000	.30094	.0020	.0005	.0118	.0000	.0017	.0000
T 1	.27488	.08519	.29966	.0011	.0003	.0040	-.0001	.0008	-.0001
T 2	.28472	.17153	.80500	.0013	.0004	.0046	-.0002	.0001	.0000
M 1	.00000	.08800	.50000	.0016	.0008	.0038	.0000	.0009	.0000
M 2	.00000	.18040	.00000	.0015	.0005	.0068	.0000	.0010	.0000

M 3	.00000	.00000	.00000	.0014	.0003	.0051	.0000	.0003	.0000
M 4	.00000	.27738	.50000	.0034	.0007	.0116	.0000	.0038	.0000
A	.00000	.50000	.00000	.0047	.0019	.0287	.0000	.0106	.0000
AM	.02411	.50000	.05648	.0092	.0011	.0341	.0000	.0128	.0000
H	.18937	.00000	.75532	1.0000	.0000	.0000	.0000	.0000	.0000
SAMPLE 33									
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.11161	.08632	.21810	.0013	.0005	.0053	-.0001	.0006	.0000
O 2	.11808	.16946	.72523	.0018	.0006	.0059	.0000	.0011	-.0002
O 3	.10675	.00000	.71194	.0017	.0008	.0067	.0000	.0010	.0000
O 4	.36214	.24857	.79520	.0033	.0008	.0081	-.0006	.0014	-.0003
O 5	.34639	.13010	.09108	.0020	.0011	.0101	.0001	.0016	.0013
O 6	.34296	.11724	.58909	.0024	.0010	.0081	.0000	.0005	-.0011
O 7	.33709	.00000	.29230	.0021	.0004	.0151	.0000	.0009	.0000
T 1	.27899	.08493	.29646	.0014	.0003	.0048	-.0001	.0005	-.0001
T 2	.28672	.17134	.80261	.0014	.0004	.0045	-.0002	.0006	.0000
M 1	.00000	.08621	.50000	.0019	.0011	.0049	.0000	.0014	.0000
M 2	.00000	.17972	.00000	.0019	.0006	.0069	.0000	.0011	.0000
M 3	.00000	.00000	.00000	.0017	.0004	.0041	.0000	.0002	.0000
M 4	.00000	.27588	.50000	.0036	.0008	.0128	.0000	.0045	.0000
A	.00000	.50000	.00000	.0074	.0101	.0301	.0000	.0129	.0000
AM	.03827	.50000	.08633	.0126	.0016	.0407	.0000	.0168	.0000
H	.19503	.00000	.75977	1.0000	.0000	.0000	.0000	.0000	.0000
SAMPLE 34									
ATOM x/a y/b z/c B11 B22 B33 B12 B13 B23									
O 1	.11157	.08668	.21967	.0013	.0008	.0088	-.0002	.0014	-.0008
O 2	.11714	.16859	.72307	.0019	.0004	.0053	-.0001	.0009	-.0003
O 3	.10562	.00000	.71098	.0025	.0009	.0047	.0000	.0010	.0000
O 4	.36149	.24933	.79818	.0033	.0009	.0112	-.0008	.0019	-.0006
O 5	.34745	.12944	.09006	.0030	.0010	.0120	.0002	.0019	.0019
O 6	.34335	.11844	.58772	.0021	.0011	.0091	.0001	.0019	-.0012
O 7	.33649	.00000	.29985	.0014	.0005	.0156	.0000	.0015	.0000
T 1	.27977	.08507	.29738	.0013	.0004	.0049	.0000	.0005	.0001
T 2	.28709	.17117	.80336	.0016	.0005	.0053	-.0002	.0003	.0004
M 1	.00000	.08357	.50000	.0023	.0013	.0062	.0000	.0017	.0000
M 2	.00000	.17997	.00000	.0010	.0005	.0062	.0000	.0010	.0000

On the correct calculation of amphibole/melt and amphibole/clinopyroxene DTi and on their use in petrogenetic studies

M 3	.00000	.00000	.00000	.0020	.0004	.0041	.0000	.0000	.0000
M 4	.00000	.27598	.50000	.0040	.0007	.0146	.0000	.0055	.0000
A	.00000	.50000	.00000	.0133	.0030	.0282	.0000	.0178	.0000
AM	.04240	.50000	.09737	.0091	.0013	.0183	.0000	.0086	.0000