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Structural, electronic, vibrational, optical, piezoelectric, thermal and thermoelectric properties of BCZT from first-principles calculations†

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Supporting Information for:

Table S. I Total Energy of all the possible structures of BCZT.

BCZT	Space Group	Total Energy (Ry)
$Ba_6Ca_2Zr_1Ti_7O_{24}$	R3m	-2247.55802
$Ba_6Ca_2Zr_2Ti_6O_{24}$	R3m	-2227.26792
$Ba_7Ca_1Zr_1Ti_7O_{24}$	R3m	-2235.23808
$Ba_7Ca_1Zr_2Ti_6O_{24}$	R3m	-2214.95241
$Ba_6Ca_2Zr_1Ti_7O_{24}$	P4mm	-2247.68725
$Ba_6Ca_2Zr_2Ti_6O_{24}$	P4mm	-2227.39514
$Ba_7Ca_1Zr_1Ti_7O_{24}$	P4mm	-2235.33208
$Ba_7Ca_1Zr_2Ti_6O_{24}$	P4mm	-2215.04743
$Ba_6Ca_2Zr_1Ti_7O_{24}$	Amm2	-2247.59229
$Ba_6Ca_2Zr_2Ti_6O_{24}$	Amm2	-2227.2906
$Ba_7Ca_1Zr_1Ti_7O_{24}$	Amm2	-2235.27292
$Ba_7Ca_1Zr_2Ti_6O_{24}$	Amm2	-2214.97084

Table S. II Piezoelectric tensors in [C/m^2] for different crystal calculated by using PBEsol.

Tensor of *a*6

$$\begin{bmatrix} 3.15987 & -0.77424 & 0.34755 & -1.72253 & -0.23244 & 0.18179 \\ -0.09720 & -4.76705 & -0.09975 & -0.09981 & -0.07497 & 0.06956 \\ 0.34746 & -0.74278 & 3.15370 & -0.23762 & -1.67957 & 0.18955 \end{bmatrix}$$

Tensor of *a*7

$$\begin{bmatrix} 4.38289 & 0.20581 & -0.35877 & -0.67328 & 0.43174 & 0.11674 \\ -0.17787 & -4.36399 & 0.35192 & 0.70495 & 0.12683 & 0.43040 \\ -1.03037 & -1.01588 & 7.54254 & 0.68552 & -2.46301 & 2.48458 \end{bmatrix}$$

Tensor of *p*6

$$\begin{bmatrix} 2.14989 & 0.01248 & 0.00912 & -0.01315 & 0.11365 & 1.38942 \\ 0.01378 & 2.14988 & 0.00913 & -0.01387 & 1.39006 & 0.11410 \\ 0.16811 & 0.16812 & 2.79267 & 0.00704 & -0.08931 & -0.08973 \end{bmatrix}$$

Tensor of *p*7

$$\begin{bmatrix} 1.98187 & -0.09543 & -0.01862 & 0.07481 & 0.03186 & 2.21970 \\ -0.09480 & 1.98190 & -0.01863 & 0.07484 & 2.22452 & 0.03148 \\ 0.56826 & 0.56825 & 2.91790 & -0.01372 & -0.11812 & -0.11781 \end{bmatrix}$$

Tensor of *r*6

$$\begin{bmatrix} -5.71262 & 1.18296 & 1.12723 & -1.09988 & 1.73278 & -1.08435 \\ 1.22756 & -5.65472 & 1.06881 & -1.16799 & -1.13123 & 1.72542 \\ 1.20482 & 1.11278 & -5.62662 & 1.72841 & -1.20312 & -1.20929 \end{bmatrix}$$

Tensor of *r*7

$$\begin{bmatrix} -5.65678 & 1.11711 & 1.08090 & -1.02823 & 1.63306 & -1.01619 \\ 1.16976 & -5.65173 & 1.07280 & -1.12704 & -1.06151 & 1.64340 \\ 1.16330 & 1.12530 & -5.64685 & 1.64436 & -1.14766 & -1.17143 \end{bmatrix}$$

Tensor of modified *a*6

$$\begin{bmatrix} 4.62068 & 0.00450 & -0.07830 & -0.83872 & 0.22394 & 0.27484 \\ 0.00050 & -4.22057 & 0.23566 & 0.60367 & 0.08169 & 0.42469 \\ -0.12966 & -0.90749 & 4.06939 & 0.33527 & -1.43563 & 1.28791 \end{bmatrix}$$

Table S. III Piezoelectric tensor in [C/m^2] for different crystal calculated by using PBE.

Tensor of $a6$

$$\begin{bmatrix} 3.03208 & -1.27302 & 0.19329 & -1.45814 & -0.10764 & 0.32434 \\ 0.13096 & -5.28716 & 0.23794 & -0.14219 & -0.23838 & 0.22214 \\ 0.17059 & -1.41737 & 3.19374 & -0.08690 & -1.50910 & 0.30679 \end{bmatrix}$$

Tensor of $a7$

$$\begin{bmatrix} 24.25580 & -19.97930 & -0.19623 & -0.39436 & 2.11617 & 1.95076 \\ 20.21559 & -24.43027 & 0.15623 & 0.81660 & 1.99094 & 2.11844 \\ -0.59971 & -0.58493 & 5.59775 & 0.42778 & -1.60319 & 1.61769 \end{bmatrix}$$

Tensor of $p6$

$$\begin{bmatrix} 1.95760 & 0.01697 & 0.04329 & -0.02252 & 0.08704 & 1.25527 \\ 0.01817 & 1.95759 & 0.04332 & -0.02329 & 1.25619 & 0.08735 \\ 0.14929 & 0.14929 & 2.63597 & 0.00709 & -0.06926 & -0.06949 \end{bmatrix}$$

Tensor of $p7$

$$\begin{bmatrix} 1.70982 & -0.06986 & 0.02243 & 0.04899 & 0.01270 & 1.94417 \\ -0.06930 & 1.70982 & 0.02244 & 0.04893 & 1.94844 & 0.01241 \\ 0.49076 & 0.49075 & 2.72699 & -0.01042 & -0.09005 & -0.08974 \end{bmatrix}$$

Tensor of $r6$

$$\begin{bmatrix} -4.72514 & 0.74254 & 0.70901 & -0.77478 & 1.10766 & -0.76227 \\ 0.78314 & -4.69030 & 0.67688 & -0.83304 & -0.79161 & 1.10675 \\ 0.76999 & 0.71703 & -4.67441 & 1.10930 & -0.85123 & -0.86054 \end{bmatrix}$$

Tensor of $r7$

$$\begin{bmatrix} -4.61509 & 0.65701 & 0.62421 & -0.71343 & 1.01772 & -0.70291 \\ 0.70401 & -4.59945 & 0.61213 & -0.77725 & -0.73205 & 1.01451 \\ 0.69141 & 0.65788 & -4.58201 & 1.01449 & -0.79792 & -0.80616 \end{bmatrix}$$

Tensor of modified $a6$

$$\begin{bmatrix} 32.41238 & -27.25899 & -0.90021 & -0.55438 & 3.96809 & -3.83357 \\ 27.18556 & -30.30513 & -0.67121 & 0.73167 & 3.77305 & -3.58438 \\ -8.32826 & 7.34462 & 3.76822 & 0.18858 & -2.26992 & 2.22970 \end{bmatrix}$$

Table S. IV BEC components (in e) of Zr1 and Zr2 in a6 and modified a6 structure.

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
a6-Zr1	6.40815	6.37792	6.43135	0.17435	-0.03443	0.02793	0.03712	-0.03038	0.17752
a6-Zr2	6.40966	6.37931	6.43358	0.17561	-0.02923	0.02573	0.03426	-0.03204	0.18166
modified a6-Zr1	6.48884	6.29009	6.46449	0.21588	-0.01675	0.19343	0.01626	-0.15530	0.19517
modified a6-Zr2	6.40408	6.25430	6.77715	0.09375	-0.05107	0.10350	0.00143	-0.08610	-0.01161

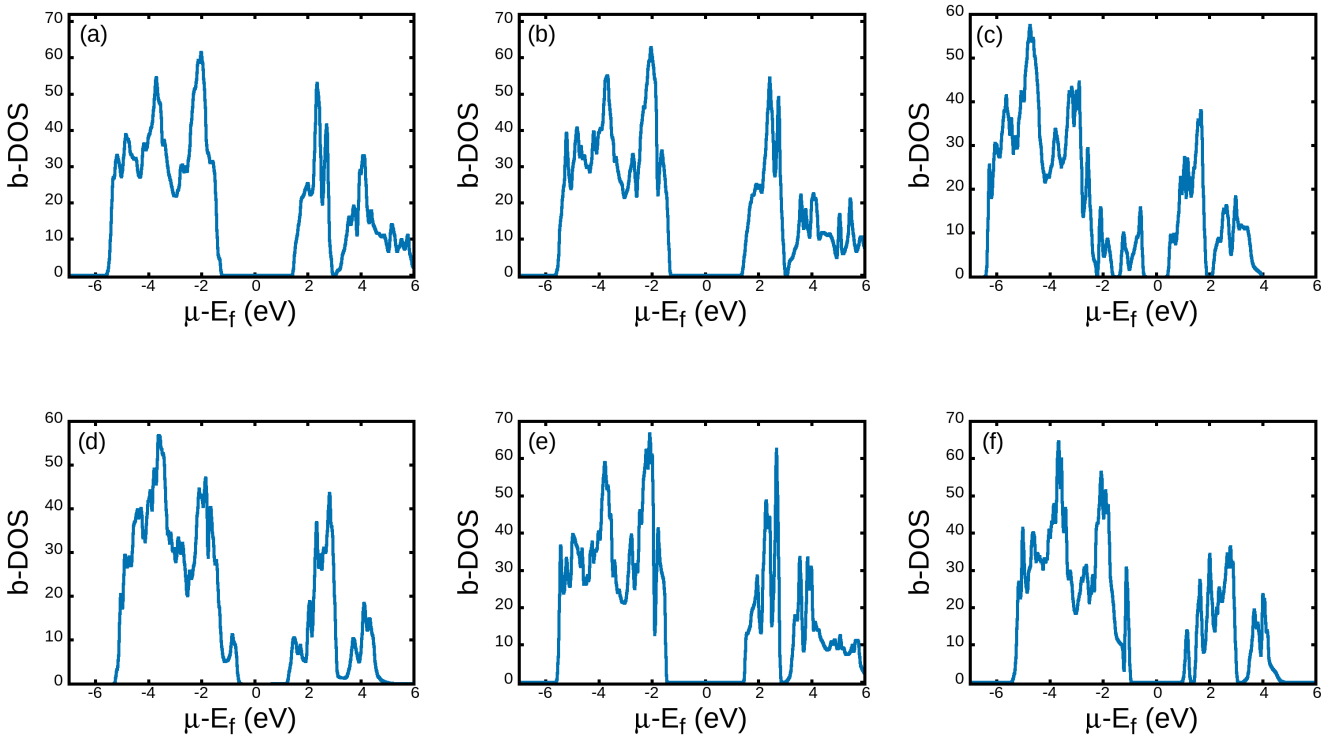

Fig. S. 1 Transport total density of state of BCZT for (a) a6 (b) a7 (c) p6 (d) p7 (e) r6 and (f) r7.

Table S. V Electrical and thermal conductivity of BCZT.

	σ ($\times 10^5 \Omega^{-1} m^{-1}$)						κ ($W m^{-1} K^{-1}$)					
Temperature	300 K		600 K		1000 K		300 K		600		1000 K	
Structures	VB	CB	VB	CB	VB	CB	VB	CB	VB	CB	VB	CB
a6	18.17	15.66	19.38	16.67	18.13	15.78	14.02	12.52	24.85	21.84	37.71	31.54
a7	20.5	18.97	19.67	18.45	18.26	17.55	14.16	13.83	24.59	24.46	36.92	33.64
p6	4.48	4.98	3.64	4.45	3.00	3.80	2.73	3.19	3.83	4.79	5.68	6.83
p7	10.97	67.40	9.94	64.30	9.76	58.43	7.25	47.23	13.58	79.63	21.42	99.96
r6	25.09	21.29	24.06	20.45	22.96	19.55	17.77	15.01	32.46	28.39	51.75	43.48
r7	12.99	7.17	12.40	6.83	12.02	6.14	6.12	3.48	14.38	7.03	23.67	12.96

Table S. VI Seebeck coefficient(mVK^{-1}) of BCZT.

S	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K
a6	3.10	3.10	2.75	2.27	1.94	1.70	1.50	1.35
a7	3.09	3.09	2.75	2.26	1.93	1.69	1.49	1.34
p6	1.54	1.16	0.92	0.76	0.65	0.56	0.50	0.40
p7	2.16	1.65	1.34	1.14	0.97	0.88	0.80	0.73
r6	3.1	3.1	2.98	2.41	2.05	1.79	1.58	1.41
r7	3.09	2.34	1.84	1.51	1.26	1.09	0.96	0.86

Table S. VII Power factor($\times 10^4 W m^{-1} K^{-2}$) of BCZT.

Structure	300 K	600 K	1000 K
a6	31.5	66.11	97.53
a7	35.28	70.88	93.26
p6	31.17	37.79	35.40
p7	10.90	35.05	48.73
r6	47.94	83.28	117.24
r7	25.53	32.76	26.87

Table S. VIII BEC Matrices (in e) for PBEsol pseudopotential in the order of a6, a7, p6, p7, r6, r7

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ba1	2.64816	2.77258	2.77974	-0.08170	0.07561	-0.04837	0.07051	-0.05249	0.11318
Ba2	2.63468	2.87952	2.62910	-0.06042	-0.06574	-0.06252	-0.06410	-0.06667	-0.05844
Ba3	2.78298	2.77519	2.64324	0.11446	-0.04556	0.07334	-0.04951	0.07590	-0.08531
Ba4	2.77866	2.77590	2.64398	0.11639	-0.04997	0.07105	-0.05097	0.07469	-0.08562
Ba5	2.62796	2.87715	2.63409	-0.05953	-0.06439	-0.06254	-0.06560	-0.06229	-0.06264
Ba6	2.64642	2.76900	2.77966	-0.08422	0.07327	-0.04514	0.07544	-0.05236	0.11817
Ti1	6.08805	5.33159	6.07329	0.06822	-0.10816	0.44221	0.44045	-0.10167	0.06682
Ti2	5.84662	4.77052	5.77181	-0.06863	0.06814	-0.08142	0.52804	0.11349	0.64651
Ti3	5.80452	4.76864	5.85366	0.64320	0.11127	0.51792	-0.08738	0.06550	-0.07547
Ti4	5.79791	4.76855	5.84119	0.64182	0.11681	0.52255	-0.08809	0.05474	-0.07839
Ti5	6.09829	5.32334	6.09326	0.06211	-0.09282	0.43954	0.44335	-0.10263	0.06212
Ti6	5.85975	4.77335	5.79612	-0.07225	0.05162	-0.08492	0.52041	0.12185	0.64959
O1	-4.66283	-1.80679	-1.96636	-0.09897	0.03464	-0.32792	-0.00944	0.12596	0.03300
O2	-4.85770	-1.84352	-2.13091	-0.11690	0.08518	-0.10170	-0.01438	0.13564	-0.02078
O3	-5.10855	-1.86748	-1.90242	0.10154	-0.11142	0.16489	-0.04853	-0.17372	-0.05243
O4	-5.10779	-1.76395	-1.76432	-0.28341	-0.10395	-0.41321	0.10773	-0.06801	0.12638
O5	-5.10284	-1.76418	-1.76104	-0.27989	-0.11087	-0.41519	0.10506	-0.06729	0.12317
O6	-5.09225	-1.87199	-1.90611	0.09964	-0.11228	0.15962	-0.04258	-0.17642	-0.04461
O7	-4.85702	-1.84201	-2.14106	-0.11957	0.08359	-0.10569	-0.01065	0.13693	-0.01640
O8	-4.66662	-1.80453	-1.97450	-0.09722	0.02126	-0.32340	-0.01511	0.11273	0.02767
O9	-1.82578	-4.74834	-1.82587	-0.22125	0.09530	-0.16859	-0.17361	0.09562	-0.23012
O10	-1.72631	-4.03221	-1.68538	-0.14616	-0.10683	-0.06746	-0.09583	-0.12382	-0.30774
O11	-1.95474	-4.29067	-1.95162	-0.03815	0.10476	0.07092	0.06598	0.10676	-0.04397
O12	-1.68698	-4.03191	-1.72445	-0.30351	-0.12501	-0.09626	-0.06105	-0.10910	-0.14287
O13	-1.68710	-4.03195	-1.72406	-0.30804	-0.12858	-0.09962	-0.06061	-0.11197	-0.14480
O14	-1.94992	-4.29227	-1.94830	-0.03594	0.10388	0.07234	0.07289	0.10435	-0.04106
O15	-1.72689	-4.03382	-1.68819	-0.14326	-0.10765	-0.06435	-0.09554	-0.12526	-0.30082
O16	-1.82316	-4.73055	-1.82543	-0.22173	0.09178	-0.17260	-0.18158	0.09211	-0.23366
O17	-1.96955	-1.80416	-4.64862	0.03024	0.12146	-0.01091	-0.32304	0.02685	-0.09540
O18	-1.76151	-1.76453	-5.09035	0.12362	-0.07291	0.10651	-0.41623	-0.10922	-0.28212
O19	-1.90732	-1.86987	-5.10033	-0.04587	-0.17374	-0.04308	0.16679	-0.11090	0.10386
O20	-2.13799	-1.84539	-4.85490	-0.01933	0.12852	-0.01250	-0.10032	0.07868	-0.11636
O21	-2.13695	-1.84734	-4.84807	-0.01799	0.13471	-0.01181	-0.09775	0.08246	-0.11364
O22	-1.90515	-1.87068	-5.09375	-0.05224	-0.17431	-0.04825	0.16363	-0.11000	0.10200
O23	-1.76586	-1.76859	-5.10210	0.11550	-0.07366	0.09899	-0.40909	-0.10987	-0.28155
O24	-1.97452	-1.80088	-4.66084	0.03321	0.11851	-0.00798	-0.31683	0.03351	-0.09027
Ca1	2.55783	2.53949	2.56206	0.09333	0.13310	0.03977	0.03325	0.13138	0.08693
Ca2	2.56139	2.54603	2.55948	0.09239	0.13377	0.04163	0.03749	0.13616	0.09112
Zr1	6.33439	5.83851	6.33271	0.32159	-0.02048	0.02863	0.02493	-0.03969	0.32715
Zr2	6.32770	5.81823	6.32558	0.31893	-0.03884	0.02551	0.02186	-0.03195	0.32680

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ba1	2.78450	2.70560	2.70258	0.06107	-0.01308	-0.04869	0.11637	-0.01599	0.10263
Ba2	2.73275	2.75184	2.70522	0.05579	0.01666	-0.03504	-0.06955	-0.01460	0.04285
Ba3	2.78239	2.78252	2.66134	-0.00979	-0.04371	-0.01016	0.04316	0.05428	-0.05354
Ba4	2.75204	2.75567	2.66032	0.13073	0.02444	0.13056	-0.02428	0.00415	-0.00380
Ba5	2.70492	2.78535	2.70260	-0.04895	-0.11664	0.05960	0.01159	-0.10257	0.01525
Ba6	2.75124	2.73309	2.70527	-0.03446	0.06934	0.05609	-0.01630	-0.04272	0.01437
Ti1	5.53461	6.03849	6.07251	0.03498	-0.44885	0.21535	0.16156	-0.41115	0.02098
Ti2	5.57075	5.52603	6.06228	0.50004	-0.41075	0.44420	0.31631	-0.32120	0.32143
Ti3	5.38454	5.39537	5.96737	0.61833	0.05529	0.61715	-0.05832	0.02743	-0.02805
Ti4	5.37529	5.38950	6.13357	0.57881	-0.17426	0.57406	0.17069	-0.09557	0.09534
Ti5	5.46611	5.47397	6.09363	0.54168	-0.24436	0.53896	0.24011	-0.42749	0.42239
Ti6	6.03580	5.53812	6.07402	0.22353	-0.16848	0.03577	0.44647	-0.02367	0.41162
Ti7	5.51445	5.58215	6.06045	0.44782	-0.32026	0.49384	0.40455	-0.32426	0.31780
O1	-4.56335	-1.76465	-1.91853	-0.05412	0.08201	-0.21046	0.06055	0.23839	0.08106
O2	-4.49108	-1.86590	-1.98919	-0.23050	0.25811	-0.36503	-0.00303	0.33428	-0.00924
O3	-5.10457	-1.93709	-1.92060	0.03297	-0.04988	0.03328	-0.10387	-0.05309	-0.10452
O4	-4.67333	-1.81701	-1.72848	-0.25324	-0.05393	-0.47163	0.11657	0.02255	0.11233
O5	-4.52771	-1.73989	-1.84306	-0.26820	0.00772	-0.46832	0.11085	0.11460	0.12771
O6	-4.66399	-1.76692	-1.80253	-0.21488	0.09243	-0.44939	-0.07570	0.26144	-0.07940
O7	-4.94812	-1.94463	-2.04383	-0.20598	0.18969	-0.22341	-0.05042	0.21989	-0.04602
O8	-4.39080	-1.88191	-1.84517	-0.23201	0.05170	-0.42506	0.05141	0.20686	0.06297
O9	-1.94016	-4.95259	-2.04348	-0.19412	0.05194	-0.17233	-0.18730	0.04825	-0.21987
O10	-1.87469	-4.39727	-1.84488	-0.40103	-0.05100	-0.20329	-0.05128	-0.06085	-0.20775
O11	-1.93809	-5.10345	-1.92027	0.06433	0.10301	0.06781	0.05291	0.10428	0.05353
O12	-1.80950	-4.68045	-1.72813	-0.44408	-0.11740	-0.22098	0.05343	-0.11197	-0.02383
O13	-1.73241	-4.53488	-1.84268	-0.44086	-0.11126	-0.23726	-0.00771	-0.12648	-0.11654
O14	-1.76007	-4.66981	-1.80225	-0.42133	0.07641	-0.18271	-0.09000	0.08220	-0.26109
O15	-1.76159	-4.56553	-1.91835	-0.18309	-0.05976	-0.02313	-0.08137	-0.07839	-0.23966
O16	-1.86002	-4.49773	-1.98895	-0.33989	0.00552	-0.20126	-0.25656	0.01299	-0.33464
O17	-1.88840	-1.74665	-5.03873	0.09887	0.34537	0.06671	-0.07669	0.18090	0.04251
O18	-1.81867	-1.82973	-4.91446	0.09576	0.27099	0.07972	-0.30821	0.07917	-0.19178
O19	-1.88614	-1.88799	-5.22981	-0.07318	-0.17325	-0.07346	0.17199	-0.12215	0.12067
O20	-2.03295	-2.03308	-4.91433	0.00448	0.14845	0.00424	-0.14596	0.13436	-0.13304
O21	-1.99075	-1.99037	-4.79581	0.03454	0.13925	0.03440	-0.13691	0.10983	-0.10894
O22	-1.79520	-1.79659	-5.23363	-0.04839	0.19302	-0.04854	-0.18986	0.11375	-0.11272
O23	-1.74815	-1.88721	-5.03912	0.06796	0.08094	0.09985	-0.34340	-0.04105	-0.18142
O24	-1.83124	-1.81742	-4.91446	0.07970	0.31172	0.09550	-0.26701	0.19214	-0.07752
Ca1	2.63384	2.63638	2.60261	0.08999	0.05701	0.08930	-0.05675	0.01626	-0.01569
Ca2	2.58416	2.58849	2.60769	0.16847	-0.03901	0.16771	0.03852	-0.01028	0.01058
Zr1	6.42361	6.42619	6.44923	0.16825	-0.03514	0.16608	0.03343	-0.17453	0.17304

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ca1	2.51606	2.51617	2.78804	0.09118	-0.06972	0.09118	-0.06976	0.00425	0.00425
Zr1	5.86368	5.86358	4.61136	-0.08453	-0.50473	-0.08453	-0.50503	-0.10889	-0.10896
O1	-1.82723	-1.82705	-3.30445	0.14876	-0.07822	0.14876	-0.07827	-0.16702	-0.16712
O2	-2.06474	-4.66303	-1.70127	0.15529	0.06495	0.08951	0.16370	-0.00464	0.14024
O3	-4.66318	-2.06459	-1.70127	0.08796	0.16366	0.15374	0.06505	0.14024	-0.00455
Ba1	2.49118	2.49113	3.20751	-0.04407	0.06277	-0.04407	0.06281	0.05388	0.05391
Ti1	5.68067	5.68061	3.70648	-0.04912	0.19173	-0.04912	0.19185	-0.25794	-0.25809
O4	-1.59786	-1.59775	-3.61366	0.08726	0.29201	0.08726	0.29218	0.17505	0.17516
O5	-1.78343	-4.74650	-1.83501	-0.03949	-0.10973	-0.05140	0.21323	-0.01080	0.28489
O6	-4.74644	-1.78348	-1.83501	-0.05317	0.21330	-0.04126	-0.10960	0.28489	-0.01063
Ba2	2.81081	2.50854	2.91479	-0.06551	-0.08743	0.05654	0.04635	-0.01019	0.01019
Ti2	5.56792	5.33226	3.81879	0.05250	-0.80730	-0.00077	0.31018	-0.43538	0.10100
O7	-1.52233	-1.57076	-3.24607	-0.15592	0.09944	-0.11405	0.29093	-0.10034	0.22670
O8	-1.98993	-4.56080	-1.94646	-0.10007	-0.05225	-0.05284	-0.15417	-0.10744	-0.15413
O9	-4.53747	-1.90800	-1.70175	0.01292	0.24718	0.06794	-0.12003	0.35369	0.00630
Ba3	2.50885	2.81067	2.91497	0.05625	0.04641	-0.06576	-0.08731	0.01018	-0.00991
Ti3	5.33162	5.56759	3.81872	-0.00118	0.31123	0.05188	-0.80722	0.10185	-0.43555
O10	-1.57069	-1.52232	-3.24589	-0.11408	0.29083	-0.15600	0.10009	0.22673	-0.09978
O11	-1.90806	-4.53693	-1.70195	0.06955	-0.12048	0.01452	0.24744	0.00592	0.35402
O12	-4.55961	-1.99022	-1.94690	-0.05435	-0.15408	-0.10161	-0.05219	-0.15405	-0.10745
Ba4	2.50854	2.81081	2.91479	0.05636	0.04640	-0.06569	-0.08740	0.01019	-0.01018
Ti4	5.33223	5.56795	3.81879	-0.00091	0.31066	0.05236	-0.80712	0.10126	-0.43532
O13	-1.57060	-1.52249	-3.24607	-0.11408	0.29087	-0.15595	0.09961	0.22676	-0.10021
O14	-1.90805	-4.53742	-1.70175	0.06951	-0.12018	0.01449	0.24711	0.00609	0.35369
O15	-4.56071	-1.99002	-1.94646	-0.05437	-0.15414	-0.10161	-0.05234	-0.15406	-0.10753
Ba5	2.81068	2.50885	2.91497	-0.06558	-0.08733	0.05643	0.04635	-0.00991	0.01017
Ti5	5.56756	5.33165	3.81872	0.05202	-0.80741	-0.00104	0.31075	-0.43561	0.10159
O16	-1.52216	-1.57085	-3.24589	-0.15597	0.09992	-0.11406	0.29089	-0.09991	0.22667
O17	-1.99013	-4.55970	-1.94690	-0.10008	-0.05210	-0.05282	-0.15411	-0.10736	-0.15412
O18	-4.53698	-1.90801	-1.70195	0.01295	0.24751	0.06798	-0.12033	0.35401	0.00614
Ba6	2.49121	2.49116	3.20715	-0.04398	0.06293	-0.04398	0.06297	0.05399	0.05402
Ti6	5.68074	5.68068	3.70606	-0.04944	0.19222	-0.04944	0.19233	-0.25784	-0.25799
O19	-1.59783	-1.59773	-3.61357	0.08693	0.29227	0.08693	0.29245	0.17542	0.17552
O20	-1.78364	-4.74639	-1.83530	-0.03959	-0.10923	-0.05117	0.21297	-0.01042	0.28462
O21	-4.74633	-1.78370	-1.83530	-0.05293	0.21303	-0.04136	-0.10911	0.28463	-0.01025
Ca2	2.51609	2.51620	2.78825	0.09125	-0.06997	0.09125	-0.07001	0.00365	0.00365
Zr2	5.86410	5.86400	4.60998	-0.08422	-0.50510	-0.08422	-0.50541	-0.10952	-0.10959
O22	-1.82710	-1.82693	-3.30390	0.14832	-0.07848	0.14832	-0.07853	-0.16707	-0.16717
O23	-2.06447	-4.66285	-1.70129	0.15552	0.06488	0.08965	0.16371	-0.00460	0.14031
O24	-4.66299	-2.06433	-1.70129	0.08810	0.16367	0.15397	0.06498	0.14031	-0.00452

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ca1	2.47087	2.47085	2.90667	-0.01868	-0.08749	-0.01868	-0.08752	-0.00301	-0.00301
Zr1	5.86108	5.86107	4.18442	-0.01572	-0.49125	-0.01572	-0.49142	-0.10397	-0.10400
O1	-1.78063	-1.78054	-3.21156	0.14279	-0.10924	0.14279	-0.10928	-0.14889	-0.14894
O2	-2.05338	-4.73489	-1.64330	0.05648	0.09796	0.02066	0.10612	-0.02403	0.05800
O3	-4.73492	-2.05335	-1.64330	0.01973	0.10608	0.05555	0.09799	0.05800	-0.02401
Ba1	2.46355	2.46355	3.27877	-0.00079	0.03345	-0.00079	0.03346	0.09175	0.09178
Ti1	5.90232	5.90229	3.63482	-0.03683	0.29352	-0.03683	0.29362	-0.14301	-0.14306
O4	-1.59995	-1.59987	-3.34397	0.11595	0.26892	0.11595	0.26901	0.18708	0.18714
O5	-1.92039	-4.82873	-1.85749	-0.00322	-0.14316	-0.00165	0.20896	0.00785	0.25479
O6	-4.82873	-1.92039	-1.85749	-0.00266	0.20901	-0.00423	-0.14308	0.25479	0.00794
Ba2	2.76415	2.47682	3.01211	0.00364	-0.03408	0.04510	0.03323	0.02930	-0.01752
Ti2	6.03594	5.44126	3.68798	0.03255	-0.67171	0.00246	0.40099	-0.24062	0.17909
O7	-1.59809	-1.55324	-3.23779	-0.14359	-0.01500	-0.11959	0.22038	-0.12447	0.17403
O8	-2.02794	-4.55914	-1.98265	-0.06262	0.02373	-0.01920	-0.14303	-0.09233	-0.15405
O9	-4.82995	-1.94183	-1.66582	-0.01529	0.12825	-0.01504	-0.08864	0.13507	0.01145
Ba3	2.48867	2.75147	2.97130	-0.00601	-0.00236	-0.03488	-0.06670	0.05389	-0.04967
Ti3	5.79291	5.76201	3.59835	-0.06343	0.27799	-0.09374	-0.72415	-0.06962	-0.38953
O10	-1.59149	-1.50312	-3.12980	-0.12523	0.28400	-0.14475	-0.01783	0.20994	-0.14145
O11	-1.98024	-4.82408	-1.63318	0.06430	-0.14749	0.01974	0.13588	0.00991	0.22149
O12	-4.82738	-1.93605	-1.84314	0.06619	0.16374	0.09261	-0.04993	0.20002	-0.08918
Ba4	2.47680	2.76417	3.01211	0.04500	0.03324	0.00354	-0.03407	-0.01753	0.02929
Ti4	5.44124	6.03596	3.68798	0.00226	0.40123	0.03234	-0.67157	0.17917	-0.24055
O13	-1.55314	-1.59818	-3.23779	-0.11957	0.22038	-0.14357	-0.01492	0.17407	-0.12441
O14	-1.94182	-4.82996	-1.66582	-0.01403	-0.08868	-0.01429	0.12822	0.01141	0.13507
O15	-4.55911	-2.02797	-1.98265	-0.02008	-0.14304	-0.06350	0.02368	-0.15402	-0.09238
Ba5	2.75148	2.48866	2.97130	-0.03479	-0.06670	-0.00592	-0.00238	-0.04969	0.05387
Ti5	5.76206	5.79286	3.59835	-0.09376	-0.72425	-0.06344	0.27774	-0.38950	-0.06975
O16	-1.50303	-1.59158	-3.12980	-0.14472	-0.01793	-0.12520	0.28399	-0.14152	0.20989
O17	-1.93611	-4.82733	-1.84314	0.09361	-0.04999	0.06719	0.16372	-0.08925	0.19999
O18	-4.82411	-1.98021	-1.63318	0.01875	0.13593	0.06331	-0.14744	0.22149	0.00998
Ba6	2.46339	2.46336	3.29544	-0.03855	0.03150	-0.03855	0.03151	-0.02971	-0.02972
Ti6	5.94995	5.94997	3.54875	0.02245	0.38014	0.02245	0.38027	0.02880	0.02881
O19	-1.57508	-1.57500	-3.24868	0.11927	0.20502	0.11927	0.20510	0.14093	0.14098
O20	-1.84989	-4.97075	-1.85969	-0.00561	-0.05954	-0.02112	0.07309	0.03299	0.07544
O21	-4.97074	-1.84990	-1.85969	-0.02221	0.07311	-0.00669	-0.05952	0.07542	0.03302
Ca2	2.47994	2.47998	2.85067	0.05810	-0.02614	0.05810	-0.02614	0.00128	0.00128
Ti7	5.75714	5.75698	3.78201	-0.22838	-0.63071	-0.22838	-0.63093	-0.34842	-0.34854
O22	-1.57386	-1.57376	-3.19547	0.14662	-0.01766	0.14662	-0.01767	-0.12073	-0.12077
O23	-2.03899	-4.76246	-1.65783	0.10803	0.06185	0.10097	0.09738	0.00665	0.18050
O24	-4.76253	-2.03892	-1.65783	0.10003	0.09736	0.10708	0.06188	0.18049	0.00672

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ca1	2.63929	2.64061	2.64316	-0.06353	-0.06266	-0.06364	-0.06204	-0.06231	-0.06109
Zr1	5.49546	5.50914	5.51995	-0.42372	-0.41799	-0.42428	-0.41230	-0.41796	-0.41156
O1	-1.83145	-4.39099	-1.83762	0.20002	0.04671	0.12186	0.15246	0.04767	0.22931
O2	-1.83135	-1.83264	-4.39539	0.04892	0.19944	0.04881	0.19616	0.12079	0.11856
O3	-4.38450	-1.83596	-1.83705	0.15526	0.15347	0.23401	0.04458	0.23102	0.04487
Ba1	2.74735	2.74990	2.69834	-0.10332	-0.05293	-0.10357	-0.05254	0.01207	0.01207
Ti1	4.82456	4.84748	5.10723	-0.74026	-0.31247	-0.73933	-0.30934	-0.43761	-0.43184
O4	-1.70586	-4.09577	-1.66390	0.51460	-0.15090	0.30704	0.15737	-0.13594	0.35650
O5	-1.90651	-1.90531	-4.32223	-0.04762	0.37686	-0.04774	0.37122	0.31573	0.31105
O6	-4.08290	-1.71690	-1.66336	0.33746	0.15541	0.54562	-0.15287	0.35481	-0.14018
Ba2	2.74749	2.69748	2.75095	-0.05401	-0.10285	0.01072	0.01259	-0.10356	-0.05139
Ti2	4.82662	5.09582	4.85437	-0.31913	-0.73562	-0.44787	-0.43331	-0.73448	-0.31126
O7	-1.90658	-4.31281	-1.91467	0.37553	-0.05236	0.31529	0.34280	-0.05152	0.40236
O8	-1.70587	-1.65760	-4.10217	-0.14415	0.51644	-0.13171	0.32457	0.30777	0.12476
O9	-4.08244	-1.66752	-1.71319	0.15965	0.33561	0.36184	-0.14113	0.54106	-0.15338
Ba3	2.69726	2.74796	2.75046	0.01143	0.01118	-0.05369	-0.10331	-0.05273	-0.10302
Ti3	5.08345	4.83677	4.85401	-0.45256	-0.44525	-0.32471	-0.72675	-0.32034	-0.72753
O10	-1.66111	-4.09161	-1.71325	0.33014	-0.13670	0.12821	0.33736	-0.14660	0.54292
O11	-1.66123	-1.70217	-4.10150	-0.13238	0.33253	-0.14473	0.51105	0.12951	0.30582
O12	-4.30179	-1.91617	-1.91447	0.34730	0.34286	0.40809	-0.05724	0.40262	-0.05683
Ba4	2.69718	2.74801	2.75060	0.01128	0.01119	-0.05375	-0.10335	-0.05292	-0.10314
Ti4	5.08351	4.83720	4.85434	-0.45389	-0.44607	-0.32598	-0.72654	-0.32004	-0.72690
O13	-1.66111	-4.09163	-1.71314	0.33027	-0.13644	0.12833	0.33727	-0.14639	0.54296
O14	-1.66120	-1.70205	-4.10147	-0.13214	0.33260	-0.14431	0.51105	0.12961	0.30587
O15	-4.30174	-1.91608	-1.91451	0.34736	0.34284	0.40816	-0.05725	0.40257	-0.05688
Ba5	2.74752	2.69746	2.75085	-0.05406	-0.10285	0.01069	0.01263	-0.10353	-0.05139
Ti5	4.82652	5.09540	4.85520	-0.31915	-0.73610	-0.44835	-0.43379	-0.73413	-0.31109
O16	-1.90654	-4.31284	-1.91475	0.37542	-0.05259	0.31508	0.34299	-0.05180	0.40243
O17	-1.70579	-1.65753	-4.10210	-0.14360	0.51642	-0.13121	0.32465	0.30766	0.12486
O18	-4.08279	-1.66768	-1.71320	0.15988	0.33583	0.36197	-0.14143	0.54131	-0.15370
Ba6	2.74733	2.74986	2.69842	-0.10337	-0.05303	-0.10354	-0.05259	0.01207	0.01202
Ti6	4.82512	4.84698	5.10649	-0.73964	-0.31389	-0.73927	-0.30745	-0.43851	-0.43203
O19	-1.70574	-4.09520	-1.66366	0.51434	-0.15044	0.30676	0.15722	-0.13561	0.35623
O20	-1.90657	-1.90529	-4.32211	-0.04752	0.37692	-0.04767	0.37133	0.31575	0.31111
O21	-4.08309	-1.71692	-1.66352	0.33790	0.15544	0.54584	-0.15285	0.35488	-0.14019
Ca2	2.63942	2.64064	2.64309	-0.06359	-0.06257	-0.06340	-0.06219	-0.06221	-0.06117
Zr2	5.49585	5.50925	5.51961	-0.42357	-0.41764	-0.42425	-0.41228	-0.41804	-0.41197
O22	-1.83151	-4.39096	-1.83744	0.19975	0.04656	0.12158	0.15270	0.04749	0.22964
O23	-1.83149	-1.83243	-4.39524	0.04925	0.19941	0.04910	0.19616	0.12074	0.11861
O24	-4.38477	-1.83590	-1.83713	0.15544	0.15364	0.23398	0.04438	0.23110	0.04459

Atom	xx	yy	zz	xy	xz	yx	yz	zx	zy
Ca1	2.63718	2.64041	2.64330	-0.09850	-0.09682	-0.09838	-0.09500	-0.09622	-0.09482
Zr1	5.58754	5.59984	5.61185	-0.43087	-0.42409	-0.43092	-0.41785	-0.42452	-0.41827
O1	-1.83376	-4.49212	-1.84064	0.18449	0.06022	0.10204	0.13943	0.06167	0.22047
O2	-1.83377	-1.83555	-4.49757	0.06274	0.18332	0.06287	0.18089	0.10061	0.09932
O3	-4.48754	-1.83903	-1.84088	0.14256	0.14050	0.22456	0.05824	0.22116	0.05833
Ba1	2.73942	2.74359	2.73440	-0.12867	-0.04394	-0.12844	-0.04310	-0.06479	-0.06392
Ti1	4.94542	4.96857	5.21415	-0.75097	-0.30812	-0.75077	-0.30254	-0.41824	-0.41277
O4	-1.75491	-4.22462	-1.65445	0.51325	-0.15843	0.28892	0.15223	-0.12707	0.33775
O5	-1.90542	-1.90429	-4.37535	-0.03600	0.37883	-0.03589	0.37327	0.32241	0.31766
O6	-4.21240	-1.76758	-1.65443	0.32661	0.15004	0.55056	-0.16098	0.33519	-0.13235
Ba2	2.73941	2.73284	2.74544	-0.04604	-0.12821	-0.06719	-0.06418	-0.12761	-0.04295
Ti2	4.94623	5.19920	4.97972	-0.31750	-0.74481	-0.43230	-0.41815	-0.74368	-0.30486
O7	-1.90527	-4.36396	-1.91500	0.37851	-0.04159	0.32264	0.35514	-0.04051	0.40979
O8	-1.75505	-1.64735	-4.23232	-0.15067	0.51536	-0.12264	0.29991	0.29008	0.11323
O9	-4.21247	-1.65861	-1.76298	0.15510	0.32402	0.34391	-0.13369	0.54512	-0.16216
Ba3	2.69863	2.76623	2.76675	-0.00465	-0.00466	-0.08137	-0.02274	-0.08017	-0.02282
Ti3	4.93391	4.94577	4.96609	-0.57770	-0.57089	-0.56316	-0.66174	-0.55495	-0.66217
O10	-1.72586	-4.11253	-1.71359	0.43913	-0.16214	0.21906	0.31116	-0.14723	0.51260
O11	-1.72607	-1.70215	-4.12452	-0.15546	0.44217	-0.14391	0.47683	0.22043	0.27486
O12	-4.05291	-1.87631	-1.87452	0.39424	0.38840	0.51403	-0.06437	0.50657	-0.06424
Ba4	2.73117	2.74139	2.74552	-0.06723	-0.06633	-0.04564	-0.12711	-0.04484	-0.12682
Ti4	5.18843	4.95692	4.97825	-0.43475	-0.42880	-0.31959	-0.73825	-0.31612	-0.74050
O13	-1.65151	-4.21877	-1.76311	0.30553	-0.12858	0.11585	0.32545	-0.15393	0.54710
O14	-1.65179	-1.75096	-4.23179	-0.12410	0.30774	-0.15226	0.51083	0.11749	0.28844
O15	-4.35346	-1.91644	-1.91469	0.35986	0.35411	0.41521	-0.04710	0.40827	-0.04674
Ba5	2.76480	2.70012	2.76664	-0.08269	-0.02281	-0.00562	-0.00429	-0.02399	-0.07992
Ti5	4.92811	4.94880	4.96561	-0.56282	-0.66915	-0.57647	-0.56157	-0.67001	-0.54336
O16	-1.86308	-4.06540	-1.87457	0.48108	-0.05860	0.36109	0.38947	-0.05653	0.50820
O17	-1.70667	-1.72127	-4.12532	-0.14423	0.48364	-0.15552	0.43473	0.27802	0.21623
O18	-4.10289	-1.73651	-1.71367	0.25540	0.30895	0.47481	-0.16688	0.51063	-0.15494
Ba6	2.76462	2.76543	2.70166	-0.02386	-0.08236	-0.02379	-0.08107	-0.00490	-0.00500
Ti6	4.92837	4.94805	4.96728	-0.67962	-0.55332	-0.67969	-0.54358	-0.56480	-0.55757
O19	-1.70649	-4.11413	-1.73177	0.48166	-0.15135	0.27608	0.25240	-0.15984	0.46963
O20	-1.86328	-1.86163	-4.07899	-0.05162	0.48220	-0.05137	0.47538	0.36142	0.35610
O21	-4.10311	-1.71845	-1.73192	0.31278	0.25029	0.51819	-0.15515	0.46668	-0.16715
Ca2	2.66049	2.66252	2.66472	-0.06299	-0.06210	-0.06279	-0.06102	-0.06170	-0.06056
Ti7	4.83487	4.85489	4.87375	-0.71550	-0.70364	-0.71507	-0.69373	-0.70450	-0.69392
O22	-1.71630	-4.20078	-1.72941	0.50097	0.01176	0.29558	0.32833	0.01501	0.52999
O23	-1.71625	-1.71694	-4.21411	0.01914	0.50059	0.01924	0.49343	0.29502	0.29080
O24	-4.18832	-1.72922	-1.72951	0.33338	0.32861	0.53814	0.00698	0.53034	0.00727