Supplemental information for Kohn, MJ *"A refined zirconium-in-rutile thermometer"*

Variance-covariance matrix for Experimental Model

	Intercept = b	a	c	d
b	1.10×10^{-1}	-9.65×10^{2}	-1.23×10^{-2}	5.81×10^{3}
a		9.02×10^{6}	7.78×10^{1}	-4.72×10^{7}
c			3.88×10^{-3}	-7.55×10^{2}
d				3.74×10^{8}

Variance-covariance matrix for Combined Model

	Intercept = b	a	c	d
b	3.87×10^{-2}	-3.45×10^{2}	1.68×10^{-4}	2.82×10^{3}
a		3.64×10^{6}	-2.80×10^{1}	-2.00×10^{7}
c			1.60×10^{-3}	-1.63×10^{2}
d				2.89×10^{8}

Variance-covariance matrix for Tomkins et al. (2007) (Roger Powell, pers. comm., 2019)

	Intercept = b	a	c
b	1.85×10^{-2}	-1.63×10^{2}	2.77×10^{-4}
a		1.69×10^{6}	-1.43×10^{1}
c			7.39×10^{-4}

Calibrations for the β-quartz stability field are:
Experimental:

$$T\,(°C) = \frac{70070 + 0.455 \cdot P(bars) - 0.114 \cdot c(ppm)}{131.17 - R \cdot ln[c(ppm)]} - 273.15$$

Combined:

$$T\,(°C) = \frac{72690 + 0.392 \cdot P(bars) - 0.130 \cdot c(ppm)}{132.06 - R \cdot ln[c(ppm)]} - 273.15$$

Supplemental Table S1: values of P, T, and X and their errors used in this study

Sample_ID	Reference	P (bars)	± (bars)	T (°C)	± (°C)	Zr (ppm)	±(ppm)	aQtz[†]	XZrO2	± (bracket error)	± (random error)	P-T method[§]
ATM-86	Tomkins et al. (2007)	1	0.001	1000	10			0.95	9.00E-03	5.00E-04	1.30E-03	Experiment
ATM-80	Tomkins et al. (2007)	1	0.001	1100	10			0.94	2.05E-02	5.00E-04	1.30E-03	Experiment
ATM-87	Tomkins et al. (2007)	1	0.001	1100	10			0.94	1.85E-02	5.0000E-04	1.30E-03	Experiment
ATM-49/68	Tomkins et al. (2007)	1	0.001	1200	10			0.92	3.30E-02	0.0000E+00	1.30E-03	Experiment
ATM-50/69	Tomkins et al. (2007)	1	0.001	1300	10			0.91	5.40E-02	3.0000E-03	1.30E-03	Experiment
ATM-52/67	Tomkins et al. (2007)	1	0.001	1400	10			0.90	8.10E-02	2.0000E-03	1.30E-03	Experiment
~~ATM-63/66~~[‡]	~~Tomkins et al. (2007)~~	~~1~~	~~0.001~~	~~1500~~	~~10~~			~~0.88~~	~~1.15E-01~~	~~1.00E-03~~	~~1.30E-03~~	Experiment
G459/506	Tomkins et al. (2007)	10000	500	1000	10			0.97	6.00E-03	2.00E-03	1.30E-03	Experiment
G464/511	Tomkins et al. (2007)	10000	500	1100	10			0.96	1.20E-02	2.00E-03	1.30E-03	Experiment
G462/522	Tomkins et al. (2007)	10000	500	1200	10			0.95	2.40E-02	2.00E-03	1.30E-03	Experiment
G457/473	Tomkins et al. (2007)	10000	500	1300	10			0.94	3.75E-02	1.50E-03	1.30E-03	Experiment
~~G463/472~~	~~Tomkins et al. (2007)~~	~~10000~~	~~500~~	~~1400~~	~~10~~			~~0.93~~	~~5.50E-02~~	~~0.00E+00~~	~~1.30E-03~~	~~Experiment~~
G500/564	Tomkins et al. (2007)	20000	500	1000	10			1.00	4.00E-03	0.00E+00	1.30E-03	Experiment
G501/566	Tomkins et al. (2007)	20000	500	1100	10			0.99	8.00E-03	1.00E-03	1.30E-03	Experiment
G502	Tomkins et al. (2007)	20000	500	1200	10			0.97	1.45E-02	1.50E-03	1.30E-03	Experiment
~~G503~~	~~Tomkins et al. (2007)~~	~~20000~~	~~500~~	~~1300~~	~~10~~			~~0.94~~	~~2.85E-02~~	~~1.50E-03~~	~~1.30E-03~~	~~Experiment~~
G499/579	Tomkins et al. (2007)	20000	500	1400	10			0.94	4.05E-02	5.50E-03	1.30E-03	Experiment
G626/627	Tomkins et al. (2007)	30000	500	1100	10			1.00	3.00E-03	0.00E+00	1.30E-03	Experiment
G624/625	Tomkins et al. (2007)	30000	500	1200	10			1.00	7.50E-03	5.00E-04	1.30E-03	Experiment
G620/621	Tomkins et al. (2007)	30000	500	1300	10			1.00	1.35E-02	5.00E-04	1.30E-03	Experiment
G618/619	Tomkins et al. (2007)	30000	500	1400	10			0.97	2.00E-02	0.00E+00	1.30E-03	Experiment
56b	Watson et al. (2006)	10000	500	925	10	3084	635	0.98	2.71E-03	0.00E+00	5.58E-04	Experiment
621	Watson et al. (2006)	14000	500	1000	10	5406	341	0.98	4.75E-03	0.00E+00	3.00E-04	Experiment
68a	Watson et al. (2006)	10000	500	950	10	4670	283	0.98	4.10E-03	0.00E+00	2.49E-04	Experiment
69a	Watson et al. (2006)	10000	500	875	10	2772	198	0.99	2.43E-03	0.00E+00	1.74E-04	Experiment
QTi13	Watson et al. (2006)	10000	500	800	10	1697	56	1.00	1.49E-03	0.00E+00	4.91E-05	Experiment
QTi14	Watson et al. (2006)	10000	500	675	10	504	167	1.00	4.42E-04	0.00E+00	1.46E-04	Experiment
QTi15	Watson et al. (2006)	10000	500	725	10	711	75	1.00	6.24E-04	0.00E+00	6.58E-05	Experiment
QS2b-2	Hofmann et al. (2013)	10000	500	1405	10			0.93	4.37E-02	0.00E+00	6.74E-04	Experiment
QS2d-1	Hofmann et al. (2013)	10000	500	1405	10			0.93	4.30E-02	0.00E+00	8.77E-04	Experiment
QS1a-1	Hofmann et al. (2013)	10000	500	1300	10			0.94	2.59E-02	0.00E+00	6.65E-04	Experiment
QS1c-1	Hofmann et al. (2013)	10000	500	1305	10			0.94	2.80E-02	0.00E+00	6.67E-04	Experiment
QS2a-1	Hofmann et al. (2013)	10000	500	1305	10			0.94	2.67E-02	0.00E+00	5.35E-04	Experiment
QS4a-1	Hofmann et al. (2013)	10000	500	1205	10			0.95	1.69E-02	0.00E+00	5.98E-04	Experiment
QS41-2	Hofmann et al. (2013)	10000	500	1205	10			0.95	1.68E-02	0.00E+00	6.62E-04	Experiment
Stillup Tal	Watson et al. (2006)	7500	1000	580	25	99	13	1.00	8.68E-05	0.00E+00	1.14E-05	GTB
Vermont	Watson et al. (2006)	3500	500	485	25	37	19	1.00	3.24E-05	0.00E+00	1.67E-05	GTB
unspecified	Baldwin et al. (2008)	28000	2000	680	80	245	69	0.92	2.15E-04	0.00E+00	6.05E-05	GTB
E1	Bukala et al. (2018)	29000	2000	702*	50	268	101	0.97	2.35E-04	0.00E+00	8.81E-05	GTB, ThMod
DB17	Cheng et al. (2009)	23000	2000	650	50	243	27	1.00	2.13E-04	0.00E+00	2.37E-05	GTB

JANW782	Chu et al. (2016)	14250	1000	710*	25	506	44	1.00	4.44E-04	0.00E+00	3.86E-05	ThMod
BU08-87	Corrie et al. (2012)	7500	1000	570	25	186	109	1.00	1.63E-04	0.00E+00	9.56E-05	GTB
Sifnos	Groppo et al. (2009) and Spear et al. (2006)	22000	2000	550	30	25	11	1.00	2.19E-05	0.00E+00	9.65E-06	ThMod
MK52	Hart et al. (2016)	10900	1800	549	32	48	7	1.00	4.21E-05	0.00E+00	6.14E-06	GTB
MK162	Hart et al. (2016)	14000	2400	613	72	97	24	1.00	8.51E-05	0.00E+00	2.10E-05	GTB
D167	Hernandez-Uribe (2018)	31500	1000	710*	25	149	34	0.93	1.31E-04	0.00E+00	2.98E-05	GTB
D161B	Hernandez-Uribe (2018)	24500	1000	630	30	96	40	1.00	8.42E-05	0.00E+00	3.51E-05	GTB
K28	Iaccarino et al. (2015)	11400	2100	722*	34	530	30	1.00	4.65E-04	0.00E+00	2.63E-05	ThMod
E-1a	Kim et al. (2019)	26000	3000	720*	80	182	30	1.00	1.60E-04	0.00E+00	2.63E-05	GTB/ThMod
E-1c	Kim et al. (2019)	26000	3000	720*	80	191	42	1.00	1.67E-04	0.00E+00	3.68E-05	GTB/ThMod
LT01-78b	Kohn (2008)	11500	1000	600	50	190	27	1.00	1.67E-04	0.00E+00	2.37E-05	GTB
LT01-66b	Kohn (2008)	10000	1000	650	50	319	48	1.00	2.80E-04	0.00E+00	4.21E-05	GTB
LT01-34	Kohn (2008)	10500	1000	700	50	495	37	1.00	4.34E-04	0.00E+00	3.25E-05	GTB
LT01-74	Kohn (2008)	10500	1000	700	50	411	60	1.00	3.60E-04	0.00E+00	5.26E-05	GTB
LT01-75a	Kohn (2008)	10500	1000	700	50	389	66	1.00	3.41E-04	0.00E+00	5.79E-05	GTB
LT01-75c	Kohn (2008)	10500	1000	700	50	308	65	1.00	2.70E-04	0.00E+00	5.70E-05	GTB
23085	Li and Massonne (2018)	10700	1400	596	25	115	44	1.00	1.01E-04	0.00E+00	3.86E-05	ThMod
23098	Li and Massonne (2018)	8500	700	629	25	199	44	1.00	1.75E-04	0.00E+00	3.86E-05	ThMod
130893	Li et al. (2017)	24400	2000	597	50	133	88	1.00	1.16E-04	0.00E+00	7.67E-05	ThMod
18193	Li et al. (2017)	19400	2000	597	50	148	43	1.00	1.29E-04	0.00E+00	3.73E-05	ThMod
Sp96-41a	Li et al. (2017)	23800	2000	653	50	145	95	1.00	1.27E-04	0.00E+00	8.33E-05	ThMod
Sp96-41b	Li et al. (2017)	17200	2000	680	50	140	110	1.00	1.23E-04	0.00E+00	9.65E-05	ThMod
18195	Li et al. (2017)	24500	2000	645	50	185	70	1.00	1.62E-04	0.00E+00	6.14E-05	ThMod
CH56	Maldonado et al. (2017)	22000	1000	600	50	161	43	1.00	1.41E-04	0.00E+00	3.73E-05	ThMod
CH9	Maldonado et al. (2017)	23000	1000	640	50	255	40	1.00	2.24E-04	0.00E+00	3.51E-05	ThMod
22	Mottram et al. (2014)	9000	1000	650	25	435	25	1.00	3.81E-04	0.00E+00	2.19E-05	ThMod
MN14A	Scodina et al. (2019)	14000	1000	715*	25	426	88	1.00	3.74E-04	0.00E+00	7.72E-05	ThMod
unspecified	Smit et al. (2008)	25500	2500	620	35	185	68	1.00	1.62E-04	0.00E+00	5.96E-05	GTB
multiple	Taetz et al. (2016)	23000	4000	550	50	70	20	1.00	6.14E-05	0.00E+00	1.75E-05	GTB/ThMod
NL01	Wang et al. (2015)	9900	800	652	25	267	100	1.00	2.34E-04	0.00E+00	8.77E-05	GTB/ThMod
L11	Wang et al. (2015)	12400	800	673	25	290	90	1.00	2.54E-04	0.00E+00	7.89E-05	GTB/ThMod
N24	Wang et al. (2015)	7300	800	639	25	378	133	1.00	3.32E-04	0.00E+00	1.17E-04	GTB/ThMod
N18	Wang et al. (2015)	6100	800	651	25	525	238	1.00	4.60E-04	0.00E+00	2.09E-04	GTB/ThMod
Y1366	Wang et al. (2018)	8900	500	660	25	305	55	1.00	2.67E-04	0.00E+00	4.82E-05	GTB/ThMod
Y1379	Wang et al. (2018)	8900	500	645	25	305	58	1.00	2.67E-04	0.00E+00	5.09E-05	GTB/ThMod
unspecified	Whitney et al. (2015)	14000	1000	725*	25	450	50	1.00	3.95E-04	0.00E+00	4.39E-05	GTB/ThMod
eclxeno	Xu et al. (2018)	26500	1500	660	25	162	12	1.00	1.42E-04	0.00E+00	1.05E-05	ThMod
Syros-SY-14	Zack et al. (2004)	18000	1000	480	50	47	12	1.00	4.12E-05	0.00E+00	1.07E-05	GTB
Syros-SY-4	Zack et al. (2004)	18000	1000	480	50	34	10	1.00	2.98E-05	0.00E+00	8.94E-06	GTB
CHM200	Zack et al. (2004)	18000	1000	600	50	112	34	1.00	9.82E-05	0.00E+00	2.95E-05	ThMod
Z6-50-13	Zack et al. (2004)	20000	1000	650	50	165	13	1.00	1.45E-04	0.00E+00	1.16E-05	ThMod
Z6-50-2	Zack et al. (2004)	20000	1000	650	50	146	50	1.00	1.28E-04	0.00E+00	4.35E-05	ThMod

Z8-59-4	Zack et al. (2004)	20000	1000	650	50	154	12	1.00	1.35E-04	0.00E+00	1.08E-05	ThMod
H713-4	Zhang et al. (2010)	25500	1500	490	25	14	5	1.00	1.23E-05	0.00E+00	4.38E-06	GTB
4Y07	Zhang et al. (2010)	30000	2000	652	25	106	40	0.94	9.29E-05	0.00E+00	3.51E-05	GTB
4Y18	Zhang et al. (2010)	30500	1500	590	25	68	11	0.92	5.96E-05	0.00E+00	9.65E-06	GTB
7X2-5	Zhang et al. (2010)	15000	1000	635	25	282	84	1.00	2.47E-04	0.00E+00	7.37E-05	GTB
7X23-1	Zhang et al. (2010)	15000	1000	635	25	228	79	1.00	2.00E-04	0.00E+00	6.93E-05	GTB
7X14-13	Zhang et al. (2010)	15000	1000	635	25	337	111	1.00	2.96E-04	0.00E+00	9.73E-05	GTB
8S57	Zhang et al. (2010)	30500	1500	659	28	144	10	0.93	1.26E-04	0.00E+00	8.77E-06	GTB
8S106	Zhang et al. (2010)	29750	2750	700	30	389	65	0.96	3.41E-04	0.00E+00	5.70E-05	GTB
2D06	Zhang et al. (2010)	30500	3500	655	56	75	22	0.93	6.58E-05	0.00E+00	1.93E-05	GTB
4C48	Zhang et al. (2010)	27000	2000	645	50	101	36	0.99	8.86E-05	0.00E+00	3.16E-05	GTB
2Q27	Zhang et al. (2010)	25900	2000	508	50	45	29	0.99	3.95E-05	0.00E+00	2.54E-05	GTB
11YM29	Zhang et al. (2014) and Song et al. (2003)	30500	1500	659	28	183	13	0.93	1.60E-04	0.00E+00	1.14E-05	GTB
HB121-8	Zhang et al. (2018)	30000	2000	552	25	15	5	0.92	1.32E-05	0.00E+00	4.38E-06	GTB
HB121-8	Zhang et al. (2018)	28000	2000	570	25	40	10	1.00	3.51E-05	0.00E+00	8.77E-06	GTB

‡Strikethroughs indicate reported experiments that were omitted from regressions because they were statistical outliers.

§GTB = geothermobarometry (calibrated specific equilibria, or multiequilibrium intersections); ThMod = thermodynamic modeling, e.g., mineral assemblage diagrams or “pseudosections”.

† Activity of α-quartz in the stability fields of other SiO_2 polymorphs, as calculated using the Berman and Aranovich (1996) thermodynamic compilation.

*Although the preferred temperature exceeds 700 °C, uncertainty limits allow T ≤700 °C.