Table S1. Summary of impurity-related paramagnetic centres in quartz

Centre T (K)	**g** Principal values	**g** Principal directions		Other Spin Hamiltonian Parameters	References
		θ°	φ°		
Atomic H, Ag, Cu and Li centres and other paramagnetic ions					
H^0 80	2.002266	132.8	270	**A**(^{1}H), **A**(^{29}Si)	Isoya *et al.* (1983)
	2.002228	90	0		
	2.002095	137.2	90		
Ag^0 20	1.99978	88.18	357.46	**A**(^{107}Ag), **A**(^{29}Si)	Davis and Weil (1978)
	1.99864	151.75	84.07		
	1.99244	61.92	88.43		
Cu^0 77	1.998	60	90	**A**(^{65}Cu), **A**(^{29}Si)	Amanis and Kliava (1977)
	2.000	150	90		
	2.000	90	0		
Li^0 35	2.001462	115.284	90	**A**(^{7}Li), **A**(^{29}Si)	Bailey and Weil (1991)
	2.000534	90	0		
	1.998795	154.716	270		
Cu^{2+} 77	2.420	65	90	**A**(^{65}Cu)	Solntsev *et al.* (1974)
	2.130	28	245		
	2.021	80	355		
Ni^+ 77	2.787	70	90		Solntsev *et al.* (1974)
	2.111	58	347		
	2.088	40	210		
Aluminum-related centres					
$[AlO_4]^0$ 35	2.060208	60.8	237.6	**A**(^{27}Al), **P** (^{27}Al)	Nuttall and Weil (1981a)
	2.008535	124.4	305.1		
	2.001948	131.6	177.5		
$[AlO_4/H]^0$ 35	2.056931	52.2	104.5	**A**(^{27}Al), **P** (^{27}Al), **A**(^{1}H)	Nuttall & Weil (1981b)
	2.008056	59.6	347.4		
	2.002495	127.4	50.8		
$[AlO_4/Li]^0$ 35	2.061016	51.7	101.5	**A**(^{27}Al), **P** (^{27}Al), **A**(^{7}Li)	Nuttall & Weil (1981b)
	2.008259	116.1	168.8		
	2.001957	130.5	53.9		
$[AlO_4/Na]^0$ 35	2.044143	126.7	97.9	**A**(^{27}Al), **P** (^{27}Al), **A**(^{23}Na), **P**(^{23}Na)	Dickson and Weil (1990)
	2.008591	113.4	168.9		
	2.002668	45.9	234.2		
$[AlO_4/Li]^q$ 15	2.055681	58.6	240.5	**A**(^{27}Al), **P**(^{27}Al), **A**(^{7}Li), **P**(^{7}Li)	Walsby *et al.* (2003)
	2.008643	127.9	302.0		
	2.002240	53.8	357.1		
$[AlO_4]^+$ 35 (*S*=1)	2.04722	131.6	270	**D**, **A**(^{29}Si), **A**(^{27}Al), **P**(^{27}Al)	Nuttall and Weil (1981c)
	2.01017	90	0		
	2.00291	138.4	90		
$[AlO_4/Ag]^0_I$	2.2667	111.5	242.6		Davis *et al.*

20	2.1020	155.1	51.7		(1978)
	2.0074	101.6	147.9		
$[AlO_4/Ag]^0_{II}$	2.2749	57.1	68.5		Davis *et al.*
20	2.1141	145.9	51.5		(1978)
	2.0061	97.7	153.4		
Germanium-related centres					
$[GeO_4]^-_I$	2.00174	45.69	17.34	**A**(^{73}Ge), **A**(^{17}O1),	McEachern and
50	2.00053	73.84	270.91	**A**(^{17}O2), **A**(^{17}O3),	Weil (1994)
	1.99349	48.76	166.19	**A**(^{17}O4)	
$[GeO_4]^-_{II}$	2.00080	68.97	90	**A**(^{73}Ge), **A**(^{17}O1),	McEachern and
50	2.00023	90	0	**A**(^{17}O2)	Weil (1994)
	1.99304	21.03	270		
$[GeO_4]^-_{av}$	2.0001	93.7	270	**A**(^{73}Ge)	Isoya *et al.*
or Ge(B)	1.9981	90	0		(1978)
220	1.9970	176.3	90		
$[GeO_4/H^-2Li^+]^0$	2.00091	114.1	52.4	**A**(^{73}Ge), **A**(^{1}H), **A**(^{7}Li1),	Weil (1971)
293	1.99726	69.0	331.9	**A**(^{7}Li2)	
	1.99292	32.9	98.3		
$[GeO_4/Li]^0_A$	2.00175	66.78	90	**A**(^{73}Ge), **A**(^{17}O1)	McEachern and
293	2.00008	90	0		Weil (1994)
	1.99089	23.22	270		
$[GeO_4/Li]^0_C$	2.00134	40.34	318.69	**A**(^{73}Ge), **A**(^{17}O1),	McEachern and
25	1.99947	85.49	54.02	**A**(^{17}O2), **A**(^{17}O3),	Weil (1994)
	1.99344	50.02	147.81	**A**(^{17}O4)	
$[GeO_4/Na]^0_A$	1.991581	156.7	270	**A**(^{73}Ge), **A**(^{23}Na),	Dickson *et al.*
293	1.999807	90	0	**P**(^{23}Na)	(1991)
	2.001152	113.3	90		
$[GeO_4/Na]^0_C$	1.99630	74.1	90	**A**(^{73}Ge), **A**(^{23}Na),	Dickson *et al.*
293	1.99728	90	0	**P**(^{23}Na)	(1991)
	2.00059	15.9	270		
$[GeO_4/Ag]^0$	2.0084	116.7	270	**A**(^{107}Ag), **A**(^{109}Ag)	Laman and Weil
293	2.0000	90	0		(1977)
	1.9884	153.3	90		
Iron-related centres					
$[FeO_4]^-$	2.00357	90	0	**D**, B_4^m	Mombourquette
293	2.00384	29.7	90		*et al.* (1986)
	2.00532	115.7	90		
$[FeO_4/H]^0_\alpha$	2.00402	115.9	17.5	**D**, B_4^m, **A**(^{1}H)	Mombourquette
20	2.00494	114.1	274.9		*et al.* (1989)
	2.00567	143.2	147.9		
$[FeO_4/H]^0_\beta$	2.00563	121	297	**D**, B_4^m, **A**(^{1}H)	Minge *et al.*
20	2.00413	78	214		(1989)
	2.00391	33	322		

$[FeO_4/Li]^0_\alpha$ 20	2.00426	90	180	**D**, B_4^m, **A**(^{7}Li)	Halliburton *et al.* (1989)
	2.00418	155.4	90		
	2.00360	65.4	90		
$[FeO_4/Li]^0_\beta$ 20	2.00537	98.8	143.8	**D**, B_4^m	Minge *et al.* (1989)
	2.00404	171.1	319.3		
	2.00303	90.7	53.6		
$[FeO_4/Na]^0_\alpha$ 20	2.0045	60.7	110.9	**D**, B_4^m	Minge *et al.* (1990)
	2.0043	118.4	38.6		
	2.0029	136.9	164.0		
Titanium-related centres					
$[TiO_4]^-$ 8	1.9932	19.95	90	**A**(^{49}Ti), **P**(^{49}Ti)	Bailey *et al.* (1992)
	1.9251	90	0		
	1.9195	70.05	270		
$[TiO_4/H]^0_A$ 20	1.9856	151.1	75.2	**A**(^{47}Ti), **A**(^{1}H)	Rinneberg and Weil (1972)
	1.9310	82.8	358.5		
	1.9151	62.1	92.3		
$[TiO_4/H]^0_B$ 20	1.990	86.6	87.7	**A**(^{1}H)	Rinneberg and Weil (1972)
	1.914	118.6	175.8		
	1.903	28.9	183.9		
$[TiO_4/Li]^0_A$ 35	1.97887	20.6	270	**A**(^{47}Ti), **A**(^{49}Ti), **A**(^{7}Li)	Isoya *et al.* (1988)
	1.93094	90	0		
	1.91193	69.4	90		
$[TiO_4/Li]^0_B$ 35	1.98022	108.6	270	**A**(^{49}Ti), **A**(^{7}Li)	Bailey and Weil (1992a)
	1.92977	90	0		
	1.91022	161.4	90		
$[TiO_4/Li]^0_\gamma$ 35	1.98056	62.69	95.56		Bailey and Weil (1992a)
	1.92711	102.21	179.14		
	1.86371	30.34	247.45		
$[TiO_4/Na]^0_A$ 35	1.89841	106.4	278.7	**A**(^{49}Ti), **A**(^{23}Na)	Bailey and Weil (1992b)
	1.95160	70.6	194.7		
	1.97046	154.1	151.2		
$[TiO_4/Na]^0_\beta$ 35	1.97863	74.62	218.51	**A**(^{49}Ti), **A**(^{23}Na), **P**(^{23}Na)	Bailey and Weil (1992a)
	1.92659	43.31	325.47		
	1.88128	50.76	115.53		
Phosphorus-related centres					
$[PO_4]^0_G$ 120	2.0012	90	0	**A**(^{31}P)	Uchida *et al*. (1979)
	2.0032	114.92	270		
	1.9991	155.08	90		
$[PO_4]^0_E$ 120	2.0013	79.194	270.50	**A**(^{31}P)	Uchida *et al*. (1979)
	2.0034	46.075	11.096		
	1.9991	45.939	169.86		
$[PO_4]^0_{AV}$ 290	2.0010	90	0	**A**(^{31}P)	Uchida *et al*. (1979)
	2.0025	117.08	90		
	2.0003	152.92	270		

$[O_3AlO^-PO_3]$ 300	2.0172	146.9	10.6	**A**(^{27}Al), **A**(^{31}P)	Maschmeyer and Lehmann (1983)
	2.0149	96.1	110.9		
	2.0105	131.6	204.5		
Hydrogarnet-like centres					
$[H_3O_4]^0$ 25	2.1351	135.5	263.3		Nuttall and Weil (1980)
	2.0047	60.5	322		
	1.9962	123.2	30.2		
$[H_4O_4]^+$ 25	2.0911	127.1	267.1		Nuttall and Weil (1980)
	2.0103	55.8	326.2		
	2.0002	124.5	28.4		
$[HLi_2O_4]^0$ 100	2.034377	115.1	70.6	**A**(^{1}H), **A**(^{7}Li1), **A**(^{7}Li2)	Lees *et al.* (2003)
	2.009657	128.4	182.3		
	2.002674	131.3	316.3		

Data in this table are updated from those in Mashkovtsev and Pan (2013) and Alessi *et al.* (2014).

Table S2. Summary of vacancy-related paramagnetic centres in quartz

Centre T (K)	**g** Principal values	**g** Principal directions θ°	 φ°	Other Spin Hamiltonian Parameters	References
***Oxygen-vacancy electron* centres (*E'*)**					
E'_1 293	2.00179 2.00053 2.00027	114.1 134.5 57.4	227.7 344.4 305.0	**A**(^{29}Si1), **A**(^{29}Si2), **A**(^{29}Si3)	Jani *et al.* (1983)
E'_2(I) 293	2.0020 2.0007 2.0005	59.9 67.2 140.7	28.4 132.5 73.3	**A**(^{29}Si), A(^{1}H)	Perlson and Weil (2008)
E'_2(II) 293	2.00161 2.00051 1.99994	45.7 129.1 109.8	72.2 109.8 2.7	**A**(^{29}Si), A(^{1}H)	Perlson and Weil (2008)
E'_3 293	2.0017 2.0007 2.0005	63.6 153.6 91.0	86.6 64.0 176.1		Perlson and Weil (2008)
E'_4 293	2.00154 2.00064 2.00059	46.3 120.6 120.8	66.2 10.7 121.4	**A**(^{29}Si1), **A**(^{29}Si2), A(^{1}H)	Isoya *et al.* (1981)
E'_9 293	2.00183 2.00079 2.00067	114 152 105	213 359 117	**A**(^{29}Si)	Mashkovtsev and Pan (2012a)
E'_{10} 293	2.00169 2.00041 2.00021	64.3 142 116	46.9 335 124	**A**(^{29}Si)	Mashkovtsev and Pan (2013)
E'_{11} 293	2.00164 2.00132 1.99938	107.3 156.9 104.6	22.5 245 117.2	**A**(^{29}Si), **A**(^{27}Al), **P**(^{27}Al)	Mashkovtsev *et al.* (2019)
E'_{12} 293	2.00171 2.00109 1.99997	144.5 64 67.8	256 209.1 311.1	**A**(^{29}Si)	Mashkovtsev and Pan (2016)
E'_{13} 293	2.00169 2.00071 2.00059	110.5 96 159	212 304 50	**A**(^{29}Si)	Mashkovtsev and Pan (2018)
E'_{14} 293	2.00573 2.00176 1..99704	74.3 40.5 53.8	338.5 87.7 236.7	**A**(^{29}Si)	Mashkovtsev *et al.* (2019)
E'_{16} 293	2.00277 2.00177 1.99896	149.3 75.8 116.5	117.5 52.8 330.1	**A**(^{29}Si), **A**(^{27}Al), **P**(^{27}Al)	Mashkovtsev *et al.* (2019)
Ge E'_1	2.00111	66.8	51.0	**A**(^{73}Ge), **P**(^{73}Ge), **A**(^{17}O1),	Mashokovtsev

293	1.99501	129.7	341.8	**A**(^{17}O2), **A**(^{17}O3), **A**(^{29}Si1), **A**(^{29}Si2)	*et al.* (2013)
	1.99399	131.3	118.8		
Ge E'_2 293	2.0009	131	208	**A**(^{1}H)	Feigl and Anderson (1970)
	1.9952	49	167		
	1.9943	68	277		
Ge(IV) 293	2.0010	114	49	**A**(^{73}Ge)	Feigl and Anderson (1970)
	1.9942	53	339		
	1.9935	47	114		

***Oxygen-vacancy electron* centres (*E''*)**

E''_1 293	2.00156	114.1	227.7	**D**, **A**(^{29}Si1), **A**(^{29}Si2)	Mashkovtsev *et al.* (2007)
	2.00081	134.5	344.4		
	2.00052	57.4	305.0		
E''_2 293	2.00133	136.3	162.1	**D**	Mashkovtsev and Pan (2011)
	2.00077	67.3	226.2		
	2.00056	125.0	299.2		
E''_3 293	2.00142	132	184	**D**, **A**(^{29}Si1), **A**(^{29}Si2)	Mashkovtsev and Pan (2013)
	2.00063	62	245		
	2.00061	125	313		
E''_4 293	2.00135	130	67	**D**	Mashkovtsev and Pan (2011)
	2.00078	95	333		
	2.00034	40	57		
E''_6 293	2.00144	114.1	304.1	**D**, **A**(^{29}Si1), **A**(^{29}Si2)	Mashkovtsev and Pan (2012b, 2013)
	2.00106	85.2	32.0		
	2.00044	155.3	111.5		
E''_7 293	2.00151	90.8	331.8	**D**, **A**(^{29}Si1), **A**(^{29}Si2)	Mashkovtsev and Pan (2012b, 2013)
	2.00079	151.1	63.3		
	2.00045	119.9	237.8		
E''_8 293	2.00178	119.9	237.8	**D**, **A**(^{29}Si1), **A**(^{29}Si2)	Mashkovtsev and Pan (2012b, 2013)
	2.00097	103.2	335.6		
	2.00060	33.2	266.5		
E''_9 300	2.00156	126.1	243.5	**D**, **A**(^{29}Si1), **A**(^{29}Si2), **A**(^{29}Si3), **A**(^{29}Si4), **A**(^{29}Si5)	Mashkovtsev and Pan (2014)
	2.00047	119	357		
	2.00025	50	295		

***Silicon-vacancy hole* centers (*H'*)**

H'_1 (#1, O_2^-) 110	2.02945	26.0	266.2	**A**(^{27}Al), **A**(^{29}Si)	Nilges *et al.* (2009)
	2.00765	64.0	91.2		
	2.00210	88.0	0.3		
H'_2(I) (B, O_2^-) 293	2.03505	22.1	172.6	**A**(^{27}Al)	Pan *et al.* (2008)
	2.00773	71.1	319.3		
	2.00234	78.6	5.32		
H'_2(II) (B', O_2^-) 293	2.03555	22.5	165.5	**A**(^{27}Al)	Pan *et al.* (2008)
	2.00771	69.5	319.5		
	2.00231	80.9	52.9		
H'_3(I)	2.04953	73.6	248.9	**A**(^{27}Al)	Pan *et al.*

(D, O_2^-)	2.00701	50.1	353.0		(2009)
115	2.00206	44.4	141.5		
H'_3(II)	2.05175	76.4	244.1	**A**(^{27}Al)	Pan *et al.*
(E, O_2^-)	2.00682	51.7	345.1		(2009)
115	2.00213	41.5	138.2		
H'_4(I)	2.03102	46.8	0.7	**A**(^{27}Al)	Nilges *et al.*
(G, O_2^-)	2.00809	84.2	265.2		(2008)
293	2.00238	43.7	169.2		
H'_4(II)	2.02925	46.8	0.7	**A**(^{27}Al)	Pan *et al*.
(G', O_2^-)	2.00809	84.2	265.2		(2008)
293	2.00238	43.7	169.2		
H'_5	2.06807	57.6	36.7		Pan *et al.*
(#6, O_2^{3-})	2.00732	69.5	293.1		(2008)
77	2.00187	39.7	176.5		
H'_6	2.05960	76.0	141.1		Pan *et al*.
(#7, O_2^{3-})	2.00759	22.1	13.6		(2008)
77	2.00179	73.0	235.4		
H'_7(I)	2.0183	26.7	270	**A**(^{27}Al)	Maschmeyer
(C, O_3^-)	2.0090	90	0		and Lehmann
293	2.0033	63.3	90		(1983)
H'_7(II)	2.01698	30.7	274.9	**A**(^{27}Al)	Pan *et al*.
(C', O_3^-)	2.00823	75.2	158.6		(2008)
293	2.00248	63.7	61.1		
H'_7(III)	2.0177	39.6	269.8		Botis *et al*.
(X, O_3^-)	2.0076	89.	0.4		(2008)
293	2.0029	50.3	90.8		

Data in this table are updated from those in Mashkovtsev and Pan (2013) and Alessi *et al*. (2014).

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