

## A genetic link between eclogitic and peridotitic diamond inclusions

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### Supplementary Information

The Supplementary Information includes:

- S1. Diamond Inclusion Database
- S2. Reaction Path Modelling and the Extended Deep Earth Water Model
- Tables S-1 to S-5
- Supplementary Information References

#### S1. Diamond Inclusion Database

The diamond inclusion database contains meta- and geochemical data for 9118 diamond inclusions including the major element data for olivine ( $n = 1334$ ), orthopyroxene ( $n = 446$ ), clinopyroxene ( $n = 926$ ), and garnet ( $n = 2628$ ) inclusions from lithospheric mantle diamonds sourced, primarily, from Stachel and Harris (2008 and references therein) supplemented with additional and more recent datasets (Gurney and Boyd, 1982; Gurney *et al.*, 1984; Viljoen *et al.*, 1999; Jacob *et al.*, 2000; Tappert *et al.*, 2005; De Stefano *et al.*, 2009; Sobolev *et al.*, 2009; Tappert *et al.*, 2009; Bulanova *et al.*, 2010; Dobosi and Kurat, 2010; Miller *et al.*, 2014; Mikhail *et al.*, 2019).

#### S2. Extended Deep Earth Water Model

The Extended Deep Earth Water Model (DEW) to calculate the apparent standard partial molal Gibbs free energies of aqueous species at high pressures and temperatures using the revised Helgeson-Kirkham-Flowers (HKF) equations of state for aqueous species (Shock and Helgeson, 1988; Shock *et al.*, 1997; Sverjensky *et al.*, 1997) calibrated with experimental solubilities of eclogite and peridotite (Huang and Sverjensky, 2019; Sverjensky, 2019). Equilibrium constants for aqueous complexes calculated using the DEW model were used in the aqueous speciation, solubility, and chemical mass transfer codes EQ3 and EQ6 (modified after Wolery,

1983, 1984, 1992 for elevated temperatures and pressures) as documented in Huang and Sverjensky (2019). Our aqueous speciation model also included a model for the variable activity of water and the activity coefficients of aqueous, neutral dissolved gases such as  $\text{H}_2\text{CO}_3$ ,  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{CO}$ , and  $\text{C}_2\text{H}_6$  as functions of the solute content of the fluid (Huang and Sverjensky, 2019).

As a first step in the modeling, EQ3 was used to generate the composition and speciation of initial C-rich fluids in equilibrium with the specified mineral compositions in a mafic eclogite (Tables S-1 and S-2). We used the mafic eclogitic mineral compositions at 1000 °C and 5.0 GPa reported in Kessel *et al.* (2015). The fluid in equilibrium with these minerals measured by Kessel *et al.* was analysed theoretically in Huang and Sverjensky (2019) as part of a calibration of the thermodynamic properties of complexes of the major elements. We used this calibration, but we also adopted a variety of values for the  $f\text{O}_2$  to ensure a range of different initial fluid chemistries.

The metasomatic interactions between these initial fluids and a variety of peridotitic substrates were simulated using the irreversible chemical mass transfer code EQ6 (results tabulated in Tables S-3–S-5). Both the initial and final rock modes are given in Table S-5. The simulations predicted the stepwise interaction of fluid and rock to yield the progressive evolution of the fluid chemistry and aqueous speciation as well as the evolution of metasomatic mineral solid solutions during reaction progress. Although the temperature and pressure of the simulations were set at 1000 °C and 5.0 GPa, preliminary calculations indicate very similar results at temperatures 100–200 °C lower and pressures 1.0–2.0 GPa lower. It should be emphasized that the initial fluid in each case is out of equilibrium with the initial peridotite reactant. During the irreversible chemical reactions, the fluid chemistry and the mineralogy, which are coupled, can therefore evolve chemically. Important parameters such as the oxygen fugacity and pH are determined throughout each run by the bulk chemistry of the reacting fluid-rock system, as is the potential for new minerals to react and even re-dissolve. All the initial reactant minerals in Table S5 are assumed to have the same relative reaction rates, which may be a reasonable assumption at the elevated temperature and pressure considered here.

The initial lherzolithic reactant minerals are progressively destroyed during reaction progress as the fluid tries to equilibrate with the rock. Each unit of the reaction progress variable ( $\xi$ ) corresponds to destruction of 1.0 mole of each of the reactant minerals. The new minerals formed during the metasomatic reactions are plotted in Figs. 2a–d (main text) as functions of the logarithm of the reaction progress variable ( $\log\xi$ ).



## Supplementary Tables

**Table S-1** The initial fluid composition and controls on the compositional variables.

Variable	Eclogitic fluid (Fluid number 3)		Eclogitic fluid (Fluid number 4.1)		Eclogitic fluid (Fluid number 5)	
	Concentration <sup>a</sup>	Set with	Concentration <sup>a</sup>	Set with	Concentration <sup>a</sup>	Set with
Na	2.50	Charge balance	1.40	Charge balance	1.40	Charge balance
Ca	1.84	Diopside (0.35)	0.66	Diopside (0.35)	0.52	Diopside (0.35)
Mg	1.65	Pyrope (0.352)	0.07	Pyrope (0.352)	0.02	Pyrope (0.352)
Fe	0.90	Almandine (0.323)	0.13	Almandine (0.323)	0.05	Almandine (0.323)
Al	1.02	Grossular (0.326)	0.79	Grossular (0.326)	0.73	Grossular (0.326)
Si	8.18	Coesite (1.0)	7.09	Coesite (1.0)	6.51	Coesite (1.0)
C	20.0	Given	20.0	Given	20.0	Given
pH	4.95	Jadeite (0.539)	4.82	Jadeite (0.539)	4.82	Jadeite (0.539)
$a_{\text{H}_2\text{O}}$	0.69		0.73		0.71	
$\log f_{\text{O}_2}$	-10.4		-11.4		-12.4	
$\Delta\text{FMQ}$	-3.0		-4.0		-5.0	

<sup>a</sup> Element concentrations refer to molality (moles/kg H<sub>2</sub>O).



**Table S-2** Model aqueous speciation results for the ten most abundant aqueous species (molal) in the initial fluid and the pH and  $fO_2$ .

Eclogitic fluid (Fluid number 3)		Eclogitic fluid (Fluid number 4.1)		Eclogitic fluid (Fluid number 5)	
Variable	Concentration <sup>b</sup>	Variable	Concentration <sup>b</sup>	Variable	Concentration <sup>b</sup>
H <sub>2</sub> CO <sub>3</sub> (aq)	6.45	CH <sub>4</sub> (aq)	8.49	CH <sub>4</sub> (aq)	13.08
HCOO <sup>-</sup>	2.74	Ethane (aq)	2.83	Ethane (aq)	2.38
CH <sub>4</sub> (aq)	2.10	H <sub>4</sub> SiO <sub>4</sub> (aq)	1.46	H <sub>4</sub> SiO <sub>4</sub> (aq)	1.38
Mg(SiO <sub>2</sub> )(HCO <sub>3</sub> ) <sup>+</sup>	1.63	Na <sup>+</sup>	1.23	Na <sup>+</sup>	1.26
Ca(HCOO) <sup>+</sup>	1.39	Propane (aq)	1.15	H <sub>8</sub> Si <sub>3</sub> O <sub>10</sub> (aq)	0.93
H <sub>4</sub> SiO <sub>4</sub> (aq)	1.30	H <sub>8</sub> Si <sub>3</sub> O <sub>10</sub> (aq)	1.03	Al(OH) <sub>3</sub> OSi(OH) <sub>3</sub> <sup>-</sup>	0.71
NaHCO <sub>3</sub>	1.26	Ethanol (aq)	0.87	H <sub>3</sub> SiO <sub>4</sub> <sup>-</sup>	0.56
Na <sup>+</sup>	1.10	Al(OH) <sub>3</sub> OSi(OH) <sub>3</sub> <sup>-</sup>	0.76	OH <sup>-</sup>	0.55
Al(OH)Si(OH) <sup>-</sup>	0.99	H <sub>3</sub> SiO <sub>4</sub> <sup>-</sup>	0.58	Propane (aq)	0.53
Fe(HCOO) <sup>+</sup>	0.87	OH <sup>-</sup>	0.55	Ca(H <sub>3</sub> SiO <sub>4</sub> ) <sup>+</sup>	0.51
pH	4.95	pH	4.82	pH	4.82
<b>log<math>fO_2</math></b>	-10.4	<b>log<math>fO_2</math></b>	-11.5	<b>log<math>fO_2</math></b>	-12.4
<b>ΔFMQ</b>	-3.0	<b>ΔFMQ</b>	-4.1	<b>ΔFMQ</b>	-5.0

<sup>b</sup> Aqueous species concentrations refer to molality (moles/kg H<sub>2</sub>O).



**Table S-3** The final fluid compositions for Run 27, 28 and 29 (see Table S-5).

Variable	Final fluid (initial $\Delta$ FMQ -3.0)		Final fluid (initial $\Delta$ FMQ -4.1)		Final fluid (initial $\Delta$ FMQ -5.0)	
	Model 27 Lherzolite + Fluid number 3		Model 28 Lherzolite + Fluid Number 4.1		Model 29 Lherzolite + Fluid Number 5	
	Concentration <sup>a</sup>	wt% oxide	Concentration <sup>a</sup>	wt% oxide	Concentration <sup>a</sup>	wt% oxide
Na	1.75	3.36	1.13	1.93	1.18	1.87
Ca	0.35	1.21	0.13	0.40	0.09	0.26
Mg	1.68	4.19	0.31	0.69	0.27	0.56
Fe	0.21	0.93	0.09	0.36	0.03	0.11
Al	0.33	1.04	0.20	0.56	0.19	0.49
Si	2.37	8.81	0.84	2.77	0.78	2.39
C	6.83	18.6	15.84	38.3	19.3	43.3
H		61.9		55.0		51.0
pH	5.09		4.98		4.99	
$a_{\text{H}_2\text{O}}$		0.86		0.79		0.76
$\log f_{\text{O}_2}$		-10.0		-11.7		-12.3
$\Delta$ FMQ		-2.6		-4.3		-4.9

<sup>a</sup> Element concentrations refer to molality (moles/kg H<sub>2</sub>O).



**Table S-4** Model aqueous speciation results for the ten most abundant aqueous species (molal) in the final fluid for Run 27, 28 and 29 (see Table S-5).

Final fluid (initial $\Delta$ FMQ -3.0)		Final fluid (initial $\Delta$ FMQ -4.1)		Final fluid (initial $\Delta$ FMQ -5.0)	
Model 27 Lherzolite + Fluid number 3		Model 28 Lherzolite + Fluid Number 4.1		Model 29 Lherzolite + Fluid Number 5	
Variable	Concentration <sup>b</sup>	Variable	Concentration <sup>b</sup>	Variable	Concentration <sup>b</sup>
H <sub>2</sub> CO <sub>3</sub> (aq)	2.80	CH <sub>4</sub> (aq)	8.26	CH <sub>4</sub> (aq)	11.42
Mg(SiO <sub>2</sub> )(HCO <sub>3</sub> ) <sup>+</sup>	1.35	Ethane (aq)	2.12	Ethane (aq)	2.02
OH <sup>-</sup>	1.05	Na <sup>+</sup>	0.94	Na <sup>+</sup>	0.99
HCOO <sup>-</sup>	1.02	OH <sup>-</sup>	0.74	OH <sup>-</sup>	0.76
NaHCO <sub>3</sub> (aq)	0.82	Propane (aq)	0.66	Propane (aq)	0.43
Na <sup>+</sup>	0.74	Ethanol (aq)	0.52	H <sub>4</sub> SiO <sub>4</sub> (aq)	0.30
H <sub>4</sub> SiO <sub>4</sub> (aq)	0.35	H <sub>4</sub> SiO <sub>4</sub> (aq)	0.33	Mg(OH) <sub>2</sub> (aq)	0.27
Mg(OH) <sub>2</sub> (aq)	0.33	Mg(OH) <sub>2</sub> (aq)	0.28	Ethanol (aq)	0.25
Al(OH)Si(OH) <sup>-</sup>	0.30	NaOH (aq)	0.18	NaOH (aq)	0.19
Ca(HCOO) <sup>+</sup>	0.28	Al(OH)Si(OH) <sup>-</sup>	0.17	Al(OH)Si(OH) <sup>-</sup>	0.16
pH	5.09	pH	4.98	pH	4.99
<b>logfO<sub>2</sub></b>	-10.0	<b>logfO<sub>2</sub></b>	-11.7	<b>logfO<sub>2</sub></b>	-12.3
<b><math>\Delta</math>FMQ</b>	-2.6	<b><math>\Delta</math>FMQ</b>	-4.3	<b><math>\Delta</math>FMQ</b>	-4.9

<sup>b</sup> Aqueous species concentrations refer to molality (moles/kg H<sub>2</sub>O).



**Table S-5** Key parameters for representative metasomatic mass transfer modes undertaken during this study. The pressure and temperature for all runs was fixed at 5 GPa and 1000 °C with the starting fluid  $fO_2$  and fluid pH fixed at  $\Delta fO_2$  -3 and 5.0, respectively.  $\Delta fO_2$  and  $\Delta pH$  express changes in the final fluid relative to the initial. Note that these changes are very small even though the mineralogical changes in the rock are very large. Runs in bold are reproductions of data from Table 1 for the sake of completeness.

Run	P GPa	T °C	$\log fO_2$ $\Delta fO_2$	pH	$\Delta \log fO_2$	$\Delta pH$	Initial Rock	Initial Mineralogy (vol %)	Final mineralogy (vol %)
3	5	1000	-3	5	0.36	0.14	Lherzolite (no garnet)	Olivine (59.99), Opx (19.80), Cpx (20.21)	Olivine (0.10), Opx (63.32), Cpx (32.77), Garnet (1.65), Diamond (0.05), Magnetite (2.11)
9	5	1000	-3	5	0.42	0.15	Lherzolite + aragonite (no garnet)	Olivine (57.43), Opx (18.95), Cpx (19.34), Aragonite (4.28)	Olivine (0.10), Opx (43.79), Cpx (52.30), Garnet (1.54), Diamond (0.07), Magnetite (2.20)
<b>27</b>	<b>5</b>	<b>1000</b>	<b>-3</b>	<b>5</b>	<b>0.35</b>	<b>0.14</b>	<b>Lherzolite</b>	<b>Olivine (54.80), Opx (20.02), Cpx (20.20), Garnet (4.98)</b>	<b>Olivine (0.11), Opx (58.62), Cpx (31.71), Garnet (7.42), Diamond (0.05), Magnetite (2.09)</b>
28	5	1000	-4.1	5	-0.30	0.16	Lherzolite	Olivine (54.80), Opx (20.02), Cpx (20.20), Garnet (4.98)	Olivine (0.05), Opx (67.44), Cpx (24.22), Garnet (8.29)
<b>29</b>	5	1000	-5	5	0.18	0.09	Lherzolite	Olivine (54.80), Opx (20.02), Cpx (20.20), Garnet (4.98)	Olivine (0.06), Opx (66.28), Cpx (24.89), Garnet (8.77)
33	5	1000	-3	5	0.35	0.14	Lherzolite (10 vol.% garnet)	Olivine (50.19), Opx (20.09), Cpx (19.92), Garnet (9.80)	Opx (54.72), Cpx (30.63), Garnet (12.49), Diamond (0.06), Magnetite (2.10)
39	5	1000	-3	5	0.35	0.14	Lherzolite (15 vol.% garnet)	Olivine (45.08), Opx (19.89), Cpx (19.87), Garnet (15.16)	Olivine (0.10), Opx (50.35), Cpx (29.86), Garnet (17.54), Diamond (0.06), Magnetite (2.09)
<b>45</b>	<b>5</b>	<b>1000</b>	<b>-3</b>	<b>5</b>	<b>-0.42</b>	<b>0.14</b>	<b>Lherzolite + aragonite</b>	<b>Olivine (52.52), Opx (19.18), Cpx (19.36), Garnet (4.77), Aragonite (4.17)</b>	<b>Olivine (0.09), Opx (40.55), Cpx (49.48), Garnet (7.62), Diamond (0.07), Magnetite (2.19)</b>
46	5	1000	-4.1	5	-0.20	0.15	Lherzolite + aragonite	Olivine (52.52), Opx (19.18), Cpx (19.36), Garnet (4.77), Aragonite (4.17)	Olivine (0.12), Opx (52.88), Cpx (37.88), Garnet (8.32), Diamond (0.78), Magnetite (0.02)



Table S-5 cont.

Run	P GPa	T °C	logfO <sub>2</sub> ΔFMQ	pH	ΔlogfO <sub>2</sub>	ΔpH	Initial Rock	Initial Mineralogy (vol %)	Final mineralogy (vol %)
47	5	1000	-5	5	0.71	0.17	Lherzolite + aragonite	Olivine (52.52), Opx (19.18), Cpx (19.36), Garnet (4.77), Aragonite (4.17)	Olivine (0.06), Opx (52.32), Cpx (38.69), Garnet (8.86), Diamond (0.07)
63	5	1000	-3	5	0.36	0.14	Dunite (no garnet)	Olivine (89.91), Opx (5.16), Cpx (4.93)	Olivine (0.17), Opx (66.38), Cpx (27.52), Garnet (3.20), Diamond (0.02), Magnetite (2.71)
69	5	1000	-3	5	0.42	0.15	Dunite + aragonite (no garnet)	Olivine (85.59), Opx (4.91), Cpx (4.70), Aragonite (4.81)	Olivine (0.18), Opx (25.59), Cpx (68.10), Garnet (3.11), Diamond (0.06), Magnetite (2.96)
<b>75</b>	<b>5</b>	<b>1000</b>	<b>-3</b>	<b>5</b>	<b>-0.06</b>	<b>0.14</b>	<b>Dunite +</b> <b>aragonite</b>	<b>Olivine (81.80), Opx</b> <b>(4.43), Cpx (4.62),</b> <b>Garnet (4.42),</b> <b>Aragonite (4.73)</b>	<b>Olivine (0.22), Opx</b> <b>(20.69), Cpx (62.87),</b> <b>Garnet (13.28),</b> <b>Diamond (0.06),</b> <b>Magnetite (2.88)</b>
76	5	1000	-4.1	5	-0.20	0.15	Dunite + aragonite	Olivine (81.80), Opx (4.43), Cpx (4.62), Garnet (4.42), Aragonite (4.73)	Olivine (0.19), Opx (47.13), Cpx (38.72), Garnet (12.59), Diamond (1.34), Magnetite (0.03)
77	5	1000	-5	5	0.71	0.16	Dunite + aragonite	Olivine (81.80), Opx (4.43), Cpx (4.62), Garnet (4.42), Aragonite (4.73)	Olivine (0.08), Opx (45.93), Cpx (40.11), Garnet (13.76), Diamond (0.12)
81	5	1000	-3	5	0.36	0.14	Harzburgite (no garnet)	Olivine (74.92), Opx (25.08)	Olivine (0.12), Opx (81.91), Cpx (13.07), Garnet (2.41), Diamond (0.03), Magnetite (2.46)
87	5	1000	-3	5	0.42	0.15	Harzburgite + aragonite (no garnet)	Olivine (71.41), Opx (23.91), Aragonite (4.68)	Olivine (0.17), Opx (53.15), Cpx (41.73), Garnet (2.27), Diamond (0.06), Magnetite (2.62)
<b>93</b>	<b>5</b>	<b>1000</b>	<b>-3</b>	<b>5</b>	<b>-0.06</b>	<b>0.14</b>	<b>Harzburgite</b> <b>+ aragonite</b>	<b>Olivine (67.89), Opx</b> <b>(22.73), Garnet</b> <b>(4.78), Aragonite</b> <b>(4.60)</b>	<b>Olivine (0.15), Opx</b> <b>(46.34), Cpx (39.92),</b> <b>Garnet (10.92),</b> <b>Diamond (0.07),</b> <b>Magnetite (2.60)</b>





Table S-5 cont.

Run	P GPa	T °C	logfO <sub>2</sub> ΔFMQ	pH	ΔlogfO <sub>2</sub>	ΔpH	Initial Rock	Initial Mineralogy (vol %)	Final mineralogy (vol %)
94	5	1000	-4.1	5	-0.20	0.14	Harzburgite + aragonite	Olivine (67.89), Opx (22.73), Garnet (4.78), Aragonite (4.60)	Olivine (0.08), Opx (61.51), Cpx (26.29), Garnet (11.01), Diamond (1.11)
95	5	1000	-5	5	0.71	0.16	Harzburgite + aragonite	Olivine (67.89), Opx (22.73), Garnet (4.78), Aragonite (4.60)	Olivine (0.06), Opx (61.06), Cpx (26.88), Garnet (11.90), Diamond (0.10)
111	5	1000	-3	5	-0.12	0.13	Dunite	<b>Olivine (85.86), Opx (4.65), Cpx (4.85), Garnet (4.64)</b>	<b>Opx (58.29), Cpx (26.61), Garnet (12.40), Diamond (0.03), Magnetite (2.67)</b>
112	5	1000	-4.1	5	-0.30	0.16	Dunite	Olivine (85.86), Opx (4.65), Cpx (4.85), Garnet (4.64)	Olivine(0.07), Opx (72.10), Cpx (15.50), Garnet (12.33)
117	5	1000	-3	5	-0.12	0.12	Harzburgite	<b>Olivine (71.16), Opx (23.83), Garnet (5.01)</b>	<b>Olivine (0.13), Opx (73.46), Cpx (13.53), Garnet (10.40), Diamond (0.04), Magnetite (2.44)</b>
118	5	1000	-4.1	5	-0.30	0.15	Harzburgite	Olivine (71.16), Opx (23.83), Garnet (5.01)	Olivine (0.06), Opx (81.66), Cpx (7.42), Garnet (10.86)
125	5	1000	-3	5	0.49	0.17	Dunite + aragonite (10 vol.%)	Olivine (78.11), Opx (4.23), Cpx (4.41), Garnet (4.22), Aragonite (9.03)	Olivine (0.13), Cpx (82.68), Garnet (14.26), Magnetite (2.93)
126	5	1000	-3	5	0.64	0.20	Dunite + aragonite (15 vol.%)	Olivine (74.73), Opx (4.05), Cpx (4.22), Garnet (4.04), Aragonite (12.96)	Olivine (0.11), Cpx (82.08), Garnet (14.81), Magnetite (3.00)



## Supplementary Information References

- Bulanova, G.P., Walter, M.J., Smith, C.B., Kohn, S.C., Armstrong, L.S., Blundy, J., Gobbo, L. (2010) Mineral inclusions in sublithospheric diamonds from Collier 4 kimberlite pipe, Juina, Brazil: subducted protoliths, carbonated melts and primary kimberlite magmatism. *Contributions to Mineralogy and Petrology* 160, 489-510.
- De Stefano, A., Kopylova, M.G., Cartigny, P., Afanasiev, V. (2009) Diamonds and eclogites of the Jericho kimberlite (Northern Canada). *Contributions to Mineralogy and Petrology*, 158, 295-315.
- Dobosi, G., Kurat, G. (2010) On the origin of silicate-bearing diamondites. *Mineralogy and Petrology* 99, 29-42.
- Gurney, J.J., Boyd, F.R. (1982) Mineral intergrowths with polycrystalline diamonds from the Orapa Mine, Botswana. *Carnegie Institute of Washington Yearbook* 81, 267-273.
- Gurney, J.J., Harris, J.W., Rickard, R.S. (1984) Silicate and oxide inclusions in diamonds from the Orapa Mine, Botswana. In: Kornprobst, J. (Ed.) *Kimberlites II: The Mantle and Crust–Mantle Relationships*. Elsevier, Amsterdam, 3-9.
- Huang, F., Sverjensky, D.A. (2019) Extended Deep Earth Water Model for predicting major element mantle metasomatism. *Geochimica et Cosmochimica Acta*, 254, 192-230.
- Jacob, D.E., Viljoen, K.S., Grassineau, N., Jagoutz, E. (2000) Remobilization in the cratonic lithosphere recorded by polycrystalline diamond (framesite). *Science* 289, 1182-1185.
- Kessel, R., Pettke, T., Fumagalli, P. (2015) Melting of metasomatized peridotite at 4–6 GPa and up to 1200 °C: an experimental approach. *Contributions to Mineralogy and Petrology* 169, 37.
- Mikhail, S., McCubbin, F.M., Jenner, F.E., Shirey, S.B., Rumble, D., Bowden, R. (2019) Diamondites: evidence for a distinct tectono-thermal diamond-forming event beneath the Kaapvaal craton. *Contributions to Mineralogy and Petrology* 174, 71.
- Miller, C.E., Kopylova, M., Smith, E. (2014) Mineral inclusions in fibrous diamonds: constraints on cratonic mantle refertilization and diamond formation. *Mineralogy and Petrology* 108, 317-331.
- Shock, E.L., Helgeson, H.C. (1988) Calculation of the thermodynamic and transport properties of aqueous species at high pressures and temperatures: Correlation algorithms for ionic aqueous species and equation of state predictions to 5 kb and 1000 °C. *Geochimica et Cosmochimica Acta* 52, 2009-2036.
- Shock, E.L., Sassani, D.C., Willis, M., Sverjensky, D.A. (1997) Inorganic Species in Geologic Fluids: Correlations among Standard Molal Thermodynamic Properties of Aqueous Cations, Oxyanions, Acid Oxyanions, Oxyacids and Hydroxide Complexes. *Geochimica et Cosmochimica Acta* 61, 907-950.
- Sobolev, N.V., Logvinova, A.M., Zedgenizov, D.A., Pokhilenko, N.P., Malygina, E.V., Kuzmin, D.V., Sobolev, A.V. (2009) Petrogenetic significance of minor elements in olivines from diamonds and peridotite xenoliths from kimberlites of Yakutia. *Lithos* 112, 701-713.
- Stachel, T., Harris, J.W. (2008) The origin of cratonic diamonds – constraints from mineral inclusions. *Ore Geology Review* 34, 5-32.
- Sverjensky, D.A. (2019) Thermodynamic modelling of fluids from surficial to mantle conditions. *Journal of the Geological Society* 176, 348-374.
- Sverjensky, D.A., Shock, E.L., Helgeson, H.C. (1997) Prediction of the thermodynamic properties of aqueous metal complexes to 1,000 °C and 5.0 kb. *Geochimica et Cosmochimica Acta* 61, 1359-1412.



- Tappert, R., Stachel, T., Harris, J.W., Shimizu, N., Brey, G.P. (2005) Mineral inclusions in diamonds from the Panda kimberlite, Slave Province, Canada. *European Journal of Mineralogy* 17, 423-440.
- Tappert, R., Foden, J., Stachel, T., Muehlenbachs, K., Tappert, M., Wills, K. (2009) The diamonds of South Australia. *Lithos* 112, 806-821.
- Wolery, T.J. (1983) *EQ3NR, A computer program for geochemical aqueous speciation-solubility calculations: User's guide and documentation*. UCRL-53414. Lawrence Livermore National Laboratory, University of California, Livermore, California.
- Wolery, T.J. (1984) *EQ6, A computer program for reaction-path modelling of aqueous geochemical systems: User's guide and documentation*. UCRL-51. Lawrence Livermore National Laboratory, University of California, Livermore, California.
- Wolery, T.J. (1992) *EQ3/6: A software package for geochemical modeling of aqueous systems: package overview and installation guide (version 7.0)*. Lawrence Livermore National Laboratory, University of California, Livermore, California.
- Viljoen, K., Phillips, D., Harris, J.W., Robinson, D. (1999) Mineral inclusions in diamonds from the Venetia kimberlites, Northern Province, South Africa. *International Kimberlite Conference: Extended Abstracts* 7, 943-945.

