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4 **Diamond's depth distribution systematics**

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11 **Abstract**

12 The thermobarometric analysis of inclusions in lithospheric diamonds has shown that these
13 diamonds may originate from a wide range of depths, with a global mode at $\sim 175 \pm 15$ km. Studies
14 based on diamond depth distribution at global scale, however, cannot clarify if this mode reflects a
15 real concentration of diamonds, preferential sampling of materials from this level by ascending
16 kimberlites, or simply a statistical distribution within the hard limits imposed by diamond stability,
17 lithosphere thickness and mantle adiabat under typical cratonic thermal regimes. We addressed this
18 problem by comparing depth distributions for peridotitic diamonds from the three localities that
19 have been the most prolific for diamond geobarometry (Cullinan, Kimberley and Voorspoed, South
20 Africa) with those of mantle xenocrysts from the same kimberlite sources. The revised P–T
21 estimates indicate that the diamonds were formed at T higher, equal or lower than the ambient
22 geotherm recorded by the xenocrysts. These conditions may represent old mantle thermal regimes
23 or local thermal perturbations related to infiltration of parental fluids or melts. Nonetheless, the
24 studied diamonds show similar depth distributions for the different localities, with a distinct mode

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25 at $\sim 180 \pm 10$ km. The similarity of these distributions with that calculated for peridotitic diamonds
26 worldwide, as well as the lack of systematic correlation with kimberlite sampling efficiency as
27 recorded by mantle xenocrysts, suggests that this mode has genetic significance. Based on observed
28 depth distributions and thermodynamic modeling of COH fluids, diamond-forming processes are
29 predicted to become less efficient with decreasing depth from at least ~ 165 km. In addition,
30 diamond endowment near the base of the lithosphere may be negatively affected by infiltration of
31 carbon-undersaturated melts or fluids after diamond formation. Considering the poor correlation
32 between diamond and xenocryst depth distributions in single kimberlites or kimberlite clusters,
33 even limited xenocryst records from diamond favorable depths (especially from the 160–190 km
34 interval) may correspond to significant diamond potential.

35
36 **Keywords** Diamond, inclusion, kimberlite, xenocryst, thermobarometry

38 **Highlights**

- 39 • Diamonds may form at T higher, equal or lower than the ambient eruption geotherm.
- 40 • Similar depth distributions at different localities for peridotitic diamonds.
- 41 • Poor correlation with xenocryst depth distributions.
- 42 • The 160–190 km depth interval is the most favorable for diamonds.

45 **1. Introduction**

46
47 Diamond is one of the most sought-after minerals, with a global annual mine production of
48 ~ 150 Mct (gem and industrial diamonds; USGS, 2019). Diamond is also the focus of extensive
49 scientific research, because it forms only at great depths, is relatively inert and can be very old.
50 Therefore, it can provide information on processes that have operated in inaccessible portions of the

51 deep Earth over long geological time-scales (e.g., Stachel and Harris, 2009; Shirey and Richardson,
52 2011). Based on the study of mineral inclusions in diamonds found in kimberlitic rocks, about 90%
53 of diamonds originated in the subcratonic lithospheric mantle (Stachel and Harris, 2008). The
54 thermobarometric analysis of these inclusions has shown that lithospheric diamonds can come from
55 a wide range of depths, extending from the graphite–diamond stability boundary to the base of the
56 lithosphere (see reviews in Stachel and Harris, 2008, and Shirey et al., 2013). The overall
57 distribution of pressure estimates for lherzolitic and harzburgitic diamonds, however, is not uniform
58 and has a mode at $\sim 5\text{--}6$ GPa, corresponding to depths of $\sim 175 \pm 15$ km (Stachel, 2014). This mode
59 has been derived by combining data for diamonds from many localities worldwide, as the number
60 of diamonds from individual localities for which pressure has been estimated is generally much too
61 small to be statistically valid. Therefore, it is generally difficult to assess possible heterogeneities in
62 the local distributions of diamonds, differences between localities, and potential links between
63 diamond depth distributions and local mantle ‘stratigraphies’. Based on geophysical evidence,
64 Garber et al. (2018) suggested that the average proportion of diamond in the cratonic lithosphere
65 can be very high (~ 2 vol.%). Direct observations on mantle xenoliths, however, show highly
66 variable diamond proportions, with the majority of samples being devoid of diamond, but with
67 individual samples having up to ~ 3 vol.% diamond (e.g., Peltonen et al., 2002; Anand et al., 2004;
68 Viljoen et al., 2004). Another recent study on six diamonds from one source suggested that some
69 kimberlites might contain diamonds that originated from a very restricted depth interval (Stachel et
70 al., 2018). From present data, it remains unclear if the 175-km mode observed at a global scale
71 reflects a real concentration of diamonds, i.e., a favored condition for diamond formation and
72 preservation at this depth, or preferential sampling of materials from this level during the ascent of
73 the carrier kimberlite through a mantle with more evenly distributed diamonds. Shirey et al. (2013)
74 even suggested that global modes obtained from diamond thermobarometry might have no genetic
75 meaning and might simply represent the statistically most probable P–T conditions within the hard

76 limits imposed by diamond stability, lithosphere thickness and mantle adiabat under typical cratonic
77 thermal regimes.

78 A more robust interpretation of diamond depth distributions would require studying large
79 numbers of diamonds from individual localities and comparing their geobarometric data with
80 independent information on the sampling efficiency of the host kimberlite. In principle, the
81 sampling efficiency of a kimberlite could be assessed by exploring the statistical distributions of
82 provenance depths for included xenoliths. However, this evaluation may be severely biased,
83 because xenoliths may undergo mechanical disruption during kimberlite ascent and their
84 preservation potential may vary with depth, lithology and eruption regime. In this respect,
85 xenocrysts derived from xenolith fragmentation, either natural or induced, allow more
86 representative sampling of kimberlite-borne mantle materials, because they are much more
87 abundant than xenoliths, are much less affected by mechanical preservation problems and are
88 routinely obtained by processing of massive kimberlite samples during diamond exploration and
89 mining (e.g., Griffin et al., 1996). Although detailed petrographic information may be lost, some
90 xenocryst types are amenable, with some caveats, to single-mineral thermobarometry (e.g., Ryan et
91 al., 1996; Nimis and Taylor, 2000; Grütter et al., 2006; Grütter, 2009; Ziberna et al., 2016) and may
92 thus conveniently be employed for this purpose. The same material may also provide information
93 on the presence and abundance of specific lithologies at depth (Griffin et al., 1996).

94 In this work, we compare diamond depth distributions for the three localities that have been the
95 most prolific for diamond geobarometry (Cullinan, Kimberley and Voorspoed, South Africa), using
96 published and unpublished chemical data. Based on inclusion compositions, the diamonds
97 considered in this work are representative of different paragenetic types: the diamonds from
98 Cullinan and Kimberley are peridotitic and belong either to the lherzolithic suite (most Cullinan
99 diamonds; Nimis, 2002; Viljoen et al., 2014; Korolev et al., 2018) or to the harzburgitic suite (most
100 Kimberley diamonds; Phillips et al., 2004); most of the diamonds from Voorspoed belong to an
101 unusual class, which is characterized by the presence of exsolved pyroxene inclusions and is

102 believed to be transitional between the lherzolitic and websteritic types (Viljoen et al., 2018). For
103 the purpose of this paper, previous thermobarometric estimates will be revised. The depth estimates
104 for diamonds will be compared with new data for chromian diopside (Cpx) and garnet (Grt)
105 xenocrysts from the same kimberlitic sources to explore potential relationships with the kimberlite
106 sampling efficiency. The results have implications for diamond genesis and for future evaluations of
107 diamond potential of kimberlites based on thermobarometric interpretation of kimberlite indicator
108 minerals.

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110

111 **2. Geological outline**

112

113 The three kimberlite localities considered in this work are representative of different geological
114 settings within the Kaapvaal craton (Fig. 1).

115 The Cullinan (formerly Premier) kimberlite was emplaced at ~1150 Ma (Wu et al., 2013)
116 through the Bushveld Igneous Complex, which intruded the northern portion of the Kaapvaal craton
117 ~2050 My ago (Hamilton, 1977; Walraven and Hattingh, 1993). Mantle xenoliths indicate the more
118 fertile nature of the Cullinan peridotitic mantle as compared with the more regular, harzburgite-rich
119 cratonic mantle of other South African diamondiferous kimberlites (Hoal, 2003). The anomalous
120 character of the Cullinan mantle has been ascribed to extensive melt-driven metasomatism, related
121 to the emplacement of the Bushveld Complex (e.g., Griffin et al., 2003a; Hoal, 2003). The ratio of
122 lherzolitic to harzburgitic diamonds is also significantly higher at Cullinan than other southern
123 African localities (Viljoen et al., 2014). Overall, eclogitic diamonds are the most abundant (69%),
124 followed by peridotitic (21%) and sublithospheric mafic types (9%) (Korolev et al., 2018).
125 Temperature estimates for inclusions in Cullinan diamonds are, on average, anomalously high
126 (Nimis, 2002; Viljoen et al., 2014; Korolev et al., 2018). Sm–Nd dating of lherzolitic and eclogitic
127 inclusions yielded ages of ~1930 Ma and ~1150 Ma, respectively, the latter being within

128 uncertainty of kimberlite emplacement (Richardson, 1986; Richardson et al., 1993). Griffin et al.
129 (2003a) suggested that few diamonds survived the Bushveld igneous event and that most grew after
130 this event.

131 The Kimberley kimberlites (i.e., Bultfontein, Wesselton, De Beers, Dutoitspan, Big Hole)
132 belong to the same Group-1 kimberlite cluster and were emplaced at ~84 Ma (Allsopp et al., 1989)
133 into the eastern portion of the Kimberley terrane, ~60 km from its boundary with the Witwatersrand
134 terrane. The two terranes were accreted through subduction beneath the Kimberley terrane, arc
135 magmatism and collisional thickening at ~2900 Ma (Schmitz et al., 2004). Based on the
136 compositions of Grt xenocrysts, the Kimberley mantle at the time of Group-1 kimberlite eruption
137 appears to have been hotter, thinner and more melt-metasomatized than that sampled by slightly
138 older (>110 Ma), Group-2 kimberlites emplaced in the same terrane (Griffin et al., 2003a).
139 Kimberley diamonds are mostly harzburgitic (>90%), with lesser abundances from eclogitic and
140 websteritic parageneses (Phillips et al., 2004). Part of the material investigated here and in previous
141 works was recovered from the De Beers mining plant, which had long been processing mixed
142 materials from four kimberlites (Bultfontein, Wesselton, De Beers and Dutoitspan). This type of
143 material is thus conveniently referred to as being derived from the De Beers Pool. Peridotitic garnet
144 inclusion composites from De Beers Pool diamonds were dated at 3.4 Ga (Sm–Nd; Richardson et
145 al., 1984), whereas eclogitic sulfide inclusions were dated at 2.9 Ga (Re–Os; Richardson et al.,
146 2001).

147 The Voorspoed kimberlite is part of the Kroonstad Group-2 kimberlite cluster and was intruded
148 at 131.9 Ma in the 3.1–3.5 Ga core of the Witwatersrand terrane (Phillips et al., 1998; Howarth et
149 al., 2011; Gibson, 2019). Inclusions in diamonds are 35% eclogitic, and 57% span a range of
150 compositions that, based on major elements, are transitional between ‘websteritic’ and ‘lherzolithic’,
151 with harzburgitic diamonds being comparatively rare (Viljoen et al., 2018). A characteristic feature
152 of Voorspoed inclusions classified as websteritic to lherzolithic is the presence of exsolved

153 pyroxenes now transformed into an intergrowth of Cpx + orthopyroxene (Opx) ± coesite ± (Ti, Cr)-
154 oxide (Viljoen et al., 2018).

155

156

157 **3. Materials and Methods**

158

159 Cpx and Grt xenocrysts from Cullinan, Voorspoed and Kimberley kimberlites were recovered
160 from kimberlite samples processed in De Beers Exploration's laboratories in Kimberley and
161 Johannesburg over a period spanning 30 years (Cullinan: 1981–2004; Kimberley: 1980–2010;
162 Voorspoed: 1986–2013). Kimberlite rock samples (drill core and hand grab samples from
163 stockpiles, underground and open pit) were crushed, wet screened and concentrated using dense
164 media separation and heavy liquids before individual mineral grains were hand-picked. The
165 majority (~75%) of the indicator mineral grains were recovered in the 0.3-1.0 mm size range. The
166 mineral separation procedure yielded 2131 Cpxs and 4486 Grts from Cullinan, ~16000 Cpxs and
167 ~24000 Grts from Kimberley and 343 Cpxs and 5082 Grts from Voorspoed.

168

169 *3.1. Chemical analyses*

170

171 Preliminary electron microprobe analyses of Cpx and Grt xenocrysts were carried out at De
172 Beers Exploration's central analytical facility, Johannesburg, South Africa. The data were used for a
173 first screening of the available material, in order to select grains of peridotitic affinity, defined as
174 Cpx with Cr₂O₃ > 0.5 wt.% and Grt with Cr₂O₃ ≥ 1 wt.% and Mg/(Mg + Fe)_{mol} > 0.65 (Ramsay and
175 Tompkins, 1994; Griffin et al., 1999). Detailed chemical analysis of randomly selected subsets of
176 the Cpx xenocrysts was then carried out using a CAMECA SX-50 electron microprobe (IGG–CNR,
177 Padua, Italy) equipped with four wavelength-dispersive spectrometers. Natural and synthetic
178 minerals (diopside for Ca and Si, albite for Na, orthoclase for K, and pure Al, Mg, Cr, Fe, and Mn-

179 Ti oxides) were used as standards. The most mobile elements (Na and K) were always analyzed
180 first in order to minimize errors due to their migration under the electron beam. Preliminary
181 compositional data were collected using a 1- μm electron beam, an accelerating voltage of 20 kV, a
182 beam current of 15 nA, and counting times of 10 s for peak and 5 s for backgrounds on each side of
183 the peak. X-ray counts were converted into weight percent oxides by using the CAMECA-PAP
184 program. Four to five point analyses were carried out on each grain and the results were averaged.
185 Relative standard deviations for the major oxides on individual grains were generally $\leq 1\%$ for SiO_2 ,
186 MgO and CaO , $\leq 5\%$ for Al_2O_3 and Na_2O , and $\leq 10\%$ for Cr_2O_3 and FeO . Grains showing significant
187 compositional zoning, i.e., relative standard deviations on major oxides greater than the above
188 values, were excluded from the dataset. Compositional filters (Ramsay and Tompkins, 1994; Nimis,
189 1998; Zibera et al., 2016) were then applied to select Cpx derived from Grt–Opx-buffered
190 ultramafic assemblages. Following Zibera et al.’s (2016) recommendation for optimum single-Cpx
191 barometry, xenocrysts showing $0.011 < a_{\text{Cr}}/\text{Cr}\# \leq 0.024$ [where $a_{\text{Cr}} = \text{Cr} - 0.81 \cdot (\text{Na} + \text{K}) \cdot \text{Cr}\#$ and
192 $\text{Cr}\# = \text{Cr}/(\text{Cr} + \text{Al})$ atoms per 6-oxygen formula unit] were reanalyzed using higher beam current
193 (40 nA) and counting times (40 s for both peak and background) for Al, Cr, and Na, and routine
194 conditions for the other elements, whereas those showing $a_{\text{Cr}}/\text{Cr}\# < 0.011$ or $\text{Cr}\# < 0.1$ were
195 discarded. The proportion of Cpx grains that were discarded based on this criterion ranged from 5 to
196 12%, thus this selection should not have significantly undermined the representativeness of the
197 dataset. The final dataset (Supplementary Table S1), including analyses performed at either 15 nA
198 or 40 nA, depending on grain compositions, comprises a total of 1435 Cpx grains (Cullinan: $n =$
199 491; Kimberley: $n = 883$; Voorspoed: $n = 61$). The smaller number for Voorspoed reflects both the
200 smaller number of sampled grains from this locality and the lower proportion of grains with
201 compositions suitable for thermobarometry (Cullinan: 66%; Kimberley: 40%; Voorspoed: 31%;
202 based on preliminary analyses on the original xenocryst population). The lower proportions for both
203 Kimberley and Voorspoed are mainly due to the abundance of Cpx grains that were not associated
204 with garnet based on compositional filters.

205 Grt xenocrysts (Cullinan: n = 507; Voorspoed: n = 507; Kimberley: n = 544) were analyzed for
206 trace elements by laser ablation inductively coupled mass spectrometry (LA-ICP-MS)
207 (Supplementary Table S2). The majority of the analyses (76%) were carried out between 2011 and
208 2015 at De Beers Exploration's central analytical facility in Johannesburg, South Africa, using a
209 ThermoFisher Scientific X-Series 2 ICP-MS and a New Wave FX193 Eximer laser. The instrument
210 was optimized on NIST SRM-610 glass before analysis for maximum sensitivity. Dwell time per
211 isotope was 30 ms with 10 s for blank background data and 60 s ablation time. Laser ablation
212 conditions were an ablation pit diameter of 100 μm , firing at 5 Hz with a fluence of 2 mJ/cm^2 , and a
213 crater depth of ~ 30 μm . Helium carrier gas was used to transport the ablated material from the laser
214 cell to the ICP-MS. ^{44}Ca was used as an internal standard in order to compensate for ionization and
215 matrix effects. Glitter 4.4.6® was used to reduce the time resolved analysis spectra and calculate the
216 concentrations of the various analytes. Typical detection limits were in the range 4–60 ppb for V,
217 Co, Ga, Sr, Y, Nb, Hf and most REEs, on the order of 0.1 ppm for Sc, Mn, Ni, Nd and Yb, and
218 approximately 0.4 ppm for Ti and 0.5 ppm for Zr. A smaller group of analyses (24%) including a
219 smaller set of elements was performed in the 1990's and early 2000's at De Beers GeoScience
220 Centre (previously Anglo American Research Laboratories) on a Perkin Elmer Sciex ELAN 6000
221 system, using a Merchantek New Wave Research Nd:YAG UV laser as described in Viljoen et al.
222 (2009). The laser was operated at a 10 Hz repetition rate, 105 μm ablation pit diameter and 60%
223 power (0.5 mJ laser pulse energy), in a high purity Ar–He mixture gas stream. A typical analysis
224 consisted of 100 replicates with each replicate representing four sweeps of the selected mass range,
225 a dwell time of 10 ms on each peak, a data collection period of 80 s during ablation, and an
226 additional 30 s for background counting. ^{44}Ca was used as an internal standard. Typical detection
227 limits were in the range 6–40 ppb for Sc, Ga, Sr, Y, Zr, Nb, Hf and REE, on the order of 0.2 ppm
228 for Ni and approximately 0.6 ppm for Ti. On both instruments, a natural garnet megacryst from
229 Monastery Mine in South Africa, GHR-1 (Viljoen et al., 2009), was used as an external standard
230 and analyzed and cross checked against the certified and accepted compositions throughout the

231 analysis periods. Accuracy and precision were better than 20% and in most cases better than 10%
232 for all elements analyzed.

233 Grt xenocrysts were classified into different compositional types using two independent
234 classification schemes (Griffin et al., 2002; Grütter et al., 2004). The classification of Grütter et al.
235 (2004) is based on major element concentrations and allows discrimination between Grts from
236 different mineral associations. In our datasets, the harzburgitic (G10), lherzolitic (G9), high-Ti
237 peridotitic (G11), wehrlitic (G12), megacrystic (G1) and pyroxenitic (G5) classes are represented
238 (Supplementary Table S2). According to the worldwide xenolith compilation of Grütter et al.
239 (2004), more than 90% of Grts falling into the harzburgitic, lherzolitic and pyroxenitic classes
240 belong to true harzburgites, lherzolites and pyroxenites, whereas the wehrlitic and megacrystic
241 classes may include significant proportions of Grts from other rock types. The CARP classification
242 tree of Griffin et al. (2002) is based on Grt trace element compositions and is best suited to
243 distinguish between geochemical associations representative of variable degrees of mantle depletion
244 and metasomatism. The individual CARP classes may contain variable proportions of harzburgitic
245 and lherzolitic Grts and can conveniently be combined into four main groups: depleted (depleted
246 harzburgites and lherzolites with little metasomatism), depleted metasomatized (depleted
247 harzburgites and lherzolites with fluid-related metasomatism), fertile (fertile to moderately depleted
248 lherzolites with fluid-related metasomatism) and melt-metasomatized (lherzolites with melt-related
249 metasomatism) (Griffin et al., 2002). The melt-metasomatized group may include Grts of the low-
250 Cr megacryst suite. For Grts that did not have measured Zn values, the original split at Zn = 22 ppm
251 in the CARP classification tree was replaced by a reversed split at Cr₂O₃ = 0.83 wt.% (W. Griffin,
252 personal communication). For garnets that did not have measured Sr values, we have simply
253 assigned them Sr values < 2.5 ppm, a concentration much higher than the upper quartile for
254 Archaean cratons (0.96 ppm; Griffin et al., 2002). This choice may have slightly underestimated the
255 proportion of Grt xenocrysts falling into the ‘fertile’ group of Griffin et al. (2002).

256

257 3.2. *Xenocryst thermobarometry and geotherm modeling*

258

259 Pressure (P) and temperature (T) estimates for the selected Cpx xenocrysts were obtained by
260 using a combination of the enstatite-in-Cpx thermometer and Cr-in-Cpx barometer of Nimis and
261 Taylor (2000). In order to make up for the recognized tendency of the Cpx barometer to
262 underestimate at high P (up to ~1 GPa at 7 GPa; Nimis, 2002; Ziberna et al., 2016) and to improve
263 consistency with other geobarometric methods, the Cr-in-Cpx pressures were corrected empirically
264 as described in the Appendix. The resulting P–T estimates were fitted with the FITPLOT program
265 (McKenzie and Bickle, 1988; McKenzie et al., 2005), as upgraded by and described in Mather et al.
266 (2011), to model geotherms for the local lithospheric mantle sections. Input values used for upper
267 and lower crustal thickness, heat production rate, thermal conductivity, and potential T for the
268 asthenospheric isentrope are summarized in Table 1. The values for upper and lower crustal heat
269 production and the differentiation between upper and lower crustal thickness are poorly constrained.
270 This uncertainty may significantly affect the shape of the shallowest portion of the model geotherm,
271 whereas at depths relevant for lithospheric diamond (4–7 GPa) the geotherm is more strongly
272 constrained by the xenocryst P–T data. The scatter of P–T points around model geotherms suggests
273 that maximum uncertainties on P–T estimates are of ~0.4 GPa and 50 °C near the graphite–diamond
274 boundary (Fig. 2–4). Uncertainties on P may increase to ~0.6 GPa near the base of the lithosphere.
275 The resulting uncertainties on the model geotherms are shown as $\pm 1 \sigma$ confidence bands in Fig. 2–4.

276 Temperatures for the Grt xenocrysts were estimated by using the P-independent Ni-in-Grt
277 thermometers of Ryan et al. (1996) and Canil (1999). The Canil (1999) version produces more
278 compressed T estimates, especially at high T, relative to that of Ryan et al. (1996). It has been
279 variously claimed that either calibrations, or even their ‘average’, agree best with other independent
280 thermometers when applied to mantle xenoliths (e.g., Ryan et al. 1996; Canil 1999; Shu et al., 2013;
281 De Hoog et al. 2019; Czas et al. 2020). We found that averaging T_{Canil} and T_{Ryan} estimates produced
282 T distributions more consistent with those obtained for Cpx xenocrysts from the same kimberlite

283 sources to at least 1350 °C. Although this is not necessarily a proof of better accuracy, our choice of
284 using the averaged $T_{\text{Ni-in-Grt}}$ probably improved consistency between estimates using different
285 thermobarometric methods. A few Grt xenocrysts, mostly from Voorspoed, still yielded
286 anomalously high temperatures, suggesting that the averaged $T_{\text{Ni-in-Grt}}$ may overestimate T above
287 1350 °C.

288 Pressures for the same Grt xenocrysts were estimated by projecting their temperatures on the
289 local model geotherm derived by fitting the Cpx P–T data. This approach is different from that
290 suggested by Ryan et al. (1996), which uses a combination of the Ni-in-Grt thermometer and Cr-in-
291 Grt barometer and defines the geotherm by the maximum $P_{\text{Cr-in-Grt}}$ at each $T_{\text{Ni-in-Grt}}$, assuming those
292 garnets coexisted with chromian spinel. Our choice of using the Cpx geotherm as reference was
293 meant to minimize the effect of potential inconsistencies between different barometric methods and
294 to allow better comparison between Cpx and Grt depth distributions. It also permitted more robust
295 estimates for Cullinan, because likely spinel-saturated Grts from this kimberlite were clustered in a
296 restricted T range (1080–1250 °C) and thus the ‘garnet geotherm’ was poorly constrained (see also
297 Griffin et al., 2003a). The typical uncertainty of the Ni-in-Grt thermometer (± 50 °C) propagates an
298 uncertainty of less than ~ 0.5 GPa on P estimates obtained by projection on the geotherm.

299

300 *3.3. Diamond inclusion thermobarometry*

301

302 P–T estimates for inclusions in diamonds were estimated by combining the results of suitable
303 geothermometers and geobarometers. Robust P estimates could not always be obtained owing to a
304 lack of suitable methods for specific minerals. In these cases, P was derived by projecting the
305 thermometric results on model ‘geotherms’. Data for multiple inclusions within the same diamond
306 were averaged, so that each computed P–T pair corresponds to one diamond. More specific details
307 on the procedures adopted are given below.

308 P–T estimates for the Cpx inclusions were obtained by using the same combination of the
309 enstatite-in-Cpx thermometer and Cr-in-Cpx barometer of Nimis and Taylor (2000) used for the
310 xenocrysts, as corrected here (see Appendix), following the same filtering protocol to select
311 inclusions belonging to Grt-bearing peridotitic assemblages. P–T estimates for the Opx–Grt
312 inclusion pairs were calculated by using a combination of the Harley (1984) thermometer with the
313 Nickel and Green (1985) barometer. Based on the scatter around conductive geotherms of P–T
314 estimates for xenoliths, the maximum uncertainty of the Nickel and Green (1985) barometer is
315 probably better than 0.5 GPa (Grütter, 2009). Using the alternative calibration of the Opx–Grt
316 thermometer of Nimis and Grütter (2010) yielded larger P–T intervals and increased scatter, but
317 would not change significantly the overall distribution of the data. None of the Opx analyses
318 showed an excess of Na relative to Cr and Ti, therefore no modification for the expression of the
319 activity of the Mg-Tschermak component was necessary (Carswell, 1991).

320 T estimates for seventeen olivine (Ol) inclusions from Cullinan (LA-ICP-MS compositional
321 data after Korolev et al., 2018) were calculated with the Al-in-Ol thermometer (Bussweiler et al.,
322 2017). The respective pressures were calculated by projecting Al-in-Ol univariant curves on model
323 geotherms, as described in the following section. Temperature estimates for thirty-two Grt
324 inclusions in diamonds and Grt in one diamondiferous xenolith from Cullinan (compositional data
325 after Viljoen et al., 2004, 2014) were calculated using the ‘average’ Ni-in-Grt thermometer in the
326 same way as the xenocrysts. Pressure estimates for the same samples were obtained by projecting
327 their $T_{\text{Ni-in-Grt}}$ on model geotherms in the same way as the Ol inclusions.

328 Fe–Mg-exchange thermometers have often been used to derive T estimates for Ol–Grt
329 inclusion pairs in diamonds, but these methods were shown to be very imprecise when applied to
330 natural samples (Nimis and Grütter, 2010). In an attempt to reduce noise in the data, Ol–Grt
331 inclusion pairs were excluded from our study, but existing data will still be considered for
332 comparison. Cpx–Grt Fe–Mg-exchange thermometers suffer from similar problems as the Ol–Grt
333 thermometers (Nimis and Grütter, 2010) and existing single-mineral thermobarometers for eclogitic

334 minerals are not sufficiently precise (e.g., discrepancies between calculated and experimental P and
335 T may exceed 1 GPa and 100 °C; Aschepkov et al., 2017). Therefore, a direct comparison between
336 depth distributions for inclusions and xenocrysts, our principal objective, is not yet possible for
337 eclogitic samples. For this reason, eclogitic diamonds are not considered in this study.

338

339 **4. Depth distributions for xenocrysts and diamonds**

340

341 *4.1. Cullinan*

342

343 The P–T estimates for most Cpx xenocrysts are aligned along a typical conductive geotherm
344 (Fig. 2a), which is close to a ~ 39 mW/m² Hasterok and Chapman (2011) theoretical geotherm. A
345 rich cluster of high-T data (~ 1350 °C) shows a tail towards higher P with a T/P slope similar to the
346 P-dependency of the Cpx thermometer. This suggests that the tail simply reflects the increased
347 uncertainty of the Cr-in-Cpx barometer at high P rather than a real spread of P–T data. The data at
348 moderate P (4 to 5 GPa) show an unusually large scatter for this P range, with six samples
349 apparently following a lower geotherm (Fig. 2a). These six anomalous xenocrysts do not show any
350 obvious compositional peculiarity and their compositions are well within the limits for optimal
351 single-Cpx barometry (cf. Zibera et al., 2016). Nonetheless, P–T estimates for these samples
352 appear to be unrepresentative of the mantle thermal state at the time of kimberlite eruption and were
353 therefore excluded from geotherm modeling.

354 Pressure data (GPa) were converted to depths (km) by using a factor of 32, which is a good
355 approximation for the cratonic lithosphere within the diamond window. The resulting depth
356 distribution for the Cpx xenocrysts is markedly bimodal, with a strong mode at ~ 205 km, a smaller
357 mode at ~ 150 km and a substantial gap at intermediate depths (Fig. 2b). When projected on the
358 model Cpx geotherm, the Grt xenocrysts show a skewed distribution, with a distinct mode at ~ 200
359 km, close to the major Cpx mode, and a tail towards shallower depths, overlapping the secondary

360 Cpx mode. The particular scarcity of Cpx xenocrysts between 165 and 185 km is consistent with the
361 Cullinan xenolith record, which indicates a predominance at about these depths of Cpx-free
362 harzburgite xenoliths containing melt-metasomatized Grts with ‘lherzolitic’ major and trace element
363 compositions (Danchin, 1979; Viljoen et al., 2009).

364 Thermobarometric calculations for eighty Cullinan diamonds have been performed using
365 compositional data for Ol (17), chromian Cpx (30), and chromian Grt (33) inclusions (Nimis, 2002;
366 Korolev et al., 2018; Viljoen et al., 2014) (Fig. 2a). P–T conditions for Grt from one
367 diamondiferous xenolith studied by Viljoen et al. (2004) were also estimated for comparison (Fig.
368 2a). Compositional data for Cpx inclusions discussed in Nimis (2002) were originally produced by
369 S.H. Richardson (personal communication) and are reported here in full for the first time
370 (Supplementary Table S3). One Cpx and one non-touching Opx–Grt pair from Korolev et al. (2018)
371 gave P–T values outside the diamond stability field, well off the xenocryst geotherm, and were
372 discarded.

373 Eleven out of twenty Cpx inclusions recording temperatures lower than 1300 °C fall along the
374 Cpx model geotherm. However, nine high-P inclusions record a colder geothermal gradient,
375 apparently falling on the same trend as the six anomalous Cpx xenocrysts (Fig. 2a). Therefore, a
376 ‘cold’ geotherm was also modeled using the six anomalous xenocrysts and the nine anomalous
377 inclusions. This ‘cold’ geotherm roughly corresponds to a ~36 mW/m² Hasterok and Chapman
378 (2011) theoretical geotherm and might reflect an old (pre-Bushveld?) lithospheric thermal state,
379 distinct from that recorded by the bulk of the xenocrysts at the time of eruption. Cpx inclusions
380 recording temperatures > 1300 °C yield, on average, higher T than Cpx xenocrysts of similar P (Fig.
381 2a), suggesting conditions hotter than the syn-eruptive geotherm for inclusions with T above ~1300
382 °C.

383 For Ol and Grt inclusions in diamonds and for the Grt from the diamondiferous xenolith, only
384 T can be directly estimated with sufficient confidence. To estimate P for the Ol inclusions, Korolev
385 et al. (2018) suggested that the Al-in-Ol T estimates could be projected onto the local xenolith

386 geotherm. According to Korolev et al. (2018), this choice is supported by the following
387 observations: (i) the consistency of the Al-in-Ol thermometer with the pyroxene thermometer that is
388 used for geotherm modeling; (ii) the small mean deviations between pressures obtained by
389 projection of Al-in-Ol temperatures onto a 40 mW/m² geotherm and those derived from
390 independent Raman barometry (Kohn, 2014) on the same olivines; (iii) the similar thermal state of
391 the lithosphere recorded by peridotitic diamonds and peridotite xenoliths of different ages. Some of
392 these observations are questionable. First, the simplified barometric formulation of Kohn (2014)
393 tends to significantly overestimate pressure relative to methods based on rigorously constrained
394 equations of state for mantle olivine (Angel et al. 2018). Even for these more rigorous methods, the
395 uncertainties are not better than ~1 GPa at lithospheric mantle conditions (Angel et al., 2018).
396 Therefore, using olivine Raman barometry to validate other P estimates is not warranted. Second,
397 high-T (>1300 °C) Cpx inclusions in Cullinan diamonds record, on average, higher T than Cpx
398 xenocrysts of similar P (Fig. 2a), indicating perturbed thermal conditions during formation of the
399 highest-T diamonds. Third, some of the lower-T Cpx inclusions record lower T than Cpx
400 xenocrysts of similar P, suggesting formation of their host diamonds under a colder thermal regime
401 (Fig. 2a). Disregarding these complications may lead to erroneous projected P estimates.

402 In an attempt to minimize possible artifacts, ‘minimum’ P estimates for Ol and Grt inclusions
403 were calculated by projecting their Al-in-Ol or, respectively, Ni-in-Grt univariant curves onto the
404 ‘hot’ model xenocryst geotherm for T < 1300 °C and on an ‘inflected’ limb passing through the
405 high-T Cpx inclusions for T > 1300 °C (Fig. 2a). The latter combination yielded P values up to 0.7
406 GPa lower than the corresponding projection onto the model conductive geotherm. The adopted
407 procedure is clearly a simplification, as we cannot establish whether the high-T Cpx inclusions fall
408 along a line (within thermobarometric uncertainties) or are simply scattered above the conductive
409 geotherm. Nonetheless, our choice should limit the general overestimation of diamond depths for
410 high-T Ol and Grt inclusions that was most probably made by Korolev et al. (2018). Given that
411 none of the high-T Cpx inclusions plot below the xenocryst geotherm (Fig. 2a), P estimates

412 calculated in this way most likely correspond to the true P conditions for Ol and Grt inclusions with
413 $T > 1300$ °C. For lower-T Ol and Grt inclusions, ‘maximum’ P estimates were obtained by
414 projecting the Al-in-Ol or Ni-in-Grt temperatures onto the ‘cold’ model geotherm (Fig. 2a).

415 In spite of the uncertainty in the depth determination for the Ol and Grt inclusions, the overall
416 diamond depth distribution is essentially unimodal (Fig. 2b). Depending on which geotherm is used
417 for the projection of the low-T Ol and Grt inclusions, the calculated mode varies from ~180 to ~210
418 km. These values straddle the Grt xenocryst depth mode of 200 km (Fig. 2b). The Cpx inclusions
419 show a distribution dissimilar from that of the Cpx xenocrysts, with about half the inclusions
420 coming from intermediate depths with very scarce Cpx xenocryst representation (Fig. 2b). If the
421 ‘hot-inflected’ geotherm is chosen for projection, then the depth mode for the Ol and Grt inclusions
422 is more similar to that of the Cpx inclusions.

423

424 *4.2. Kimberley*

425

426 Cpx xenocrysts from the Kimberley mines fall along a typical conductive geotherm, roughly
427 corresponding to a ~ 38 mW/m² Hasterok and Chapman (2011) theoretical geotherm, but are mostly
428 concentrated at low to moderate depths, with a main mode at 135 km (Fig. 3a). Two outliers plot
429 considerably below the geotherm, suggesting a derivation from an Opx-free, wehrlitic assemblage,
430 which could not be discriminated by the adopted compositional filters. P–T estimates for these two
431 samples are unreliable and were not considered any further. When projected on the Cpx geotherm,
432 the Grt xenocrysts show a distinct mode at ~145 km, that is only 10 km deeper than and within
433 errors of the Cpx xenocryst mode (Fig. 3a). The distribution is broadly similar for both harzburgitic
434 and lherzolitic Grts, although the lherzolitic Grts show more pronounced skewness at lower depth.
435 There is an abrupt decrease in the abundance of xenocrysts (Cpx and Grt) from depths greater than
436 ~160 km. This observation is consistent with all previous abundant data for xenocrysts and

437 xenoliths from this locality (Finnerty and Boyd, 1987; Nimis and Taylor, 2000; Griffin et al.,
438 2003a; Creighton et al., 2009).

439 P–T estimates for thirty-four Opx–Grt inclusion pairs from the De Beers Pool were recalculated
440 using compositional data obtained by Phillips et al. (2004). A single record, which showed clear
441 indications of disequilibrium between the untouched Grt and Opx (Phillips et al., 2004), was not
442 considered. The results essentially confirm previous estimates by Phillips et al. (2004) and indicate
443 an extended depth range with a mode at ~190 km and a distinctly deeper average provenance than
444 for the xenocrysts (Fig. 3b). Moreover, as noted by Weiss et al. (2018), P–T trends for touching and
445 non-touching inclusions depart markedly from the model xenocryst geotherm and mostly fall at
446 much lower T for a given P (Fig. 3a). Note that the Harley (1984) Opx–Grt thermometer tends to
447 overestimate T at $T < 1100^{\circ}\text{C}$ and to underestimate T at $T > 1100^{\circ}\text{C}$ for natural peridotites (Nimis
448 and Grütter, 2010), but that this has little bearing on the P–T distribution of the touching inclusions,
449 which mostly record temperatures around 1100°C . The modified version of the Opx–Grt
450 thermometer proposed by Nimis and Grütter (2010), which was meant to reduce these systematic
451 discrepancies for mantle peridotites equilibrated under ‘average’ redox conditions, at the cost of
452 larger overall scatter, would shift the higher-T, non-touching inclusions to even higher P–T (by up
453 to 170°C and 1 GPa), roughly parallel to the conductive geotherm. This shift would only reinforce
454 the discrepancy between xenocryst and diamond depth distributions. Temperature estimates for
455 touching and non-touching Ol–Grt inclusion pairs in De Beers Pool diamonds reported by Phillips
456 et al. (2004) are consistent with those obtained for touching and non-touching Opx–Grt inclusions,
457 respectively, further supporting the reliability of our estimates.

458

459 *4.3. Voorspoed*

460

461 Most of the Cpx xenocrysts from Voorspoed follow a conductive geotherm close to a ~38
462 mW/m^2 Hasterok and Chapman (2011) theoretical geotherm, but a few samples at very low and

463 very high P yielded anomalous P–T estimates (Fig. 4a). The low-P anomalous xenocrysts gave
464 lower P than other xenocrysts of similar T. Detailed inspection revealed that most of these
465 xenocrysts contain fine exsolution lamellae of Opx and spinel. This suggests that these xenocrysts
466 originated from spinel peridotites rather than garnet peridotites and erroneously survived
467 compositional filtering. In this case, the Cr-in-Cpx P estimates, which assume equilibrium of Cpx
468 with Grt, are meaningless (see also Read et al., 2004). The two high-P anomalous xenocrysts have
469 almost identical compositions and give T estimates which are much lower than expected at this P
470 (Fig. 4a). An origin from Opx-free wehrlitic assemblages would explain the low calculated T, as
471 only minimum T could be estimated in this case. The presence of occasional Grt xenocrysts with
472 wehrlitic composition recording $T_{\text{Ni-in-Grt}}$ as high as ~ 1400 °C (Supplementary Table 2),
473 corresponding to a geotherm P of 6.7 GPa, is consistent with this hypothesis. Both the low-P and
474 the high-P anomalous Cpx xenocrysts were excluded from geotherm modeling.

475 When projected on the Cpx geotherm, the Grt xenocrysts show a smeared depth distribution,
476 with one main broad peak at ~ 165 km and broad shoulders at shallower and, especially, greater
477 depths (Fig. 4b). The distribution of the Cpx xenocrysts is less well defined due to the much smaller
478 number of samples, but shows a major peak at ~ 150 km, which is close to the depth mode for the
479 lherzolitic Grts (~ 155 km; Fig. 4b).

480 Pressure estimates for the exsolved Cpx inclusions cannot be directly derived, since the
481 inclusions reequilibrated in the absence of Grt. Thermobarometry for the recalculated pre-
482 exsolution Cpx compositions (Viljoen et al., 2018), assuming original equilibrium with Opx *and*
483 Grt, yields $T \geq 1335$ °C, but generally too low P values to be compatible with diamond (Fig. 4a).
484 Detailed review of raw data for inclusions analyzed by Viljoen et al. (2018) revealed that some
485 point analyses had weight percent totals < 99 or sums of cations per formula unit < 3.99 , or
486 represented mixed Cpx–Opx analyses. However, analytical quality filtering did not improve
487 compatibility with diamond and only reduced the overall dispersion of T data, with most estimates
488 falling between 1335 and 1384 °C and a single estimate of 1474 °C. Since original equilibrium with

489 Opx, which is pre-requisite for enstatite-in-Cpx thermometry, is suggested by the occurrence of
490 Opx exsolution lamellae, the inconsistent P–T estimates are entirely ascribed to barometric errors.
491 This suggests that the assumption of equilibrium with Grt, which is pre-requisite for Cr-in-Cpx
492 barometry, is incorrect, consistent with the absence of exsolved Grt. Temperature estimates for the
493 exsolved inclusions are ~200 °C lower than those for the reconstructed homogeneous Cpxs.
494 Assuming that the exsolved inclusions reequilibrated to the last thermal conditions recorded by the
495 xenocrysts, P estimates for the exsolved pyroxenes can be derived by projecting their T estimates on
496 the xenocryst geotherm (Fig. 4a). The resulting depth distribution is distinctly unimodal, with a
497 mode at ~170 km (i.e., 5.3 GPa) (Fig. 4b). At this or slightly higher P, the thermobarometric
498 estimates for the reconstructed pre-exsolution pyroxenes would move into the diamond stability
499 field, supporting the reliability of the geotherm-projected P estimates. Incidentally,
500 thermobarometric data based on a combination of nitrogen-aggregation thermometry and elastic
501 modeling of a kyanite inclusion in a single eclogitic diamond from Voorspoed (Nestola et al., 2018)
502 yielded conditions falling right on the xenocryst geotherm and at the peridotitic diamond mode (Fig.
503 4a).

504

505 **5. Discussion**

506

507 *5.1. Locality-specific diamond P–T distributions*

508

509 *5.1.1. Cullinan*

510 The P–T distribution for Cullinan diamonds has been previously investigated by Nimis (2002)
511 using chromian Cpx inclusions and by Korolev et al. (2018) using a more comprehensive set of
512 inclusion types (Ol, peridotitic Grt and Cpx, and eclogitic Cpx–Grt pairs). Nimis (2002) noticed the
513 existence of both high- and low-T Cpx inclusions at high P, whereas Korolev et al. (2018)
514 emphasized the frequency of inclusions recording unusually high and even super-adiabatic T. These

515 findings were ascribed to a perturbed state of the mantle lithosphere at the time of diamond
516 formation, related to plume activity and intrusion of the large Bushveld Complex.

517 Our partially revised estimates essentially confirm previous findings in terms of T distribution,
518 although the T range that we obtained is smaller, due to the slightly different procedure adopted to
519 estimate P for the Ol inclusions (Fig. 2a). Also, assuming a slightly higher potential T for the
520 Proterozoic mantle (Ganne and Feng, 2017), there is no need to invoke super-adiabatic conditions
521 for any of the inclusions. Some very high-P, but relatively low-T Cpx inclusions may record old,
522 deep lithospheric conditions pre-dating thermal perturbation. This suggests that some Cullinan
523 diamonds were formed in a relatively cold cratonic lithosphere, but this conclusion requires further
524 verification based on more extensive data.

525 Despite the complex genetic environment and variable thermal regime, the overall diamond
526 depth distribution remains essentially unimodal and shows no apparent relationship with ‘hard’
527 restrictions, such as those imposed by diamond stability and lithosphere thickness (Fig. 2b).
528 Depending on which geotherm is used for the projection of the Ol and Grt inclusions, the mode
529 varies from ~180 to ~210 km. The latter value is most likely biased to the high side, because it
530 assumes that all Ol and Grt inclusions with $T < 1300$ °C recorded conditions falling on the ‘cold’
531 geotherm, whereas more than half of Cpx inclusions in this T range appear to fall on the ‘hot’
532 geotherm (Fig. 2a). Moreover, probably only few ‘cold’ diamonds survived the Bushveld igneous
533 event and many grew in a hotter mantle after this event (Griffin et al., 2003a; Viljoen et al., 2014).
534 Also, the depth mode for the Cpx inclusions is more similar to that for the Ol and Grt inclusions if
535 all of the Ol and Grt inclusions are projected onto the ‘hot’ geotherm (Fig. 2b). All these
536 observations suggest that the ~180 km mode is the most representative for Cullinan diamonds.

537

538 *5.1.2. Kimberley*

539 At Kimberley, the P–T estimates for inclusions mostly fall off the xenocryst geotherm and their
540 calculated T range is smaller than that expected for a conductive mantle over the same P range (Fig.

541 3a). As regards the non-touching inclusions, their apparent displacement towards lower T/P
542 gradients might reflect an old, relatively cold mantle thermal state. This hypothesis, however,
543 cannot hold for the touching inclusions, which should have re-equilibrated to the last ambient
544 conditions in the same way as the xenoliths and xenocrysts. The possibility that the offset of the
545 touching inclusions is an artifact due to incomplete chemical resetting during eruption is also
546 unlikely, because non-touching inclusions show a similar displacement (Fig. 3a).

547 Weiss et al. (2018) estimated broadly similar P–T conditions for microinclusions in fluid-rich
548 diamonds from the same kimberlite sources. The chemical analysis of these microinclusions was
549 challenging and required linear regression of the mixing lines between minerals and associated
550 high-density fluids (Weiss et al., 2018). Therefore, the reported compositional data may not be of
551 the quality required for robust thermobarometry. Nonetheless, several independent thermometers
552 yielded relatively cold conditions at any given P (e.g., 889–1081 at 5 GPa; Weiss et al., 2018).
553 Based on these data and the low nitrogen-aggregation state of these diamonds, Weiss et al. (2018)
554 suggested a young formation of diamond from cold, slab-derived fluids, which largely left the
555 ambient mantle thermally unperturbed. This scenario would explain the low T estimates for
556 relatively high-P diamonds, but is at variance with the very old Sm–Nd ages (3.4 Ga) obtained on
557 composite garnet inclusions from De Beers Pool diamonds (Richardson et al., 1984). Therefore,
558 either many of the dated garnets were protogenetic and were not isotopically reset during diamond
559 formation (cf. Nestola et al., 2019a) or both old and young diamonds occur at Kimberley. The
560 occurrence of multiple generations of diamonds at Kimberley is likely, because the gem- or near-
561 gem quality diamonds dated by Richardson et al. (1984) and the cloudy or cuboid-coated diamonds
562 studied by Weiss et al. (2018) belong to totally different genetic populations. An alternative
563 scenario is that the diamonds resided in a deep mantle region that escaped the thermochemical
564 modifications that variably affected the cratonic mantle in the Kimberley area between 120 and 90
565 Ma (cf. Griffin et al., 2003a; Kobussen et al., 2009). This scenario is challenged, however, by the

566 fact that the scarce xenocrysts from depths greater than 160 km plot along the extension of the
567 xenocryst geotherm instead of below it (Fig. 3a).

568 Whatever the significance of the cold signature of Kimberley diamonds, the reason why the
569 kimberlites could efficiently sample diamonds, *but not xenoliths*, from depths greater than 160 km
570 remains mysterious. The strong metasomatic and rheological modifications of the deep lithosphere
571 that occurred in the Cretaceous (Griffin et al., 2003a; Kobussen et al., 2009) may have played a role
572 in this respect. This metasomatism, however, must have been diamond friendly, rather than
573 diamond destructive, if not actually growing diamonds again.

574

575 5.1.3. Voorspoed

576 At Voorspoed, the exsolved texture and composition of the pyroxene inclusions (Viljoen et al.,
577 2018) indicate reequilibration of originally homogeneous pyroxenes as a result of a ~200 °C cooling
578 from initial conditions near the mantle adiabat (~1350–1400 °C at ~5.3 GPa; Fig. 4a). The presence
579 of Cpx and Opx in broadly constant proportions among different inclusions in different diamonds,
580 as well as the occurrence of coesite always at the inclusion margin and often at diamond–Cpx–Opx
581 triple junctions, indicates that exsolution occurred after the incorporation in the diamond. The high
582 nitrogen-aggregation state of most of Voorspoed diamonds is consistent with diamond residence in
583 the mantle at unusually high T (Viljoen et al., 2018). The presence of exsolved coesite and the lack
584 of exsolved Grt indicate that the original Cpx contained a small proportion of Ca-Eskola or
585 supersilicic component (e.g., Harlow, 1999) and could have formed in a silica-saturated, but Grt-
586 undersaturated environment. These considerations, as well as the unreasonable P estimates obtained
587 for the reconstructed pre-exsolution Cpx using the Cr-in-Cpx barometer, indicate that the Cpxs are
588 not derived from garnet peridotites/pyroxenites, despite their compositions being similar to those of
589 websteritic to lherzolitic chromian diopsides, but from unusual (Ca, Si, Cr)-rich, relatively Al-poor
590 mineral assemblages. To our knowledge, the only reported example of this unusual inclusion type is
591 that described by Leost et al. (2003), who found texturally and compositionally similar inclusions in

592 some placer diamonds from Namibia. Leost et al. (2003) interpreted these inclusions as products of
593 extensive carbonation of mantle peridotite. They also ascribed the lack of Grt exsolutions to
594 reequilibration under decreasing T and P (by ~1.5 GPa) after diamond incorporation. This
595 interpretation, however, relied on the assumption that the original pyroxene was Grt-saturated,
596 which is only supported by a single finding of a *non-touching* Cr-rich Grt in one of their diamonds.
597 Similarly, Viljoen et al. (2018) only found *non-touching* Grt in association with some of their
598 exsolved inclusions, namely those with compositions the most similar to lherzolitic. The associated
599 Grts may thus represent relicts of a former peridotitic paragenesis, which was extensively modified
600 by non-equilibrium reactions with the infiltrating hot melt. Accordingly, we consider a decrease of
601 P unnecessary to explain the textures observed in Voorspoed diamonds. An isobaric thermal
602 relaxation from ~1350–1400°C at ~5.3 GPa would equally well explain their textural and
603 compositional features and would avoid the need for large (~50 km) vertical displacement of
604 diamonds through the cratonic lithosphere. The diamond depth distribution which results from
605 projecting the final pyroxene equilibrium T onto the geotherm is, again, distinctly unimodal and
606 unrelated to ‘hard’ petrological or rheological restrictions (Fig. 4b).

607

608 *5.2. Diamond distribution vs kimberlite sampling efficiency*

609

610 Garnet is virtually ubiquitous in cratonic peridotites at P greater than ~2 GPa (Zibera et al.,
611 2013). Clinopyroxene instead is absent in some refractory lithologies, which may be unevenly
612 distributed with depth (e.g., Griffin et al., 2003a). Clinopyroxene is also more prone than Grt to
613 resorption during kimberlite transport (Chepurov et al., 2013) and to alteration after kimberlite
614 emplacement. Therefore, the depth distribution of Grt xenocrysts should generally provide a better
615 assessment of the kimberlite sampling efficiency at different mantle depths.

616 Garnet xenocrysts from the three investigated kimberlite localities (Cullinan, Voorspoed and
617 Kimberley) show either unimodal or polymodal depth distributions, with a principal mode varying

618 between ~150 and ~190 km (Fig. 2–4). Although depths could not be estimated for some Grt types,
619 and specifically for those that classified as eclogitic, the relative abundances of these Grts were very
620 low (1–5%), therefore the obtained depth distributions should not be significantly biased by their
621 exclusion. The Grt distributions show that the sampling of deep-seated material by the respective
622 kimberlites was not uniform throughout the lithospheric mantle, but preferentially concentrated at
623 intermediate depths. The preferential sampling level may vary by several tens of km from one case
624 to another. It should be noted that the Grt xenocrysts do not provide information on Grt-free, spinel
625 peridotites, which may be abundant at relatively shallow depths. The Grt distributions may thus
626 underestimate the kimberlite sampling efficiency at shallow mantle depths, which are, however, not
627 relevant for diamond growth.

628 The depth distributions for peridotitic diamonds from the same kimberlitic sources are
629 essentially unimodal (Fig. 2–4). The value of the mode varies only slightly among the different
630 localities and is centered at $\sim 180 \pm 10$ km. This is somewhat surprising, considering that the
631 diamonds contain different inclusion types, may have very different ages (even within the same
632 kimberlite), and may have been formed by different processes (e.g., fluid-driven vs. melt-driven)
633 under different thermal regimes. At Cullinan, considering the uncertainty in depth estimates for the
634 Grt and Ol inclusions, the diamond mode is not significantly distinct from the Grt xenocryst mode
635 (Fig. 2b). However, the majority of Cpx-bearing lherzolitic diamonds appear to have derived from a
636 mantle level where Cpx-rich material was rare or, at least, undersampled (Fig. 2b). At Voorspoed,
637 the diamond mode (170 km) is close to the main Grt xenocryst mode (165 km), but the diamond
638 depth distribution is very sharp, whereas the xenocryst distributions are polymodal and smeared
639 over a much larger depth interval (Fig. 4b). Finally, at Kimberley, the diamond mode is
640 significantly different from that of the mantle material sampled by the host kimberlite, being shifted
641 to ~40 km greater depths (Fig. 3b). In fact, there is very little xenocryst record (either Cpx or Grt)
642 from mantle levels from which most of the investigated Kimberley diamonds were derived. The fact

643 that formerly spinel-associated xenocrysts from relatively shallow levels were probably
644 undersampled may only reinforce the observed discrepancies.

645 The absence of systematic correlation between the diamond and xenocryst depths suggests that
646 the diamond depth distributions are not a sampling artifact produced by selective kimberlite
647 transport. By extension, the similar diamond mode at ~175 km depth that is observed at global scale
648 (Stachel, 2014) may also reflect a true statistical distribution of diamond in the cratonic lithosphere.
649 Notably, T estimates based on diamond N-aggregation state for eclogitic diamonds worldwide, with
650 the exception of the unusual Argyle diamonds, show a unimodal distribution around ~1150 °C,
651 which is identical to that of peridotitic diamonds (Stachel and Harris, 2008). This suggests that the
652 global mode at ~175 km depth that is observed for peridotitic diamonds may apply to eclogitic
653 diamonds as well. This is despite the tendency for eclogitic xenoliths at many localities to cluster
654 near the lithosphere base (O'Reilly and Griffin, 2010). We also note that a systematic increase in
655 diamond abundance at about this depth would provide the best match between average cratonic
656 shear wave velocities (V_S) according to the SEMUCB_WM1 model (French and Romanowicz,
657 2014) and calculated V_S profiles in the diamond stability field (Garber et al., 2018). This may be
658 independent evidence for higher average concentration of diamond at intermediate lithospheric
659 mantle levels. Possible reasons for the unimodal vertical distribution of diamond are discussed
660 below.

661

662 *5.3. Efficiency of diamond formation/preservation vs. depth*

663

664 In an attempt to derive information on the efficiency of diamond-forming processes vs. depth,
665 we have calculated the amount of diamond precipitated from originally C-saturated COH fluids on
666 their ascent through the mantle using the GFluid model by Zhang and Duan (2010) (Fig. 5). In an
667 earlier study of this type by Huizenga et al. (2012), redox conditions were assumed to be buffered
668 by mantle rocks and were forced to follow P–T and fO_2 –P trends observed in mantle xenoliths. Luth

669 and Stachel (2014) then showed that the redox buffering capacity of cratonic peridotites is actually
670 very low, but that isochemical precipitation of carbon from COH fluids during isobaric cooling or
671 ascent along a cratonic geotherm may be an efficient mechanism of diamond crystallization (see
672 also Stachel and Luth, 2015). In our calculations, and more similar to Luth and Stachel (2014), f_{O_2}
673 was assumed to be controlled by the fluid and to evolve by carbon precipitation or dissolution,
674 while the O/(O + H) molar ratio (hereafter X_O) remained fixed. Different from Luth and Stachel
675 (2014), who used a theoretical cratonic geotherm as reference for their calculations, we calculated
676 the rate of diamond precipitation as a function of depth along P–T trends observed in real diamonds
677 from our investigated kimberlites.

678 Our results for different P–T paths show that the rate of diamond precipitation for a given X_O
679 depends strongly on the P/T gradient and, therefore, on the geometry of the P–T trajectory (Fig. 5).
680 Along a Cullinan-type conductive geotherm (Fig. 2a), roughly corresponding to a ~ 39 mW/m²
681 Hasterok and Chapman (2011) theoretical geotherm, diamond is continuously precipitated from the
682 base of the lithosphere to the diamond–graphite boundary. Overall, the rate of diamond
683 precipitation decreases on ascent, but the most reduced fluids ($X_O < 0.3$) show a peak of diamond
684 formation between 190 and 175 km (Fig. 5a). This peak is shifted to greater depths for fluids along
685 a colder geotherm (Fig. 5b). Along a perturbed geotherm characterized by a lower P/T gradient
686 above ~ 1300 °C, as defined by the highest-T Cullinan diamonds (Fig. 2a), diamond precipitation is
687 significantly boosted for relatively oxidized fluids ($X_O \geq 0.3$) along the inflected limb, reflecting the
688 strong decrease of carbon solubility with decreasing T (Fig. 5c). Along a cold, nearly adiabatic
689 trend, similar to that shown by Kimberley touching inclusions (Fig. 3a), followed by cooling along
690 the conductive geotherm, only relatively reduced fluids precipitate diamond on ascent, whereas
691 those near and beyond the water maximum, i.e., those having an $X_O \geq 0.32$, become increasingly C-
692 undersaturated (Fig. 5d). This is in marked contrast with the high diamond potential of thermally-
693 equilibrated water-rich fluids ascending along conductive cratonic geotherms (cf. Luth and Stachel,
694 2014 and Fig 5a–c). A trajectory similar to that inferred for diamond parent media at Voorspoed,

695 consisting of initial ascent along the mantle adiabat followed by nearly isobaric cooling down to the
696 conductive geotherm (Fig. 4a), would precipitate a large amount of diamond along the cooling path
697 for all but the most reduced fluids (Fig. 5e).

698 Taken at face value, the model rates of diamond precipitation calculated for reduced ($X_{\text{O}} < 0.3$)
699 fluids along conductive or perturbed geotherms would explain the main features of the distribution
700 of diamonds at Cullinan and, specifically, the mode at intermediate depths and even the greater
701 average depth for diamonds falling on the colder geotherm (Fig. 2 and 5a–c). This hypothesis,
702 however, requires that the compositional features of the inclusions, which point to melt-induced
703 metasomatism (Viljoen et al., 2014), are inherited and not directly related to diamond-forming
704 processes. Moreover, the prominent mode in diamond $\delta^{13}\text{C}$ at -5 ± 1 ‰ that is observed at global
705 scale (Cartigny, 2005) and isotopic fractionation modeling imply that, if most diamonds formed
706 from $\text{CH}_4\text{--H}_2\text{O--CO}_2$ fluids, then their $\text{CO}_2/(\text{CO}_2+\text{CH}_4)$ molar ratios should vary within a restricted
707 range, constraining most diamond-producing fluids to more oxidized compositions near the water
708 maximum (Stachel et al., 2017). Such fluids are not expected to produce the mode at intermediate
709 depths that is observed at Cullinan (compare Fig. 2b and 5a–c).

710 The P–T trajectory of diamond parent fluids at Kimberley is not unequivocally determined.
711 Touching inclusions seem to describe a nearly adiabatic, relatively cold path, which intersects the
712 xenocryst geotherm at ~150 km (Fig. 3a). Non-touching inclusions rather seem to follow a
713 relatively cold conductive geotherm running below the xenocryst geotherm (Fig. 3a), intermediate
714 between the hot and cold Cullinan geotherms (cf. Fig. 2a). The overall decrease in the calculated
715 amount of precipitated diamond for CH_4 -rich, very reduced fluids ($X_{\text{O}} = 0.2\text{--}0.3$) along the
716 Kimberley ‘cold adiabatic’ trend (Fig. 5d) might explain the progressive decrease of diamonds at
717 depths shallower than 185 km at this locality, but not the smaller concentration of diamonds near
718 the base of the lithosphere (Fig. 3b). As mentioned above, the involvement of very reduced
719 diamond fluids seems in contrast with isotopic evidence at the global scale (Stachel et al., 2017) and
720 is also challenged by the oxidized nature of fluids entrapped in eight inclusion-rich De Beers Pool

721 diamonds, for which f_{O_2} values less than 1 log unit below the EMOD buffer have been estimated
722 (Weiss et al., 2018). Under these redox conditions, at the P and T recorded by Kimberley diamonds
723 the fluid X_{O} would be greater than ~ 0.32 (Zhang and Duan, 2010). However, based on
724 thermodynamic modeling, these oxygen-rich fluids should not precipitate much diamond along
725 Kimberley-type, ‘cold adiabatic’ trends (Fig. 5d), but only along less steep P/T gradients, such as
726 along a conductive geotherm (cf. Fig. 5a–c). On the other hand, ascent of these fluids along a
727 cratonic geotherm would explain the progressive decrease of diamonds at depths shallower than 185
728 km (cf. Fig. 5a–c), but, again, not the smaller concentration of diamonds near the base of the
729 lithosphere (Fig. 3b).

730 The prominent peak in diamond precipitation rate at ~ 170 km that is observed for the
731 Voorspoed P–T trend, especially for fluids near the water-maximum (Fig. 5e), shows an interesting
732 correspondence with the diamond depth mode at this locality (Fig. 4b). This peak reflects the strong
733 decrease in diamond solubility that is determined by a decrease of T and supports the potential role
734 of isobaric cooling in producing diamonds (Luth and Stachel, 2014). A possible scenario for such a
735 process might be fluid exsolving from a crystallizing magma and precipitating diamond on cooling
736 to ambient mantle temperature (Luth and Stachel, 2014). Alternatively, diamond may directly
737 precipitate from the cooling crystallizing magma, due to concentration of carbonate components
738 and reduction of the redox stability field of the melt (Stagno et al., 2015). Both scenarios seem
739 indeed suitable for Voorspoed diamonds, given the high-T, melt-metasomatic nature of their
740 inclusions.

741 Despite the apparent success of simplified COH fluid models to reproduce the diamond depth
742 distribution at Voorspoed, their apparent inability to fully predict the observed diamond
743 distributions at Cullinan and Kimberley suggests that either these models are not representative of
744 real diamond-forming media or additional factors other than carbon solubility played a significant
745 role. A possible reason for the limitations of traditional COH models is because they do not
746 consider the influence of dissolved species other than $\text{CH}_4\text{--H}_2\text{O--CO}_2\text{--H}_2\text{--C}_2\text{H}_6$ (Sverjensky and

747 Huang, 2015). For instance, Tiraboschi et al. (2018) found that carbon solubility increased in (Mg,
748 Si)-bearing COH fluids relative to pure COH in experiments at relatively low P–T (1.0–2.1 GPa,
749 700–1200 °C) and high fO_2 (NNO buffer). Real mantle fluids certainly contain Mg, Si and other
750 non-COH species, even in significant concentrations (cf. the high-density fluids found in many
751 fibrous and some monocrystalline diamonds; e.g., Schrauder and Navon, 1994; Klein-BenDavid et
752 al., 2007; Jablon and Navon, 2016; Weiss et al., 2014, 2018), but the behavior of these complex
753 systems at P–T– fO_2 relevant for diamond precipitation is still unknown. A further complication is
754 that some diamond-forming fluids were reported to contain significant or even dominant
755 proportions of a variety of hydrocarbons heavier than methane (Sobolev et al., 2019), which are not
756 contemplated in available fluid models. Finally, many diamonds may form from carbonate-bearing
757 melts rather than from COH fluids (Stachel and Luth, 2015). This might be relevant particularly for
758 Voorspoed diamonds, as the unusual nature of their inclusions would be consistent with a hot, melt-
759 rich environment, and probably also for most Cullinan diamonds (Korolev et al., 2018).

760 Even in the absence of robust thermodynamic models for natural diamond-forming
761 fluids/melts, some qualitative considerations can be made. All calculated fluid models for a variety
762 of possible P–T paths predict overall decreasing precipitation rates for diamond with decreasing
763 depth from at least 165–185 km (Fig. 5). This suggests that the progressive decrease in diamond
764 concentrations at shallower depths (Fig. 2–4), a feature that seems to be shared by diamonds at
765 global scale (Stachel, 2014), may be due to decreasing precipitation rates for diamond from
766 ascending mantle fluids and melts. Alternatively, the observed decrease of diamonds may reflect
767 progressive volume reduction of infiltrating fluids/melts at shallower levels and consequent
768 reduction of the carbon load transported upwards. The progressive decrease of diamonds near the
769 base of the lithosphere that is shown by Cullinan, Kimberley and Voorspoed diamonds (Fig. 2–4)
770 also seems to be shared by diamonds at global scale (Stachel, 2014). An increasing diamond
771 endowment with increasing distance from the lithosphere base might reflect a positive balance
772 between the opposed effects that a decrease of P and a decrease of T may have on carbon solubility

773 in rising fluids/melts, similar to what predicted for some model COH fluids under moderately hot
774 cratonic conditions (Fig. 5a). Moreover, deep lithospheric regions are exposed to infiltration of
775 asthenospheric melts, which may be undersaturated relative to diamond (e.g., Malkovets et al.,
776 2001; Bobrov and Litvin, 2009). Therefore, their diamond endowment might have decreased over
777 time due to diamond resorption. Possible supporting evidence is the increasing proportion of melt-
778 metasomatized lithologies towards the base of the lithosphere as indicated by the trace-element
779 composition of Grt xenocrysts at the investigated localities (Fig. 6; see also Griffin et al., 2003a), a
780 feature that, again, is shared by many cratonic lithosphere sections (Griffin et al., 2003b).
781 Remobilization of carbon from the deepest cratonic roots by these metasomatic agents could
782 eventually contribute to build the global diamond mode some distance into the shallower
783 lithosphere. Under some conditions, infiltration of relatively cold (e.g., subduction-related),
784 thermally non-equilibrated, water-rich fluids might also contribute to diamond resorption in these
785 deep lithospheric regions (Fig. 5d), but this hypothesis awaits confirmation based on modeling of or
786 experiments in complex fluid-bearing systems.

787

788 **6. Conclusions**

789

790 Diamonds may form at temperatures higher, equal or lower than the ambient geotherm
791 recorded by mantle xenocrysts at eruption time. They may record old mantle thermal regimes or
792 local thermal perturbation in the lithosphere related to infiltration of parental fluids and melts.
793 These thermal perturbations may be both positive and negative.

794 Inclusion-bearing diamonds belonging to harzburgitic, lherzolithic and even undetermined,
795 metasomatic parageneses show similar depth distributions at different localities, with a distinct
796 mode at $\sim 180 \pm 10$ km. Several lines of evidence indicate that this locality-specific mode has global
797 significance: (i) similarity with the overall depth distribution calculated for inclusion-bearing
798 diamond worldwide (~ 175 km); (ii) lack of correlation with kimberlite sampling efficiency as

799 recorded by mantle xenocrysts; (iii) compatibility with independent inferences derived from shear-
800 wave velocity profiles for cratonic mantle.

801 Based on observed diamond depth distributions at both local and global scale, diamond-
802 forming processes are predicted to become less efficient with decreasing depth from at least ~165
803 km, probably irrespective of the diamond-forming process (e.g., fluid-driven vs. melt-driven). In
804 addition, diamond endowment near the base of the lithosphere may be negatively affected by
805 infiltration of carbon-undersaturated melts or fluids.

806 Considering the poor correlation between diamond and xenocryst depth distributions in single
807 kimberlites or kimberlite clusters, even limited xenocryst records from diamond favorable depths
808 (especially the 160–190 km interval) may correspond to significant diamond potential. This interval
809 should be considered as indicative of high diamond potential in mineralogical exploration for
810 diamond.

811 Despite the large number of published electron microprobe analyses for inclusions in diamonds
812 from worldwide localities, after rigorous compositional screening for robust thermobarometry there
813 are still very limited analyses that can be used, particularly for pressure estimation. The
814 interpretation of diamond depth distribution data would greatly benefit from additional P–T
815 estimates for diamonds from the same localities studied here, as well as from statistically significant
816 datasets for diamonds from other localities. Alternate methods for diamond barometry that are
817 independent of chemical equilibria, such as the still underutilized and, in part, underdeveloped
818 elastic methods (Nimis, 2018; Nestola et al., 2018, 2019b), may greatly increase the variety of
819 diamonds amenable to barometry and should be undertaken whenever possible.

820

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829

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- 1076

1077 **Appendix**

1078

1079 **Empirical correction to the Nimis and Taylor (2000) single-Cpx barometer**

1080

1081 We have compared independent P estimates for 424 well-equilibrated Cpx–Opx–Grt-bearing mantle
1082 xenoliths using the single-Cpx barometer of Nimis and Taylor (2000) and the Opx–Grt barometer of
1083 Nickel and Green (1985), as modified by Carswell (1991) (Fig. A1). The xenoliths were derived
1084 from the compilation of Nimis and Grütter (2010), filtered following recommendations in Ziberna
1085 et al. (2016) (cf. Fig. 4b in Ziberna et al., 2016). For both barometers, input T for P calculation was
1086 derived by using the Taylor (1998) thermometer and both P and T were then calculated by iteration.
1087 The Taylor (1998) thermometer has been evaluated to be the most robust for natural peridotites and
1088 pyroxenites and yields T estimates very similar to those obtained by using the Nimis and Taylor
1089 (2000) single-Cpx thermometer (Nimis and Grütter, 2010). The results show the well-known
1090 tendency of the Cpx barometer to underestimate P at high P (Nimis, 2002; Ziberna et al., 2016). The
1091 scatter of the points around the best-fit line suggests an overall precision of better than ± 0.5 GPa for
1092 each of the two barometers.

1093 An empirical correction was then determined based on a second-order polynomial fit through the
1094 xenolith data. We preferred to use xenoliths rather than experimental data because most
1095 experimental Cpxs other than those used for the barometer calibration were either too high-T (at or
1096 above peridotite solidus) or had compositions that would have not survived the Ziberna et al. (2016)
1097 filters for optimum thermobarometry. The correction is formulated as follows:

1098

1099 $P_{\text{NT,corr}} = 0.05024(0.022) \cdot P_{\text{NT}}^2 + 0.7633(0.17) \cdot P_{\text{NT}} + 0.1257(0.34),$

1100

1101 where P_{NT} is the P (GPa) calculated with the original Nimis and Taylor (2000) formulation and
1102 numbers in parentheses are standard errors from the fitting procedure. When applied to the natural

1103 xenoliths, the correction improves the overall consistency between the two barometers, but at the
1104 expense of somewhat increased scatter (Fig. A2). The correction should therefore be considered as a
1105 band aid measure, which is meant to reduce systematic discrepancies between independent P
1106 estimates when comparing large datasets, rather than a working ‘improvement’ of the Nimis and
1107 Taylor (2000) barometer.
1108

1109 **Figure captions**

1110

1111 **Fig. 1.** Sketch map of the Kaapvaal craton (modified after Eglington and Armstrong, 2004) with
1112 location of the kimberlites studied. K: Kimberley cluster; V: Voorspoed; C: Cullinan.

1113

1114 **Fig. 2.** (a) P–T estimates for xenocrysts, diamond inclusions and diamondiferous xenolith from the
1115 Cullinan kimberlite. Two Cpx geotherms (black solid lines with 95% confidence bands) are
1116 modeled by FITPLOT by fitting P–T estimates for xenocrysts plotting above and, respectively,
1117 below the dashed line. Minimum and maximum P estimates for the Ol and Grt inclusions were
1118 obtained by projecting their Al-in-Ol or Ni-in-Grt temperatures on the hot and cold model
1119 geotherms, respectively. For the hot geotherm, an inflection relative to the xenocryst geotherm was
1120 assumed at $T > 1300$ °C. Only Ol and Grt inclusions recording a $T < 1300$ °C were projected also
1121 on the cold geotherm, as no Cpx inclusions recording higher T fall on this geotherm. The two open
1122 symbols indicate two high-P Cpx inclusions with compositions close to the limit for reliable single-
1123 Cpx barometry. (b) Depth distributions for xenocrysts and diamond inclusions from the Cullinan
1124 kimberlite. Depths for low-T (< 1300 °C) Ol and Grt inclusions in the two lower graphs were
1125 calculated by projection onto ‘hot’, inflected and ‘cold’, non-inflected model geotherms,
1126 respectively (cf. (a)). Classification of Grt xenocrysts (HZB: harzburgitic; LHZ: lherzolitic; HTi:
1127 high-Ti peridotitic; WEH: wehrlitic; MEG: megacrystic) after Grütter et al. (2004). GD: graphite-
1128 diamond boundary after Day (2012). LA: lithosphere-asthenosphere boundary, corresponding to the
1129 depth where the projection of the conductive geotherm intersects the isentrope. Compositional data
1130 for diamond inclusions and diamondiferous xenolith after (Korolev et al., 2018; Viljoen et al., 2004,
1131 2014; and this work)

1132

1133 **Fig. 3.** (a) P–T estimates and FITPLOT model geotherm (black solid line with 95% confidence
1134 bands) and (b) relative depth distributions for xenocrysts and diamond inclusions from Kimberley

1135 kimberlites. Encircled outliers in (a) may belong to Opx-free parageneses; therefore, their P–T
1136 estimates are unreliable and were excluded from geotherm fitting. Note that the few xenocrysts
1137 recording $T > 1200^{\circ}\text{C}$ have negligible influence on the shape of the model geotherm. The dashed
1138 lines marked *t* and *nt* in (a) are the best fits of P–T estimates for the touching (Opx–Grt) and non-
1139 touching (Opx–Grt and Cpx) inclusions, respectively. Classification of Grt xenocrysts (HZB:
1140 harzburgitic; LHZ: lherzolitic; HTi: high-Ti peridotitic; WEH: wehrlitic; MEG: megacrystic) after
1141 Grütter et al. (2004). GD: graphite-diamond boundary after Day (2012). LA: lithosphere-
1142 asthenosphere boundary, corresponding to the depth where the projection of the conductive
1143 geotherm intersects the isentrope. Compositional data for diamond inclusions after Phillips et al.
1144 (2004).

1145

1146 **Fig. 4.** (a) P–T estimates and FITPLOT model geotherm (black solid line with 95% confidence
1147 bands) and (b) relative depth distributions for xenocrysts and diamond inclusions from the
1148 Voorspoed kimberlite. Encircled outliers in (a) may belong to Grt-free (<3 GPa) or Opx-free (6-7
1149 GPa) parageneses; therefore, their P–T estimates are unreliable and were excluded from geotherm
1150 fitting. P estimates for the reconstructed, pre-exsolution Cpx inclusion compositions are
1151 incompatible with diamond, suggesting derivation from very unusual, possibly Grt-free mineral
1152 assemblages. The hatched area in (a) indicates the most probable conditions of diamond growth.
1153 The dashed arrow in (a) indicates a possible P–T trajectory for the diamond-forming fluids.
1154 Classification of Grt xenocrysts (HZB: harzburgitic; LHZ: lherzolitic; HTi: high-Ti peridotitic;
1155 WEH: wehrlitic; MEG: megacrystic; PRX: pyroxenitic) after Grütter et al. (2004). GD: graphite-
1156 diamond boundary after Day (2012). LA: lithosphere-asthenosphere boundary, corresponding to the
1157 depth where the projection of the conductive geotherm intersects the isentrope. Compositional data
1158 for diamond inclusions after Viljoen et al. (2018). Data for kyanite inclusion in single eclogitic
1159 diamond after Nestola et al. (2018).

1160

1161 **Fig. 5.** Moles of precipitated C from 1 mole of initial C-saturated COH fluid evolving along
1162 different P–T paths: (a) the conductive geotherm defined by most Cullinan xenocrysts (Fig. 2a); (b)
1163 the colder conductive geotherm defined by some Cullinan xenocrysts and diamonds (Fig. 2a); (c) a
1164 ‘hot inflected’ geotherm which follows the P–T trend of high-T Cullinan diamonds at $T > 1300$
1165 (Fig. 2a) and the Cullinan ‘hot’ geotherm at lower T; (d) the cold, nearly adiabatic trend described
1166 by touching inclusions in Kimberley De Beers Pool diamonds (Fig. 3a), followed by cooling along
1167 the xenocryst geotherm; (e) the path inferred for parent fluids of Voorspoed diamonds, comprising
1168 adiabatic ascent at high T, followed by nearly isobaric cooling down to the xenocryst geotherm and
1169 further cooling along the geotherm (Fig. 4a). Calculations were made at 0.5-GPa steps for fluids
1170 with fixed X_{O} of 0.2 to 0.4 using the GFluid model of Zhang and Duan (2010), starting from 7 GPa
1171 (6.5 GPa for the Cullinan inflected geotherm). Pressures are plotted at mid-step values. Ranges of
1172 X_{O} calculated with GFluid at the enstatite–magnesite–olivine–diamond buffer (Luth and Stachel,
1173 2014) for the different P–T conditions are reported for reference. In gray areas, the fluids are
1174 undersaturated with respect to diamond. The hatched regions indicate the depths of maximum
1175 frequency for peridotitic diamonds worldwide (Stachel, 2014).

1176
1177 **Fig. 6.** Relative proportions of Grt xenocrysts from different compositional classes, plotted against
1178 depth, for Cullinan, Kimberley and Voorspoed kimberlites. Depth sections with less than ten
1179 records were not plotted. The numbers of the xenocrysts used for the plots and of the entire data sets
1180 are given in parentheses after the locality names. Grt classification after Griffin et al. (2002). D –
1181 depleted; DM – depleted, fluid-metasomatised; F – fertile; MM – melt-metasomatised; OTH –
1182 others.

1183
1184 **Fig. A1.** Comparison between P estimates for 767 well-equilibrated mantle xenoliths (Nimis and
1185 Grütter, 2010) using the single-Cpx barometer of Nimis and Taylor (2000) and the Opx–Grt
1186 barometer of Nickel and Green (1985), as modified by Carswell (1991). The red line with shaded

1187 95% confidence bands is the second order polynomial fit through the data. A single outlier (gray
1188 filled circle) was excluded from fitting.

1189

1190 **Fig. A2.** Same data as in Fig. A1, but using the empirically corrected expression for the Nimis and
1191 Taylor (2000) barometer.