

1 Pressure induced speciation changes in the aqueous
2 Al^{3+} system.

3 *Supplementary Information*

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5 *Stuart Bogatko, Paul Geerlings*

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7 Eenheid Algemene Chemie, Vrije Universiteit Brussel (VUB), Faculteit Wetenschappen,
8 Pleinlaan 2,
9 1050 Brussels, Belgium.

10 CORRESPONDING AUTHOR FOOTNOTE:

11 Email: stuart.bogatko@gmail.com

12 Telephone: +32-2-629-3316

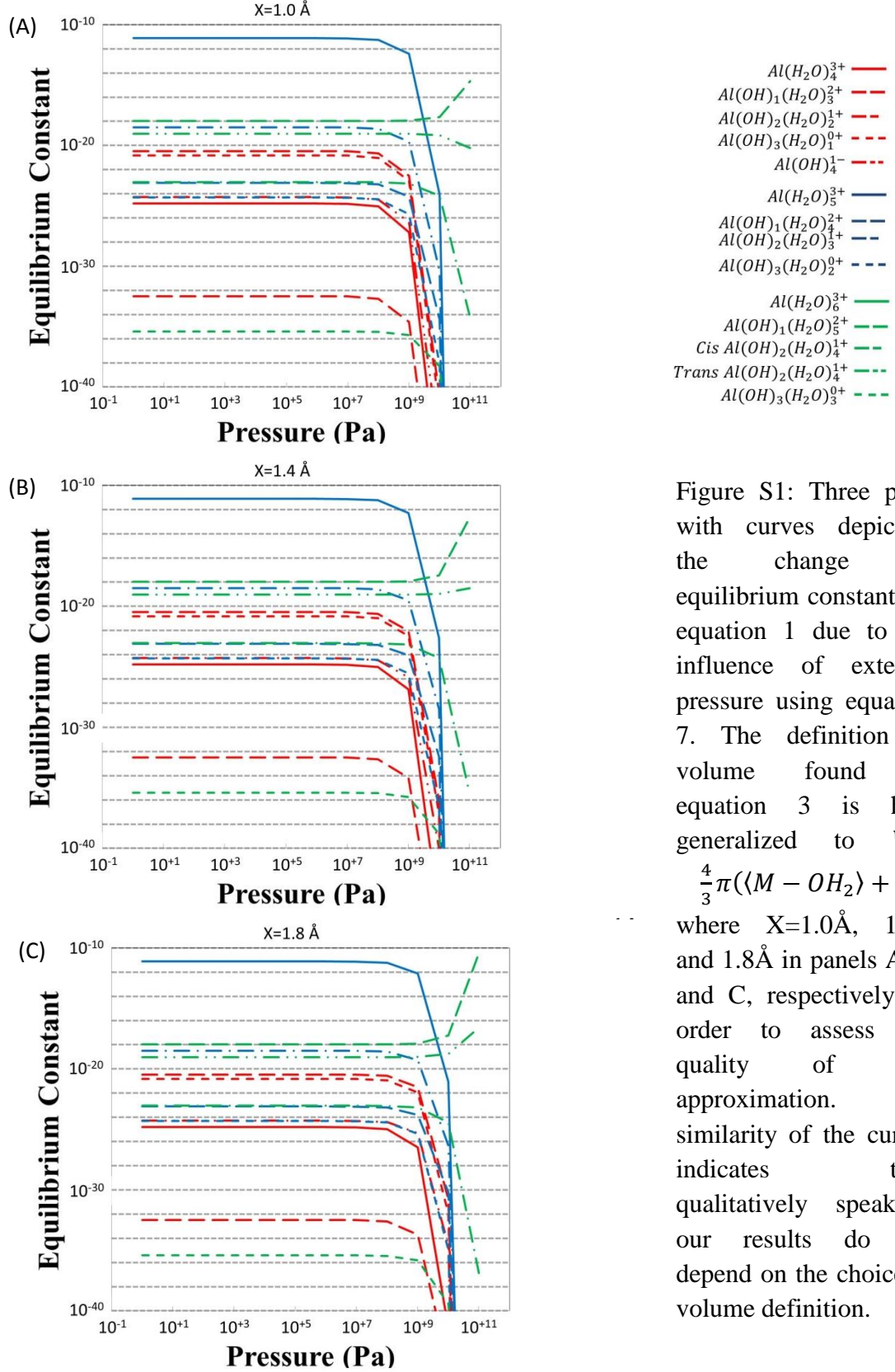


Figure S1: Three plots with curves depicting the change in equilibrium constants of equation 1 due to the influence of external pressure using equation 7. The definition of volume found in equation 3 is here generalized to $V = \frac{4}{3}\pi(\langle M - OH_2 \rangle + X)^3$ where $X=1.0\text{\AA}$, 1.4\AA and 1.8\AA in panels A, B and C, respectively, in order to assess the quality of this approximation. The similarity of the curves indicates that, qualitatively speaking, our results do not depend on the choice of volume definition.

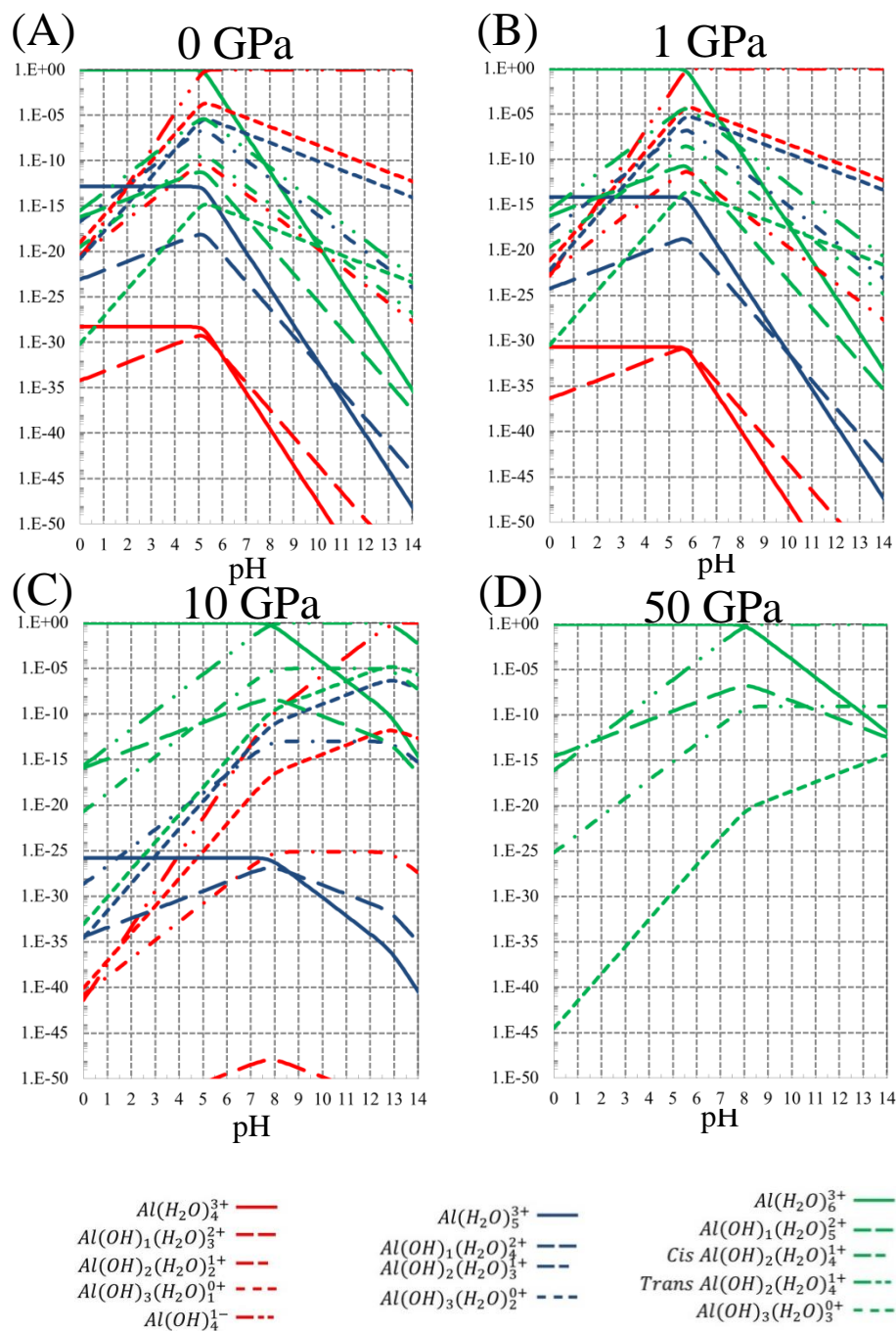


Figure S2: Mole fraction distributions computed at modelled external pressures of 0 (A), 1 (B), 10 (C) and 50 (D) GPa following the procedure outlined in the text except for the substitution of 1.0Å in place of 1.4Å in equation 3. Comparison of Figure 2 in the manuscript suggests only minor effects arising from changes in the species volume definition. The similarity of the curves indicates that, qualitatively speaking, our results do not depend on the choice of volume definition.

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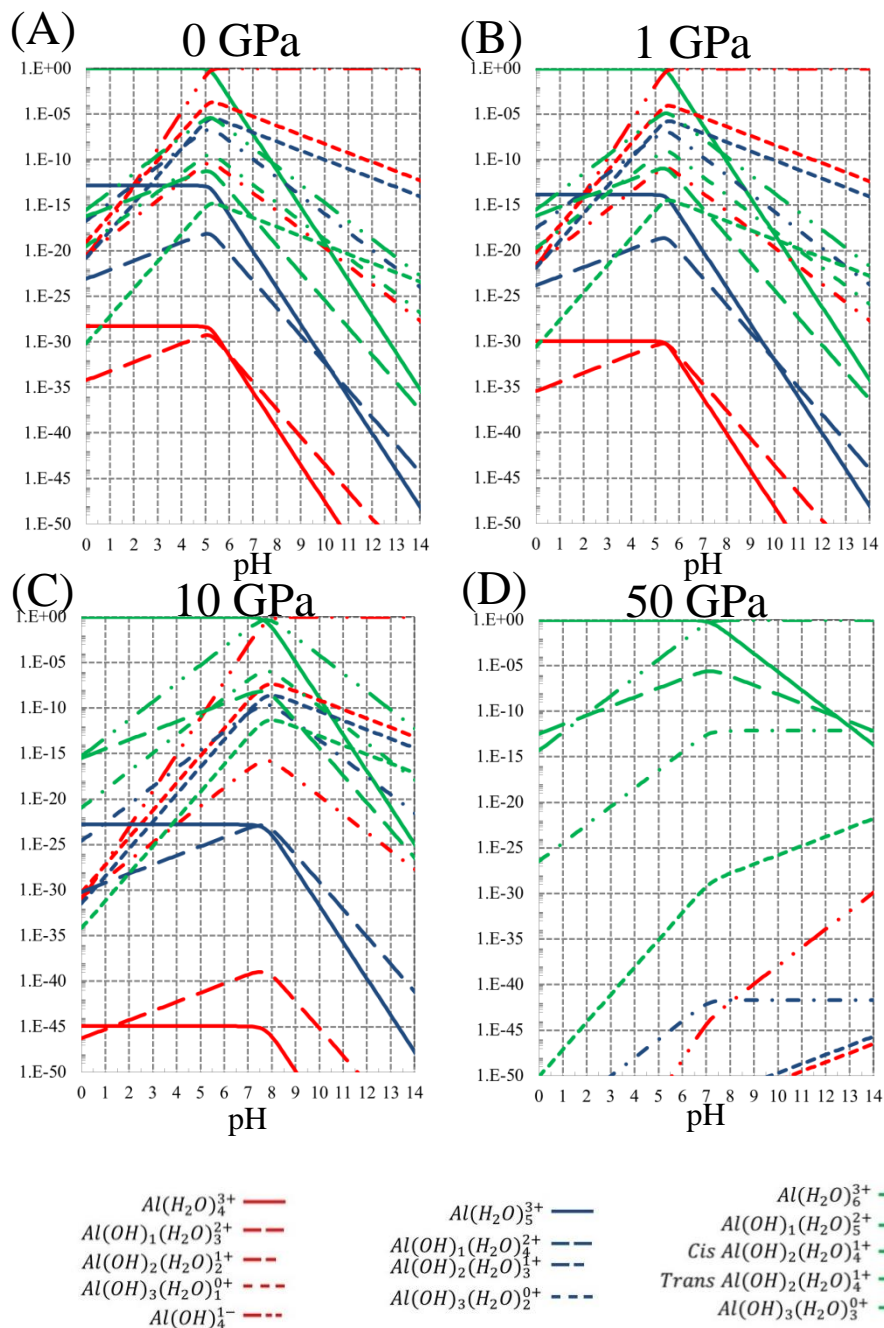


Figure S3: Mole fraction distributions computed at modelled external pressures of 0 (A), 1 (B), 10 (C) and 50 (D) GPa following the procedure outlined in the text except for the substitution of 1.8Å in place of 1.4Å in equation 3. Comparison of Figure 2 in the manuscript suggests only minor effects arising from changes in the species volume definition. The similarity of the curves indicates that, qualitatively speaking, our results do not depend on the choice of volume definition.

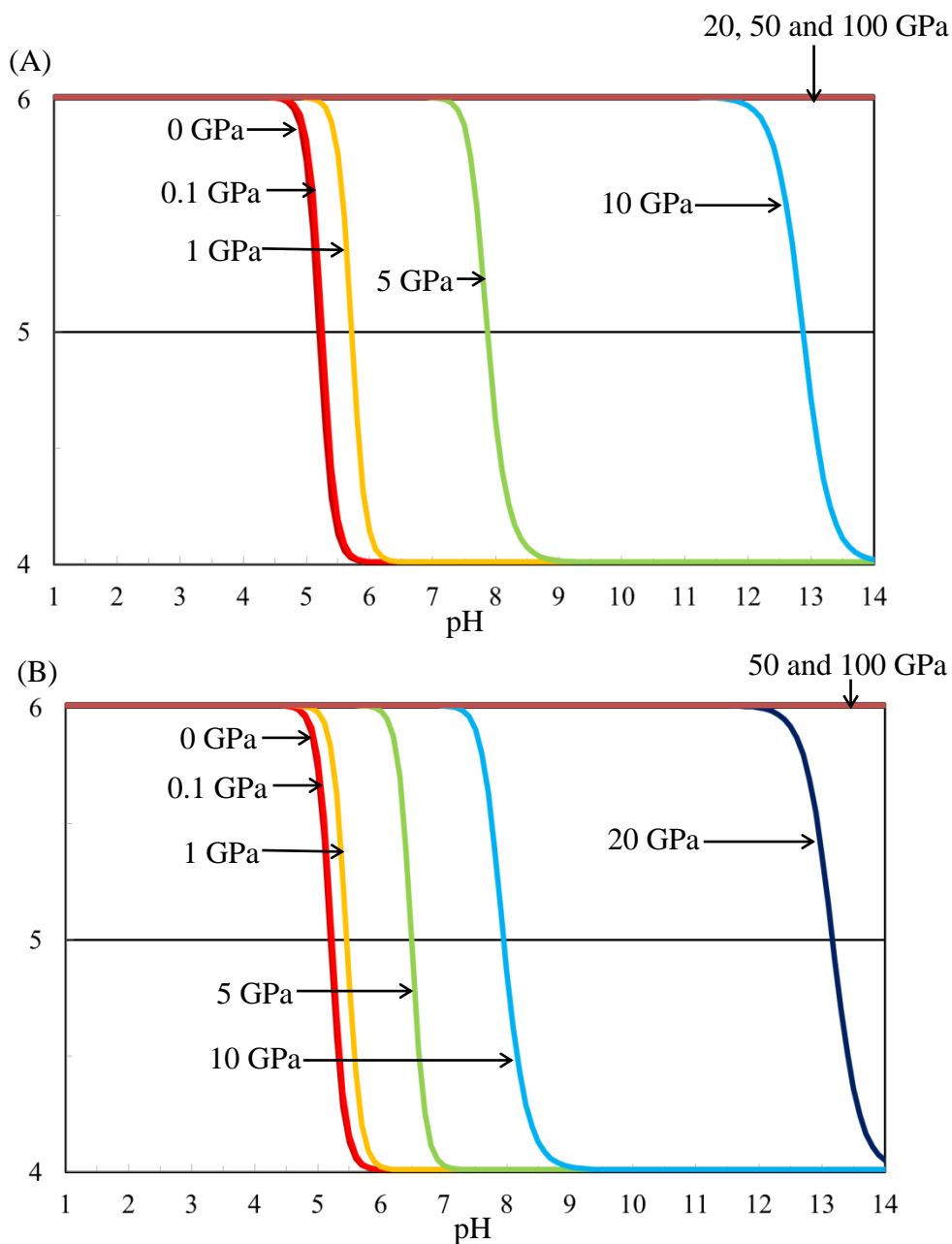


Figure S4: The average total coordination number (CN) of all species is plotted against solution pH for 8 contours corresponding to external pressures of 0, 0.1, 1, 5, 10, 20, 50 and 100 GPa. Panels A and B indicate data generated using a variant of equation 3 in the manuscript wherein 1.4\AA is replaced by 1.0\AA (A) and 1.8\AA (B). Note that curves for 0 and 0.1 GPa are overlying in A and B; those for 20, 50 and 100 GPa are also superimposed in panel A while only 50 and 100 GPa curves are overlying in panel B. Comparison with Figure 3 in the manuscript indicate that all three volume definitions result in the same behavior. The similarity of the curves indicates that, qualitatively speaking, our results do not depend on the choice of volume definition.