# Compensation of the Meyer-Neldel Compensation Rule – Online Auxiliary Supplementary material

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### 1) Arrhenius model parameters reported in the literature for hydrogen diffusion in minerals.

Table S1: Arrhenius model parameters reported in the literature for hydrogen diffusion in minerals. The underlined italicized values, labelled D or E in the Deleted/Excluded/Culled/Removed column, were not used in the regressions, either because they are suspect or they are repeats that appear in another publication. Values culled during Least Trimmed Squares robust linear regression are indicated by a "C" in the Deleted/Excluded/Culled/Removed column with the number denoting the iteration that the point was culled. Values removed from the datasets due to considerations of experimental issues indicated by an "X".

| **Reference** | **E (eV)** | **E (kJ/mol)** | **$\log_{10}(D_0$ [$m^2/s$])** | **Comment** | **Duplicate (D) or Excluded (E). Iteratively Culled (C) or Removed (X)** |
|---|---|---|---|---|---|
| **Olivine – 24 values for LTS iteration, 15 subjectively selection** | | | | | |
| *Mackwell and Kohlstedt* [1990] | 1.35 | 130 | -4.22 | [100], 0.3 GPa | |
| | *1.35* | *130* | *-5.30* | [001], 0.3 GPa, assumed same ΔH as for [100] so is suspect value | E |
| *Kohlstedt and Mackwell* [1999] | 1.50 | 145 | -3.85 | [100] | |
| | 1.87 | 180 | -3.82 | [010] | |
| | 1.14 | 110 | -6.83 | [001] | |
| *Demouchy and Mackwell* [2003] | 2.18 | 210 | -3.30 | Forsterite [001] | |
| | 2.12 | 205 | -4.10 | Forsterite [010] | |
| | 2.33 | 225 | -3.80 | Forsterite [100] | |
| *Demouchy and Mackwell* [2006] | 2.11 | 204 | -4.5 | [100] & [010] analysed together, 0.2 GPa | |
| | 2.67 | 258 | -1.4 | [001], 0.2 Gpa | |
| *Ingrin and Blanchard* [2006] | 1.39 | 134 | -7.50 | Forsterite with 0.25 wt% Fe; based on *Libowitzky and Beran* [1995] < 100 ppm $H_2O$. Not a direct measurement. | X, C2 |
| | 1.45 | 140 | -5.80 | γ-Spinel (synthetic, Mg2GeO4) | X |
| *Zhao and Zheng* [2007] review | 1.19 | 115 | -7.91 | Ionic porosity. Not experimental data | X, C3 |
| | *2.18* | *210* | *-3.30* | Forsterite – *Demouchy and Mackwell* [2003] result | D |
| | *2.12* | *205* | *-4.10* | Forsterite – *Demouchy and Mackwell* [2003] result | D |
| | *2.33* | *225* | *-3.80* | Forsterite – *Demouchy and Mackwell* [2003] result | D |
| | *1.35* | *130* | *-4.22* | Olivine – *Mackwell and Kohlstedt* [1990] result | D |
| *Demouchy* [2010]; 2012] | 0.74 | 71 | -6.2 | Effective diffusion; grain boundary & grain interior; fine-grained aggregate, 0.3 GPa | X |

| | | | | | |
|---|---|---|---|---|---|
| | 0.56 | 54 | -3.4 | Grain boundary diffusion, 0.3 GPa | X, C1 |
| *Farver* [2010] review | *1.39* | *134* | *-7.49* | Forsterite (0.25 wt% Fe), natural single Xal - *Ingrin and Blanchard* [2006] result | D |
| | *1.35* | *130* | *-4.22* | Olivine (Mg0.91Fe0.09Ni0.003)2SiO4, natural singal Xal - *Mackwell and Kohlstedt* [1990] result | D |
| | *1.35* | *130* | *-5.30* | Olivine (Mg0.91Fe0.09Ni0.003)2SiO4, natural single Xals - *Mackwell and Kohlstedt* [1990] excluded result | D |
| | 1.14 | 110 | -6.59 | Olivine (Mg0.91Fe0.09Ni0.003)2SiO4, natural single Xals – *Kohlstedt and Mackwell* [1998] | |
| | 1.50 | 145 | -3.52 | Olivine (Mg0.91Fe0.09Ni0.003)2SiO4, natural single Xals – *Kohlstedt and Mackwell* [1998] | |
| | 1.87 | 180 | -3.21 | Olivine (Mg0.91Fe0.09Ni0.003)2SiO4, natural single Xals – *Kohlstedt and Mackwell* [1998] | |
| | *2.18* | *210* | *-3.30* | Forsterite, synthetic single Xals - *Zhao and Zheng* [2007] result | D |
| | *2.12* | *205* | *-4.10* | Forsterite, synthetic single Xals - *Zhao and Zheng* [2007] result | D |
| | *2.33* | *225* | *-3.80* | Forsterite, synthetic single Xals - *Zhao and Zheng* [2007] result | D |
| *Brady and Cherniak* [2010] online database (http://diffusion.smith.edu/) | *2.11* | *204* | *-4.5* | Olivine - *Demouchy and Mackwell* [2006] result | D |
| | *2.67* | *258* | *-1.4* | Olivine - *Demouchy and Mackwell* [2006] result | D |
| | *1.35* | *130* | *-4.22* | Olivine – in *Farver* [2010] compilation | D |
| | 1.27 | 123 | -5.02 | Wadsleyite | X |
| *Du Frane and Tyburczy* [2012] | 1.52 | 147 | -4.60 | [100] (data modelled by Jones) | |
| *Zhang* [2012] | 1.60 | 154 | -4.88 | cBΩ model, [001] | X |
| | 1.84 | 177 | -3.80 | cBΩ model, [010] | X |
| | 1.56 | 151 | -3.56 | cBΩ model, [100] | X |
| *Padrón-Navarta et al.* [2014] | 3.07 | 296 | -1.1 | [Ti] + [Si] in Ti-doped fosterite | |
| | 4.78 | 461 | 3.3 | [Si] in undoped MgO-buffered fosterite | |
| **Pyroxenes – 15 values for LTS iteration, 15 subjectively selected [M]: monoclinic [O]: orthoclinic** | | | | | |
| *Ingrin et al.* [1995] | 1.41 | 136 | -6.30 | [M] Diopside, fit to all three crystallography directions | |
| *Stalder and Skogby* [2003] | 3.06 | 295 | 0.14 | [O] Pure enstatite | |
| | 2.21 | 213 | -1.74 | [O] Orthopyroxene | |
| *Ingrin and Blanchard* [2006] review | 1.54 | 149 | -3.40 | [M] Diopside Fe/(Fe+Mg) = 0.036; ~10-40 ppm H2O, *Hercule and Ingrin* [1999] | |
| | 1.48 | 143 | -5.00 | [M] Diopside Fe/(Fe+Mg) = 0.036; ~10-40 ppm H2O, *Hercule and Ingrin* [1999] | |
| *Zhao and Zheng* [2007] review | *1.41* | *136* | *-6.30* | Diopside, *Ingrin et al.* [1995] | D |
| | *1.88* | *181* | *-2.10* | Diopside – in *Farver* [2010] compilation | D |
| | *1.59* | *153* | *-3.40* | Diopside – in *Farver* [2010] compilation | D |
| | *1.54* | *149* | *-3.40* | Diopside, *Hercule and Ingrin* [1999] – in *Ingrin and Blanchard* [2006] compilation | D |
| | *1.48* | *143* | *-5.00* | Diopside, *Hercule and Ingrin* [1999] – in *Ingrin and Blanchard* [2006] compilation | D |

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|---|---|---|---|---|---|
| | *3.06* | *295* | *0.13* | Enstatite, *Stalder and Skogby* [2003] result | D |
| | *2.21* | *213* | *-1.75* | Orthopyroxene, *Stalder and Skogby* [2003] result | D |
| *Sundvall et al.* [2009b] | 3.43 | 331 | 0.90 | [M] Diopside, [010], very large error on $\log_{10}(D_0)$ of (0.9 ±2.3) | |
| | 3.23 | 312 | 0.50 | [M] Diopside, [100], very large error on $\log_{10}(D_0)$ of (0.5 ±2.4) | |
| *Sundvall et al.* [2009a] | 3.02 | 292 | -1.9 | [M] Synthetic Fe-poor diopside [010], very large error on $D_0$ (-1.9 ±2.3) | |
| *Farver* [2010] Review paper | *1.54* | *149* | *-3.40* | Diopside, (Fe/Fe+Mg)=0.036, natural single Xal, *Hercule and Ingrin* [1999] – in *Ingrid and Blanchard* [2006] compilation | D |
| | *1.48* | *143* | *-5.00* | Diopside, (Fe/Fe+Mg)=0.036, natural single Xal, *Hercule and Ingrin* [1999] – in *Ingrin and Blanchard* [2006] compilation | D |
| | 1.88 | 181 | -2.10 | [M] Diopside (Fe/(Fe+Mg)=0.07), natural single Xals, *Carpenter-Woods et al.* [2000] | |
| | 1.59 | 153 | -3.40 | [M] Diopside (Fe/(Fe+Mg)=0.07), natural single Xals, *Carpenter-Woods et al.* [2000] | |
| | 1.31 | 126 | -6.70 | [M] Diopside (Fe/(Fe+Mg)=0.036), natural single Xals, *Ingrin et al.* [1995] | |
| | *1.31* | *126* | *-6.70* | Diopside (Fe/(Fe+Mg)=0.036), natural single Xals, *Hercule and Ingrin* [1999] – combined with data from *Ingrin et al.* [1995] | D |
| | 1.11 | 107 | -6.64 | [M] Diopside (Fe/(Fe+Mg)= 0.05, natural, *Hercule* [1996] | |
| | 1.13 | 109 | -5.70 | [M] Diopside (Fe/(Fe+Mg)=0.126, natural, *Hercule* [1996] | |
| | *3.06* | *295* | *0.15* | Enstatite, synthetic single Xals, *Stalder and Skogby* [2003] | D |
| | 2.00 | 193 | -4.69 | [O] Enstatite-Ferrosilite synthetic single Xals, Fe-doped, *Stalder et al.* [2007] | |
| | *3.43* | *331* | *0.90* | Diopside, synthetic single Xals, *Sundvall et al.* [2009b] | D |
| | *3.23* | *312* | *0.48* | Diopside, synthetic single Xals, *Sundvall et al.* [2009b] | D |
| *Brady and Cherniak* [2010] online database (http://diffusion.smith.edu/) | *3.23* | *312* | *0.50* | Diopside – in *Farver* [2010] compilation | D |
| | *3.43* | *331* | *0.90* | Diopside – in *Farver* [2010] compilation | D |
| | *1.59* | *153* | *-3.40* | Diopside – in *Farver* [2010] compilation | D |
| | *1.88* | *181* | *-2.10* | Diopside – in *Farver* [2010] compilation | D |
| | *3.06* | *295* | *-0.14* | Enstatite – in *Farver* [2010] compilation | D |
| | *2.21* | *213* | *-1.74* | Orthopyroxene - *Stalder and Skogby* [2003] | D |
| | 1.79 | 173 | -6.18 | [O] Orthopyroxene, *Stalder et al.* [2007] | C1 |
| | *2.00* | *193* | *-4.69* | Orthopyroxene – in *Farver* [2010] compilation | D |
| **Rutile – 13 values for LTS iteration, 9 subjectively selected** | | | | | |
| *Ingrin and Blanchard* [2006] review | 1.25 | 121 | -4.55 | Rutile $TiO_2$; ~17 ppm $H_2O$, *Johnson et al.* [1975] | X |

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| | 1.25 | 121 | -4.72 | Rutile TiO2; ~17 ppm H2O, *Johnson et al.* [1975] | |
| | 0.58 | 56 | -6.78 | Rutile TiO2; ~17-45 ppm H2O, *Johnson et al.* [1975] | X |
| | 0.58 | 55 | -6.92 | Rutile TiO2; ~17-45 ppm H2O, *Johnson et al.* (1975) | |
| | 1.10 | 106 | -5.84 | Rutile TiO2; ~3 ppm H2O, *Cathcart et al.* [1979] | X |
| | 0.73 | 70 | -6.25 | Rutile TiO2; ~3 ppm H2O, *Cathcart et al.* [1979] | X |
| *Zhao and Zheng* [2007] review | *1.25* | *121* | *-4.55* | Rutile – in *Ingrin and Blanchard* [2006] compilation | D |
| | *0.58* | *56* | *-6.78* | Rutile – in *Ingrin and Blanchard* [2006] compilation | D |
| *Farver* [2010] review | 0.39 | 38 | -9.12 | Rutile, synthetic single Xals – *Caskey* [1974] | C3 |
| | 0.57 | 55 | -9.57 | Rutile, synthetic single Xals – *Caskey* [1974] | C2 |
| | 0.59 | 57 | -6.74 | Rutile, synthetic single Xals - *Johnson et al.* [1975] recalculated fit | |
| | 1.29 | 125 | -4.42 | Rutile, synthetic single Xals - *Johnson et al.* [1975] recalculated fit | |
| | 0.75 | 72 | -6.07 | Rutile, synthetic single Xals- *Cathcart et al.* [1979] recalculated fit | |
| | 1.11 | 107 | -5.75 | Rutile, synthetic single Xals- *Cathcart et al.* [1979] recalculated fit | |
| | 1.94 | 187 | -5.05 | Rutile, synthetic single Xals - *Cathcart et al.* [1979] recalculated fit | C1 |
| **Other NAMs – 2 values** | | | | | |
| *Zhao and Zheng* [2007] review | 1.78 | 171.7 | -3.21 | Adularia, *Kronenberg et al.* [1996] | |
| | 4.53 | 437.1 | 6.01 | Corundum, *Ramirez et al.* [1997] | |
| **Garnet – 12 values for LTS iteration, 12 subjectively selected** | | | | | |
| *Wang et al.* [1996] | 2.63 | 254 | 0.25 | Natural pyrope (Py70Alm16Grm14) containing 22-112 wt ppm H2O | |
| | 2.50 | 241 | 0.13 | | |
| *Blanchard and Ingrin* [2004a] | 1.45 | 140 | -5.80 | Pyrope (Gr3Alm15Py81); ~13-36 ppm H2O | |
| *Blanchard and Ingrin* [2004b] | 2.87 | 277 | 0.5 | Natural pyrope ((Py88Al9Gr3), OHa band | |
| | 3.41 | 329 | 1.9 | Natural pyrope ((Py88Al9Gr3), OHb band | C2 |
| *Kurka et al.* [2005] | 1.06 | 102 | -7.60 | Grossular (Gr84And14Py2); 220 ppm H2O, H-D exchange deuteration | |
| | 3.35 | 323 | 1.0 | Grossular (Gr73And23Py2); H extraction | C1 |
| *Ingrin and Blanchard* [2006] review | *1.45* | *140* | *-5.80* | Pyrope (Gr3Alm15Py81); ~13-36 ppm H2O, *Blanchard and Ingrin* [2004a] | D |
| | *1.06* | *102* | *-7.60* | Grossular (Gr84And14Py2); 220 ppm H2O, *Kurka et al.* [2005] | D |
| | 1.92 | 185 | -3.80 | Grossular (Gr73And23Py2); 1400 ppm H2O, *Kurka* [2005] | |
| | 0.73 | 70 | -8.90 | Andradite (Gr1And99); 1500 ppm H2O, *Kurka* [2005] | |
| *Zhao and Zheng* [2007] review | *2.63* | *254* | *0.25* | Pyrope, *Wang et al.* [1996] | D |
| | *2.50* | *241* | *0.13* | Pyrope, *Wang et al.* [1996] | D |
| | *1.45* | *140* | *-6.80* | Pyrope, *Blanchard and Ingrin* [2004a] (the value of $D_0$ incorrectly calculated by Zhao & Zheng) | D |
| | *2.87* | *277* | *0.50* | Pyrope – in *Farver* [2010] review (the value of $D_0$ incorrectly calculated by Zhao & Zheng) | D |
| | *3.41* | *329* | *0.90* | Pyrope – in *Farver* [2010] review (the | D |

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|---|---|---|---|---|---|
| | | | | value of $D_0$ incorrectly calculated by Zhao & Zheng) | |
| *Farver* [2010] review | *1.45* | *140* | *-5.80* | Pyrope (Gr3Alm15Py81), natural single Xal, *Blanchard and Ingrin* [2004] | D |
| | *1.06* | *102* | *-7.60* | Grossular (Gr84And14Py2), natural single Xal, *Kurka et al.* [2005] | D |
| | *1.92* | *185* | *-3.80* | Grossular (Gr73And23Py2), natural single Xal, *Kurka* [2005] – in *Ingrin and Blanchard* [2006] compilation | D |
| | *0.73* | *70* | *-8.89* | Andradite (Gr1And99), natural single Xal, *Kurka* [2005] – in *Ingrin and Blanchard* [2006] compilation | D |
| | *2.62* | *253* | *0.57* | Pyrope (Py67-72Alm14-21Gr10-14) natural single Xals, average of *Wang et al.* [1996] | D |
| | *2.87* | *277* | *0.50* | Pyrope (Gr3Alm15Py81) natural single Xals, *Blanchard and Ingrin* [2004b] | D |
| | *3.41* | *329* | *1.90* | Pyrope (Gr3Alm15Py81) natural single Xals, *Blanchard and Ingrin* [2004b] | D |
| | *3.35* | *323* | *1.00* | Grossular (Gr84And14Py2), natural single Xal, *Kurka et al.* [2005] – in *Ingrin and Blanchard* [2006] review | D |
| | 1.87 | 180 | -3.70 | Grossular (Gr73And23Py2), natural single Xal, *Kurka* [2005] | |
| | 2.81 | 271 | 0.0 | Andradite (Gr1And99), natural single Xal, OH3620, *Kurka* [2005]. | |
| | 2.16 | 209 | -1.8 | Andradite (Gr1And99), natural single Xal, OH3560, *Kurka* [2005]. | |
| | **Quartz – 11 values for LTS iteration, 7 subjectively selected** | | | | |
| *Ingrin and Blanchard* [2006] review | 0.72 | 69 | -8.95 | α-Quartz; ~30 ppm H2O, *Kats et al.* [1962] | X |
| | 1.75 | 169 | -3.66 | β-Quartz; ~30 ppm H2O, *Kats et al.* [1962] | X |
| | 2.23 | 215 | -0.45 | β-Quartz; ~13 ppm H2O, *Kronenberg et al.* [1986] | X |
| | 1.62 | 156 | -3.45 | β-Quartz; ~13 ppm H2O, *Kronenberg et al.* [1986] | X |
| *Zhao and Zheng* [2007] review | 2.07 | 200 | -0.86 | β-Quartz, refitting data in *Kronenberg et al.* [1986] | |
| | 0.82 | 79.5 | -8.30 | α-Quartz, refitting data in *Kats et al.* [1962] | |
| | 1.82 | 175.7 | -3.30 | β-Quartz – refitting data in *Kats et al.* [1962] | |
| | 0.97 | 93.7 | -10.55 | β-Quartz, *Shaffer et al.* [1974] | |
| | 1.04 | 100 | -10.19 | β-Quartz, *Shaffer et al.* [1974] | |
| | 1.08 | 104.2 | -10.04 | β-Quartz, *Shaffer et al.* [1974] | |
| | 1.12 | 108.4 | -10.07 | β-Quartz, *Shaffer et al.* [1974] | |
| *Farver* [2010] review | 0.82 | 79.5 | -8.30 | α-Quartz, natural single Xal, *Kats et al.* [1962] refitted in *Zhao and Zheng* [2007] | D |
| | 1.82 | 175.5 | -3.30 | β-Quartz, natural single Xal, *Kats et al.* [1962] refitted in *Zhao and Zheng* [2007] | D |
| | *2.23* | *215* | *-0.46* | β-Quartz, natural single Xals, *Kronenberg et al.* [1986] – in *Ingrin and Blanchard* [2006] compilation | D |
| | *1.62* | *156* | *-3.46* | β-Quartz, natural single Xals, *Kronenberg et al.* [1986] – in *Ingrin and Blanchard* [2006] compilation | D |
| | *1.04* | *100* | *-10.37* | β-Quartz, natural single Xal, from *Shaffer et al.* [1974] | D |

| | | | | | |
|---|---|---|---|---|---|
| | *2.07* | *200* | *-0.85* | β-Quartz, natural single Xal, from *Kronenberg et al.* [1986] | D |
| *Brady and Cherniak* [2010] online database (http://diffusion.smith.edu/) | *2.07* | *199.7* | *-0.85* | β-quartz – in *Farver* [2010] compilation | D |
| **Feldspar, Feldspathoids – 2 values, both selected** | | | | | |
| *Zhao and Zheng* [2007] review | *1.78* | *172* | *-3.21* | Adularia, *Kronenberg et al.*[1996] – in *Farver* [2010] compilation | D |
| *Farver* [2010] review | 1.78 | 172 | -3.21 | Adularia (Ab9Or90Cs1), natural single Xals, *Kronenberg et al.* [1996] | |
| | 2.32 | 224 | -3.24 | Andesine (Ab66An30Or3), natural single Xals, *Johnson* [2006] | |
| **Amphibole – 5 values for LTS iteration, none selected** | | | | | |
| *Farver* [2010] review | 0.82 | 79 | -4.70 | Hornblende, powdered natural sample, *Graham et al.* [1984] | C1 |
| | 0.87 | 84 | -11.60 | Hornblende, powdered natural sample, *Graham et al.* [1984] | |
| | 0.74 | 71.5 | -10.00 | Tremolite, powdered natural Xals, *Graham et al.* [1984] | C2 |
| | 1.03 | 99 | -9.20 | Actinolite, powdered natural Xals, *Graham et al.* [1984] | |
| | 1.08 | 104 | -8.70 | Kaersutite, natural single Xal, *Ingrin and Blanchard* [2000] | |
| **Hydroxyl-bearing minerals – 53 values for LTS iteration, none selected** | | | | | |
| *Zhao and Zheng* [2007] review | 1.02 | 98.75 | -9.20 | Actinolite, *Graham* [1981] | |
| | 1.22 | 118 | -7.59 | Actinolite, *Suzuoki and Epstein* [1976] | |
| | 1.06 | 102.5 | -11.62 | Actinolite, *Suzuoki and Epstein* [1976] | |
| | 0.27 | 26.4 | -17.30 | Alunite, *Stoffregen et al.* [1994] | |
| | 0.62 | 60.1 | -6.94 | Analcime, *Dyer and Molyneux* [1968] | C1 |
| | 0.56 | 54.2 | -7.79 | Analcime, *Dyer and Molyneux* [1968] | |
| | 1.21 | 116.3 | -10.47 | Biotite, *Suzuoki and Epstein* [1976] | |
| | 1.27 | 122.6 | -7.12 | Biotite, *Suzuoki and Epstein* [1976] | |
| | 1.78 | 171.7 | -5.21 | Chlorite, *Graham et al.* [1987] | |
| | 1.73 | 166.9 | -7.32 | Chlotite, *Graham et al.* [1987] | |
| | 1.33 | 128 | -3.91 | Epidote, *Graham* [1981] | |
| | 0.60 | 57.7 | -9.48 | Epidote, *Graham* [1981] | |
| | 1.33 | 128.5 | -3.03 | Epidote, *Graham* [1981] | C3 |
| | 0.54 | 52.3 | -9.01 | Epidote, *Graham* [1981] | |
| | 0.84 | 81.38 | -12.81 | Epidote, *De et al.* [2000] | |
| | 0.82 | 79.5 | -10.80 | Hornblende, *Graham et al.* [1984] | |
| | 0.87 | 84.1 | -11.62 | Hornblende, *Graham et al.* [1984] | |
| | 1.23 | 118.5 | -7.37 | Ilvaite, *Qian and Guo* [1993] | |
| | 1.20 | 115.5 | -7.01 | Ilvaite, *Qian and Guo* [1993] | |
| | 0.63 | 60.9 | -11.86 | Kaolinite, *O'Neil and Kharaka* [1976] | |
| | 0.78 | 74.8 | -11.67 | Kaolinite, *O'Neil and Kharaka* [1976] | |
| | 0.87 | 83.7 | -12.06 | Kaolinite, *Liu and Epstein* [1984] | |
| | 0.75 | 72.4 | -11.26 | Kaolinite, *Liu and Epstein* [1984] | |
| | 0.83 | 80 | -9.02 | Kaolinite, *Vennemann et al.* [1996] | |
| | 0.38 | 37 | -13.25 | Manganite, *Hariya and Tsutusmi* [1981] | |
| | 0.52 | 49.8 | -13.19 | Montmor, *O'Neil and Kharaka* [1976] | |
| | 0.55 | 52.7 | -11.35 | Montmor, *O'Neil and Kharaka* [1976] | |
| | 1.24 | 119.7 | -11.00 | Muscovite, *Graham* [1981] | |
| | 1.26 | 121.3 | -7.98 | Muscovite, *Graham* [1981] | |
| | 0.26 | 25.4 | -9.85 | K-Natrolite, *Dyer and Faghihian* [1998b] | |
| | 1.33 | 128.6 | -10.11 | Phlogopite, *Suzuoki and Epstein* [1976] | |
| | 1.61 | 155.2 | -5.65 | Phlogopite, *Suzuoki and Epstein* [1976] | |
| | 0.51 | 48.8 | -9.90 | Serpentine, *Sakai and Tsutsumi* | |

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|---|---|---|---|---|---|
| | | | | [1978] | |
| | 0.49 | 47.2 | -11.12 | Serpentine, *Sakai and Tsutsumi* [1978] | |
| | 0.20 | 19 | -10.79 | Na-Stilbite, *Dyer and Faghihian* [1998a] | |
| | 0.12 | 11.8 | -11.70 | Ca-Stilbite, *Dyer and Faghihian* [1998a] | |
| | 1.33 | 127.9 | -9.96 | Tourmaline, *Guo and Qian* [1997] | |
| | 1.27 | 122.9 | -9.64 | Tourmaline, *Guo and Qian* [1997] | |
| | 0.75 | 72.4 | -10.75 | Tremolite, *Graham et al.* [1984] | |
| | 0.74 | 71.1 | -12.05 | Tremolite, *Graham et al.* [1984] | |
| | 1.04 | 100 | -7.79 | Zoisite, *Graham* [1981] | |
| | 1.06 | 102.5 | -8.35 | Zoisite, *Graham* [1981] | |
| | 0.54 | 52.3 | -8.49 | Zoisite, *Graham et al.* [1980] | |
| | 0.54 | 52.3 | -7.76 | Zoisite, *Graham et al.* [1980] | C2 |
| *Brady and Cherniak* [2010] online database (http://diffusion.smith.edu/) | *1.78* | *171.7* | *-5.21* | Chlorite – in *Zhao and Zheng* [2007] | D |
| | *0.60* | *57.9* | *-9.48* | Epidote – in *Zhao and Zheng* [2007] | D |
| | *1.26* | *121.6* | *-7.98* | Muscovite – in *Zhao and Zheng* [2007] | D |
| | *0.69* | *66.6* | *-12.20* | Tourmaline – in *Farver* [2010] | D |
| | *1.10* | *106.1* | *-9.80* | Tourmaline – in *Farver* [2010] | D |
| | *1.06* | *102.3* | *-8.35* | Zoisite – in *Zhao and Zheng* [2007] | D |
| *Farver* [2010] review | **Sheet Silicates** | | | | |
| | 1.25 | 121 | -9.52 | Muscovite, powdered natural Xals, *Graham* [1981] | |
| | 1.06 | 102 | -8.00 | Zoisite (Ca2Fe0.1Al2.9Si3O12OH), powdered natural Xals, *Graham* [1981] – *Farver* [2010] notes possible capsule leak | E |
| | 0.57 | 55 | -9.15 | Epidote (Ca2Fe0.9Al2.1Si3O12OH), powdered natural Xals, *Graham* [1981] – *Farver* [2010] notes possible capsule leak | E |
| | 1.33 | 128 | -3.52 | Epidote (Ca2Fe0.9Al2.1Si3O12OH), powdered natural Xals – *Farver* [2010] notes possible capsule leak | E |
| | 0.69 | 67 | -13.60 | Epidote (Ca2FeAl2Si3O12OH), natural single Xals, *Suman et al.* [2000] | |
| | 0.83 | 80 | -9.00 | Lawsonite (CaAl2Si3O12(OH2)H2O), powdered natural Xals, *Marion et al.* [2001] | |
| | 1.75 | 169 | -7.00 | Chlorite, powdered natural Xals, *Graham et al.* [1987] | |
| | 1.21 | 117 | -7.15 | Ilvaite, powdered natural Xals, *Yaqian and Jibao* [1993] | |
| | **Other Silicates** | | | | |
| | 1.30 | 125.5 | -9.82 | Tourmaline (14.27% FeO, 1.93% MgO, 31.34%Al2O3) powdered natural Xal, *Jibao and Yaqian* [1997] | |
| | 1.10 | 106.3 | -9.80 | Tourmaline (elbaite), natural single Xals, *Desbois and Ingrin* [2007] | |
| | 0.69 | 66.8 | -12.20 | Tourmaline (elbaite), natural single Xals, *Desbois and Ingrin* [2007] | |
| | 1.38 | 133 | -6.60 | Beryl, synthetic single Xals, *Fukuda et al.* [2009] | |

**2) Fitting a robust line to noisy data with outliers**

Linear regressions are fit to the various datasets considered within this paper of the form

$$Y = a + b\,X \qquad (1)$$

where *a* is the gradient and *b* is the intercept. The results of these regressions are going to be interpreted in detail, therefore it must be ensured that the regressions are undertaken in the most careful statistical manner possible. There are two major problems with applying standard least squares linear regression. The first is that in the standard approach, such as implemented in Excel for example, one variable, usually designated as the X-variable and plotted along the abscissa when the data are displayed visually, is defined as the independent variable and is assumed to be free of error. The other variable, Y and plotted along the ordinate, is the dependent variable and may have error. In reality, in most observational scenarios, both X and Y data are in error, so assuming one is error free will lead to a biased result.

As a simple example of the problem, consider 41 data from the process *Y* = *X*, i.e., *a*=0 and *b*=1, sampled uniformly in *X* in the range [-1,+1]. We will consider three situations; (1) *X* is error free and *Y* is noise contaminated, (2) *X* is contaminated and *Y* is error free, and (3) both *X* and *Y* are contaminated by noise. We will assume that the noise is Gaussian with a mean of 0.0 and a standard deviation of 0.10. Estimates of the slope and intercept from standard linear regression of these three cases for sample runs are listed in Table S2, where the downward bias in the estimate of the slope *b* for Case 2 and Case 3 caused by noise in *X* is shown. If noise in *X* is suspected, and it is thought to be greater than noise in *Y*, then one can assume that *Y* represents the independent variable and *X* the dependent variable, in which case the slope estimates *b* from the regressions for Case 1 and Case 3 are then upward biased by noise in *Y*, as shown in Table S2.

Table S2: Slope and intercept (with their standard errors) for three cases studied of 41 data from the process Y = X with X in the range [-1,+1] using standard LS regression assuming noise only in Y for X as the independent variable, or noise only in X for Y as the independent variable.

| Case | Slope (b) | Intercept (a) | Correlation coefficient |
|---|---|---|---|
| *X* independent variable, *Y* dependent variable | | | |
| Case 1: Noise in Y | 0.996 ±0.024 | 0.0014 ±0.0141 | 0.989 |
| Case 2: Noise in X | 0.974 ±0.028 | -0.0065 ±0.0165 | 0.987 |
| Case 3: Noise in X and Y | 0.969 ±0.039 | -0.0023 ±0.0238 | 0.970 |
| *X* dependent variable, *Y* independent variable | | | |
| Case 1: Noise in Y | 1.042 ±0.026 | 0.0014 ±0.0157 | 0.986 |
| Case 2: Noise in X | 1.004 ±0.028 | -0.0067 ±0.0167 | 0.985 |
| Case 3: Noise in X and Y | 1.015 ±0.034 | -0.0026 ±0.0207 | 0.977 |

To combat this bias problem, the methods of *York* [1966; 1969] and *Fasano and Vio* [1988], in which both data are assumed to be contaminated by noise, need to be applied. Using the Fasano-Vio method, the estimates of slope and intercept for the three cases are listed in Table S3, and there is no bias in the estimates.

Table S3: Slope and intercept (with their standard errors and 95% confidence intervals) for three cases studied of 41 data from the process *Y = X* with *X* in the range [-1,+1] using *York* [1966] LS regression assuming error in both *X* and *Y*.

| Case | Slope (b) | Intercept (a) | Correlation coefficient |
|---|---|---|---|
| Case 1: Error in Y | 1.028 ±0.027 | 0.0014 ±0.0161 | 0.986 |
| Case 2: Error in X | 0.989 ±0.028 | -0.0067 ±0.0165 | 0.985 |
| Case 3: Error in X and Y | 0.991 ±0.034 | -0.0264 ±0.0665 | 0.977 |

The second problem with standard LS regression is the potential overwhelming influence of outliers [e.g., *Cook*, 1977]. Linear regression in particular is easily biased by the presence of a small number of outliers that can act as leverage points. In statistical parlance standard LS lacks robustness, the L2 norm is unbounded. Outliers can be identified, and their effect(s) on the regression reduced, by using robust statistical methods pioneered by *Tukey* [1960; see *Huber*, 2002] and established by *Huber* [1964; 1981] and *Hampel* [1973; 1974; 1986], amongst others.

As an example of the problem, consider the prior dataset from the process *Y = X* with *X* sampled in the range [-1, +1] but with an extreme leverage point outlier at [+10,+20] with noise added to *Y* or *X* or both for each of the 3 cases respectively (Table S4). Standard LS regression and York-type LS regression estimates for Case 3, noise in both *X* and *Y*, are listed in Table S4 and shown in Figure S1 (red and blue lines), and these appear statistically to be reasonable models that fit the data; the correlation coefficients are large and the standard error estimates are small. Huber replacement and reweighting also poorly identifies the leverage point; a regression result using the simple replacement approach of *Huber* [1981, p. 18, c=1.345, 50 iterations] with 10 of the 42 datapoints replaced by pseudodata is listed in Table S4 and is clearly biased by the influence of the leverage point (Figure S1a, green line). When zooming in to focus on the region [-1,+1] (Figure S1b), then clearly the problem of misfitting the data is obvious.

A statistical technique to efficiently identify outliers and especially leverage points is Least Trimmed Squares (LTS) proposed and established by *Rousseeuw* [*Rousseeuw*, 1984; *Rousseeuw and Van Driessen*, 2006]. The method uses the so-called Cook's distance [*Cook*, 1977], which estimates the influence of each data point by removing it, fitting the statistical model, and assessing the summary statistics in the absence of each data point in turn. An equivalent approach to LTS using Cook's Distance was proposed independently in the geosciences by *Jones* [*Jones and Joedicke*, 1984, method 6; *Jones et al.*, 1989] for determining the best estimates of magnetotelluric response functions. Applying the LTS technique to this dataset rejects the leverage point outlier in the first iteration as its inclusion massively increases the standard error for the model fit to the data. Allowing the scheme to iterate until the standard error is minimised results in a further 19 points being rejected, with the final regression model given in Table S4 and shown in Figure S1a,b (black line), together with the 95% confidence intervals of that regression line (dashed black lines). Figure S2 shows the decrease of the standard error at each iteration as the point identified by Cook's Distance that increases the standard error the most is rejected. The first point rejected is the leverage outlier at nominally [+10,+20], and its exclusion reduces the standard error by more than half. On the 25$^{th}$ iteration, no points could be reduced that would lead to a smaller ensemble standard error. The 24 points rejected are shown as red diamonds on Figure S1a,b, and the regression model is listed in Table S4. The change in the estimates of the slope and intercept, and their standard deviations, with iteration as points are culled are shown in Figure S2. The slope stabilizes within a few iterations to a value of just above 1, whereas the intercept is less stable.

Allowing the process to run to the point where no more data values can be rejected to lower the ensemble standard error is the most extreme culling. A more conservative limit is to take the same approach as Hansen's L-curve [*Hansen*, 1992; *Hansen and O'Leary*, 1993], and to iterate to the point on the "knee" of the standard error descent curve (Figure S2), which is approximately 10 iterations. Those 10 points are shown as blue squares on Figure S1a,b and the regression model is listed in Table S4 and plotted on Figure S1a,b together with the 95% confidence intervals of the model.

Table S4: LS regressions for 42 point dataset from the process *Y* = *X* with 41 points in the *X*-range [-1,+1] with noise in both *X* and *Y* and with an extreme outlier at [+10,+20] (plus noise).

| Case | Slope (b) | Intercept (a) | Correlation coefficient |
|---|---|---|---|
| Case 3: Standard LS regression, independent *X* variable | 1.858 ±0.049 | 0.0526 ±0.0816 | 0.986 |
| Case 3: Standard LS regression, independent *Y* variable | 1.910 ±0.027 | 0.0398 ±0.0433 | 0.986 |
| Case 3: Fasano-Vio LS regression | 1.900 ±0.050 | 0.0426 ±0.0826 | 0.986 |
| Case 3: Robust Fasano-Vio LS regression using Huber replacement and reweighting with a *c* factor of 1.1 (10 points replaced) | 1.881 ±0.033 | -0.0524 ±0.0556 | 0.994 |
| Case 3: Robust Fasano-Vio LS regression using Rousseeuw LTS with Cook's Distance based rejection iterating until no more improvement possible (39 points culled) | 1.050 ±0.0003 | 0.0289 ±0.00005 | 1.000 |
| Case 3: Robust Fasano-Vio LS regression using Rousseeuw LTS with Cook's Distance based rejection iterating to the knee in the standard error descent curve (8 points culled) | 1.051 ±0.022 | 0.0319 ±0.0130 | 0.993 |

Figure S1: 41 (black circles, blue squares and red diamonds) points from the process *Y* = *X* with *X* sampled uniformly in the range [-1,+1] and with Gaussian noise added to both *X* and *Y* with a mean of 0.0 and a standard deviation of 0.1. An additional $42^{nd}$ outlier point exists at [+10,+20] (with noise at same level as other data). LS regression fits to the 42 points are shown. The 8 blue squares are those rejected by applying Rousseeuw's Least Trimmed Squares (LTS), with standard error of misfit used as the Cook's Distance, to the "knee" of the standard error descent curve (Figure S2). The 95% confidence intervals of the robust regression to the remaining 34 points (black) are shown as dashed black lines. Plot (a) is the whole data space, and plot (b) zooms in on the *X,Y* range of [-1.2,+1.2].

Figure S1a

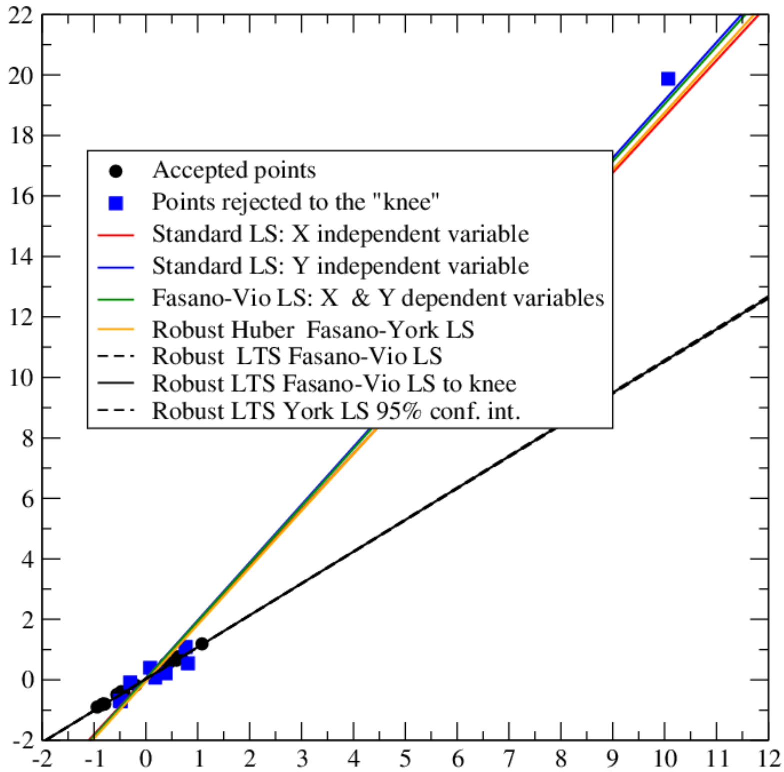



Figure S1b

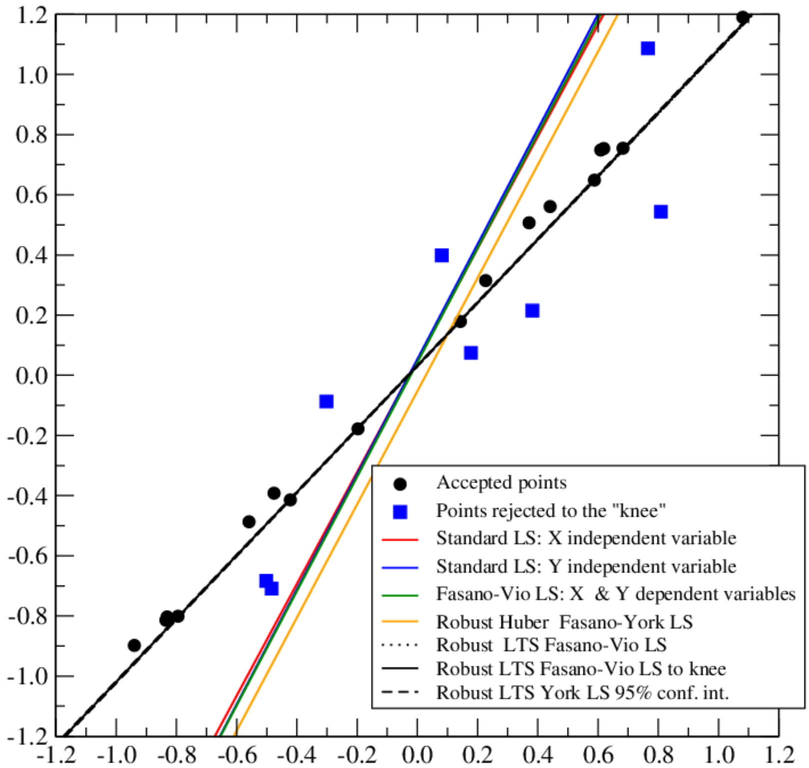
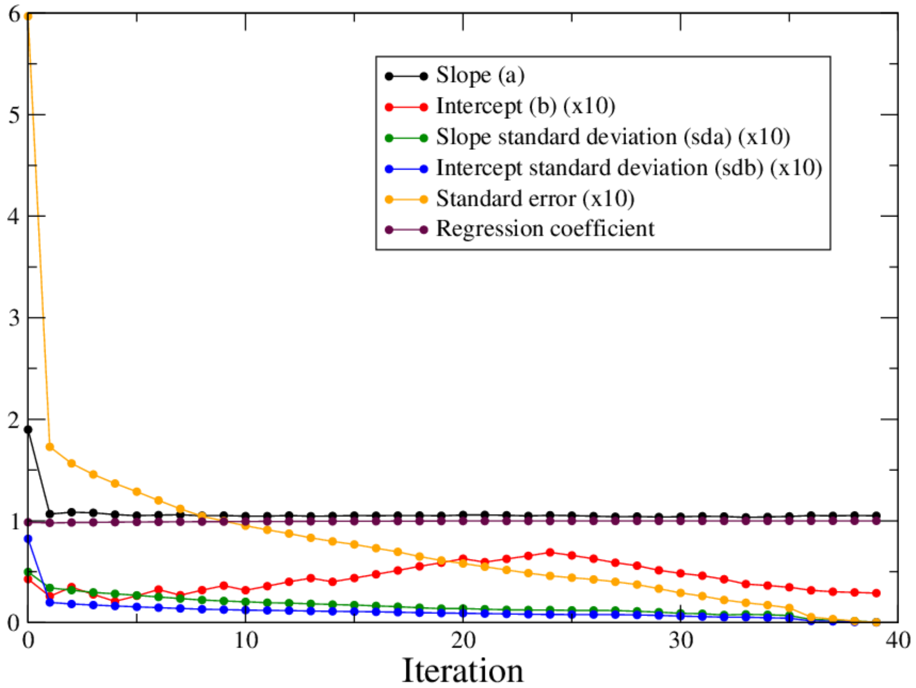


Figure S2: Variation of slope and intercept, and their errors and the regression coefficient, with increasing iteration of the robust Fasano-Vio LTS regression for the data shown in Figure S1.



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