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| --- | --- | --- | --- | --- | --- | --- |
| **Publication** | **Name** | **T-sens?** | **P-sens?** | **H2O-sens?** | ***f*o2 or Fe3/FeT-sens?** | **Sulfide comp?** |
| **SCAS models** | | | | | | |
| Chowdhury & Dasgupta (2019) | “calculate\_CD2019\_SCAS” | **🗸** | **✗** | **🗸** | **✗** | **✗** |
| Zajacz & Tsay (2019) | “calculate\_ZT2022\_SCAS” | **🗸** | **✗** | **🗸** | **✗** | **✗** |
| **SCSS models** | | | | | | |
| Li and Zhang (2022) | “calculate\_LZ2022\_SCSS” | **🗸** | **🗸** | **🗸** | **🗸** | **🗸** |
| O’Neill (2021) | “calculate\_O2021\_SCSS” | **🗸** | **🗸** | **✗** | **🗸** | **🗸** |
| Smythe et al. (2017) | “calculate\_S2017\_SCSS” | **🗸** | **🗸** | **✗** | **🗸** | **🗸** |
| Fortin et al. (2015) | “calculate\_F2015\_SCSS” | **🗸** | **🗸** | **🗸** | **✗** | **✗** |
| **Sulfide composition models** | | | | | | |
| O’Neill (2021) | “Calc\_ONeill” | **✗** | **✗** | **✗** | **🗸** |  |
| Smythe et al. (2017) adaptation of Kiseeva et al. (2015) method | “Calc\_Smythe” | **🗸** | **✗** | **✗** | **🗸** |  |
| **S6+ Correction/ SCSS total corrections** | | | | | | |
| Jugo et al. (2010) | “calculate\_S6St\_Jugo2010” | **✗** | **✗** | **✗** | **🗸** | **✗** |
| Nash et al. (2019) | “calculate\_S6St\_Nash2019” | **🗸** | **✗** | **✗** | **🗸** | **✗** |

**Other functions**

|  |  |
| --- | --- |
| “calculate\_SCSS\_Total” | Calculates S total for a S6St\_Liq ratio, and a calculated SCSS value |
| “calculate\_S\_Tot\_Kleinsasser2022\_dacite” | Calculates S tot for an entered deltaFMQ value, and either a calculated SCSS2 or SCAS value |
| “crystallize\_S\_incomp” | Calculates S left in the melt for a given F\_melt, assuming S is entirely incompatible |
| “calculate\_mass\_frac\_sulf” | Calculates mass fraction of sulfide/sulfate removed for a fractional crystallization path where the SCSS or SCAS is modelled |