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## 1. History

Human fascination with crystals has a long history. 105,000 years ago, someone had a collection of calcite crystals (Iceland spar) (Wilkins *et* al., 2021). Theophrastus (ca. 372-287 B.C.), a student of Plato and successor to Aristotle, wrote the first known treatise on gems ("On Stones") (Wikipedia contributors, 2022).

Figure 1 notes a few key events in cataloging crystal properties. We start with (Kepler, 1611) (translated in (Kepler *et* al., 1966)) and Steno (see (Authier, 2013)) who conjectured on the structures of crystals. (Haüy, 1800) created the first catalog of minerals.

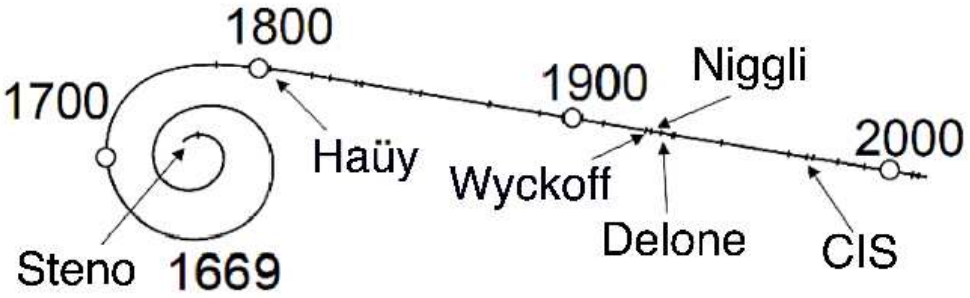


Fig. 1. Some key dates in the history of modern crystallography

## 2. References to Sources for Information about the Calculations

- No operation: simply check the input for errors
- generate four C6 test cells
- compute Selling-reduced primitive cells: Delone/Delaunay/Selling reduction

  (Delaunay, 1932)

  (Delone *et* al., 1975)

  (Andrews *et* al., 2019a)
- compute NCDist and CS6Dist distances

  (Andrews & Bernstein, 2014)

  (Andrews *et* al., 2019b)
- apply Lattice Matching algorithm to listed cells

  (Mighell, 2002)

  (Andrews & Bernstein, 2021)
- compute Niggli-reduced primitive cells

  (Niggli, 1928) (Gruber, 1973)
- compute path between pairs of cells

(Andrews & Bernstein, 2023)

- compute perturbed versions of input cells

  (Andrews & Bernstein, 2022)

- apply S6 reflections to input cells

  (Andrews *et* al., 2019b)

- apply Sella algorithm

  (Andrews *et* al., 2023)

- compute Bravais tetrahedron (B4)

  (Delone *et* al., 1975)

- compute Selling-reduced complex cell presentation (C3)

  (Andrews *et* al., 2019b)

- compute side-angle cells (a, b, c, $\alpha$, $\beta$, $\gamma$)

- compute raw Dirichlet cells (DC13)

  (Bernstein *et* al., 2023)

- computed sorted Dirichlet cells (DC)

  (Bernstein *et* al., 2023)

- compute Niggli-reduced cells (G6)

  (Andrews & Bernstein, 2014)

- compute Selling-reduced cells (S6)

  (Andrews *et* al., 2019b)

- compute unsorted Dirichlet cells (dc7unsrt)

  (Andrews *et* al., 2019b)

- compute volumes of listed cells

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