Subject: Re: Sorting, counting and deleting different elements (e.g., lodine) in a dataset

Posted by Paul on Wed, 28 Sep 2022 19:02:47 GMT

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Many years ago, this problem was presented as an Excel challenge that could not use macros/VBA.

I've kept and still use the spreadsheet because it's so simple and addresses the need.

Formulas from DataWarrior are pasted into the sheet and elemental composition data can then be pasted into a text file and merged back into the DWAR file. If Data Warrior has comparable CHAR functions perhaps a similar approach is possible. Granted, it does require moving data to then from Excel, but it's straight forward.

The attached spreadsheet handles only 10 formulas/rows at a time to keep the attachment size small. Expanding the formula rows in Excel is trivial, but the spreadsheet can get rather slow for thousands of rows at a time.

File Attachments

1) ATOMCALCS.xlsx, downloaded 300 times