COMPUTATIONAL OPTIMAL TRANSPORT FOR MOLECULAR SPECTRA

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The use of computational optimal transport for the comparison of molecular spectra is presented. Computational optimal transport provides a comparator, the transport distance, which can be used in machine learning applications and for the comparison of theoretical and experimental spectra. Unlike many other comparators, the transport distance encodes line positions and intensities. It can be used to compare two discrete spectra, a discrete spectrum and a continuous spectrum, as well as two continuous spectra. Because the transport distance reflects the movement of density from one spectrum to another, the two spectra being compared do not have to have the same number of lines or features and need not closely match up in frequency space.

Several well-chosen examples will be shown to demonstrate how computational optimal transport is used and its overall utility. In addition, it is used to make quantitative comparisons between theoretical and experimental spectra including a rotational spectrum of 1-hexanal and an electronic absorption spectrum of $SO2$.[a]

[a]This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences operating under Contract Number DE-AC02-06CH11357.