

## A MULTIMODE-LIKE SELECTION OF CENTERS OF GAUSSIAN BASIS FUNCTIONS WHEN COMPUTING VIBRATIONAL SPECTRA USING COLLOCATION

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When computing vibrational spectra with collocation and localized basis functions such as Gaussian functions, one can choose the distribution of points and of function centers to increase the accuracy or decrease the cpu cost. Here, we compute vibrational energy levels using Gaussian basis functions whose centers are in slabs that include the lower-dimensional hyperplanes on which the Multimode approximation to the potential is based. We use more potential points than basis functions to increase the accuracy, i.e. we use rectangular collocation. The number of Gaussian basis functions is smaller than the number required using the best existing methods. For formaldehyde, the first 50 (100) levels we compute, using 30,000 Gaussians and 120,000 points, in 4D-like slabs, differ from numerically exact levels by 0.3 (0.6) cm<sup>-1</sup> (mean absolute error). With 3D-like slabs, the mae for the first 50 (100) levels is 0.17 (0.47) cm<sup>-1</sup> with 30,000 basis functions and 0.95 (2.06) cm<sup>-1</sup> with 20,000 basis functions. Although we use a multimode-like idea to select Gaussian centers, we use a single point set and there is no need to write the potential in multimode form and no need to neglect high-order terms.