DDD: DYNAMIC DATABASE FOR DIATOMIC MOLECULES

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We are developing a web-based program to deliver high resolution spectra of diatomic molecules. A unique feature is that data for molecules not yet present in the database will be automatically generated by *ab initio* methods. Because the calculations will be carried out on massively parallel computers, the time to solution will be minimized. The goal is the accurate prediction of rotational, vibrational, and electronic transitions for valence states of any diatomic. Certainly there will be limitations in the automatic procedure, but preliminary applications show astonishing robustness and the ability to predict many states that have not been characterized by experiment. Some results for CO and TiO will be presented.