Abstract. We present CDSD-296 a version of the Carbon Dioxide Spectroscopic Databank aimed at processing signals from the satellite based sensors. The databank contains line parameters (positions, intensities as well as HITRAN air- and self-broadened halfwidths and coefficients of temperature dependence of air-broadened halfwidths) of the four most abundant isotopic species of CO$_2$. The reference temperature is $T_{ref}=296$ K, the intensity cutoff is $I_{cut}=10^{-28}$ cm$^{-1}$/molecule cm$^{-2}$ and the spectral range is 405-12784 cm$^{-1}$. The databank was generated within the framework of the method of effective operators and based on the global fittings of parameters of the models to observed data collected from the literature. Calculated line positions were systematically replaced where possible by the differences between experimental term values derived from recalibrated observed line positions with the help of the combination Ritz principle. The databank includes statistically justified confidence intervals for each line position and intensity.

Keywords: carbon dioxide; databank; radiative properties; HITRAN; atmospheric applications
1. Introduction

Precise knowledge of the radiative properties of CO$_2$ is required for many scientific and industrial applications. Carbon dioxide is one of the major greenhouse gases and plays an important role in the chemical-physical processes in the terrestrial atmosphere and in planetology. Spectroscopic rovibrational line parameters (positions, intensities, halfwidths, etc.) of CO$_2$ are used by various radiative transfer codes to model properties of the terrestrial atmosphere as well as atmospheres of Venus and Mars. Information of CO$_2$ data are used by a number of already working or planned satellite-borned sensors (MIPAS, IASI, OCO) to retrieve atmospheric temperature profile and to monitor the column amount of CO$_2$ across the globe. Spectroscopic line parameters of atmospheric gases are accumulated in a well known database HITRAN. The carbon dioxide HITRAN data are in fact a mixture of measured and calculated line parameters. According to the adopted approach, when possible high-quality measurements are put into the database. In situations where direct measurements are unavailable, the calculated data either from the previous version of the CDSD atmospheric databank or (if required data are absent from CDSD) from the DND calculations were used. The accuracy of calculated line positions covers the 0.0001 – 0.01 cm$^{-1}$ range. The accuracy of calculated line intensities depends on the experimental data used for fitting the parameters of theoretical dipole models and varies from 2% to 50%.

Modern requirements of the accuracy of this data are stricter. For example in order to provide a 0.5% measurement precision in retrieved values of total column CO$_2$ in the 1.6 μm region the line position uncertainties less than 0.5 ×10$^{-4}$ cm$^{-1}$ are required. As for line intensities, they must be known with accuracy ~0.3% according to the OCO specifications. It is clear that neither CDSD nor DND calculations fail to meet these requirements.

Another important point is availability of realistic confidence intervals for calculated line parameters. HITRAN-2004 provides IER integer codes for position and intensity uncertainties. Their values, however, often do not reflect the actual uncertainties. The inclusion of statistically justified confidence intervals for line parameters into a spectroscopic database is an important requirement posed by the IASI-METOP working group.

In this study we present a database of line positions and line intensities of CO$_2$ aimed at spectroscopic applications and called CDSD-296. The principal goal is to supply the scientific community with enlarge and more precise data on four most abundant isotopologues $^{12}$C$^{16}$O$_2$, $^{13}$C$^{16}$O$_2$, $^{12}$C$^{18}$O$^{18}$O, and $^{12}$C$^{16}$O$^{17}$O of the carbon dioxide molecule.