Readme for **CDSD-HITEMP**

CDSD-HITEMP is a version of the Carbon Dioxide Spectroscopic Databank (CDSD) and is a part of new version of the HITEMP database [1].

CDSD-HITEMP was developed in V.E. Zuev Institute of Atmospheric Optics Siberian Branch, Russian Academy of Sciences. All queries and comments about the CDSD-HITEMP databank should be addressed to:

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CDSD-HITEMP contains **calculated** parameters of spectral lines of 7 most abundant in the Earth's atmosphere isotopologues of the carbon dioxide molecule: $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$, $^{16}O^{12}C^{17}O$, $^{16}O^{13}C^{18}O$, $^{16}O^{13}C^{17}O$, and $^{12}C^{18}O_2$. The databank covers the 6 - 12784 cm^{-1} spectral range and contains more than 11 million entries.

Reference temperature of the databank is T_{ref} = 296 K.

CDSD-HITEMP is the result of merging 3 previous versions of CDSD, namely

1. enlarged version of CDSD-1000 [2] which has reference temperature T_{ref} = 1000 K and intensity cutoff $I_{cut} = 10^{-27}$ cm^{-1}/(molecule cm^{-2})
2. version of CDSD called CDSD-Venus adapted for Venus conditions with T_{ref} = 750 K and $I_{cut} = 10^{-30}$ cm^{-1}/(molecule cm^{-2})
3. atmospheric version of CDSD which is partly included into present version of the HITRAN database [3] with T_{ref} = 296 K and $I_{cut} = 10^{-30}$ cm^{-1}/(molecule cm^{-2}).

Format of the databank is compatible with HITRAN-2008 [3].

Structure of CDSD-HITEMP

Line positions

All line positions are **calculated** values based on global fits of measured positions using the effective Hamiltonian approach [4,5]. Measured positions in MHz were converted to cm^{-1} using the factor 1./29979.2458.

Line intensities

All line intensities are **calculated** values based on global fits of measured positions using the effective operator approach [4,6]. Measured at temperature T intensities in cm^{-2}/atm were converted to cm^{-1}/(molecule cm^{-2}) using factor T/(2.679e19*273.15). Isotopic abundances are the same as in the HITRAN database.

Pressure broadening parameters

Air-broadened halfwidths g_{air}, self-broadened halfwidths g_{self}, coefficients of temperature dependence of air-broadened halfwidths n_{air} and coefficients of temperature dependence of self-broadened halfwidths n_{self} are **calculated** values based on a semi-empirical approach [2,7].

Air-broadened pressure shifts

Air-broadened pressure shifts d_{air} were **calculated** using a FORTRAN function Shift_CO2_air [8].

Format of the databank

The CDSD databank format is conformed with the current HITRAN format [3].
Each databank entry has the following fields

field number	parameter	field length	Fortran descriptor	meaning	type	units and comments
1	M	2	I2	HITRAN molecule	integer	
2	I	1	I1	HITRAN isotopologue	integer	
3	ν	12	F12.6	vacuum wavenumber	real	cm^{-1}
4	s	10	E10.3	intensity	real	$cm^{-1}/(molecule\ cm^{-2})$ at 296 K
5	A	10	E10.3	Einstein A-coefficient	real	s^{-1}
6	g_{air}	5	F5.4	air-broadened half-width	real	$cm^{-1}atm^{-1}$ at 296 K
7	g_{self}	5	F5.4	self-broadened half-width	real	$cm^{-1}atm^{-1}$ at 296 K
8	E''	10	F10.4	lower-state energy	real	cm^{-1}
9	n_{air}	4	F4.2	temperature-dependence exponent for g_{air}	real	
10	d_{air}	8	F8.6	air pressure-induced line shift	real	$cm^{-1}atm^{-1}$ at 296 K
11	n_{self}	4	F4.2	temperature-dependence exponent for g_{self}	real	
12	v_1'	3	I3	upper state vibrational numbers $v_1v_2l_2v_3r$	integer	Spectroscopic assignment adopted for HITRAN
13	v_2'	2	I2		integer	
14	l_2'	2	I2		integer	
15	v_3'	2	I2		integer	
16	r'	1	I1		integer	
17	v_1''	8	5x,I3	lower state vibrational numbers $v_1v_2l_2v_3r$	integer	
18	v_2''	2	I2		integer	
19	l_2''	2	I2		integer	
20	v_3''	2	I2		integer	
21	r''	1	I1		integer	
22	p'	3	I3	upper state polyad, Wang symmetry and ranking number	integer	Generalized assignment discussed in detail in [2]. $p=2v_1+v_2+3v_3$ c= 1 or 2 n=1,2,…
23	c'	2	I2		integer	
24	n'	4	I4		integer	
25	p''	3	I3	lower state polyad, Wang symmetry and ranking number	integer	
26	c''	2	I2		integer	
27	n''	4	I4		integer	
28	branch	3	2x,a1	P, Q, R	char	
29	j''	3	I3	lower state j	integer	
30	w''	1	a1	lower state Wang symmetry	char	'e' or 'f'
31	t_CDSD	5	I5			Origin of a line: 296 – CDSD-296 750 – CDSD-Venus 1000 – CDSD-1000

Isotopic composition of CDSD-HITEMP

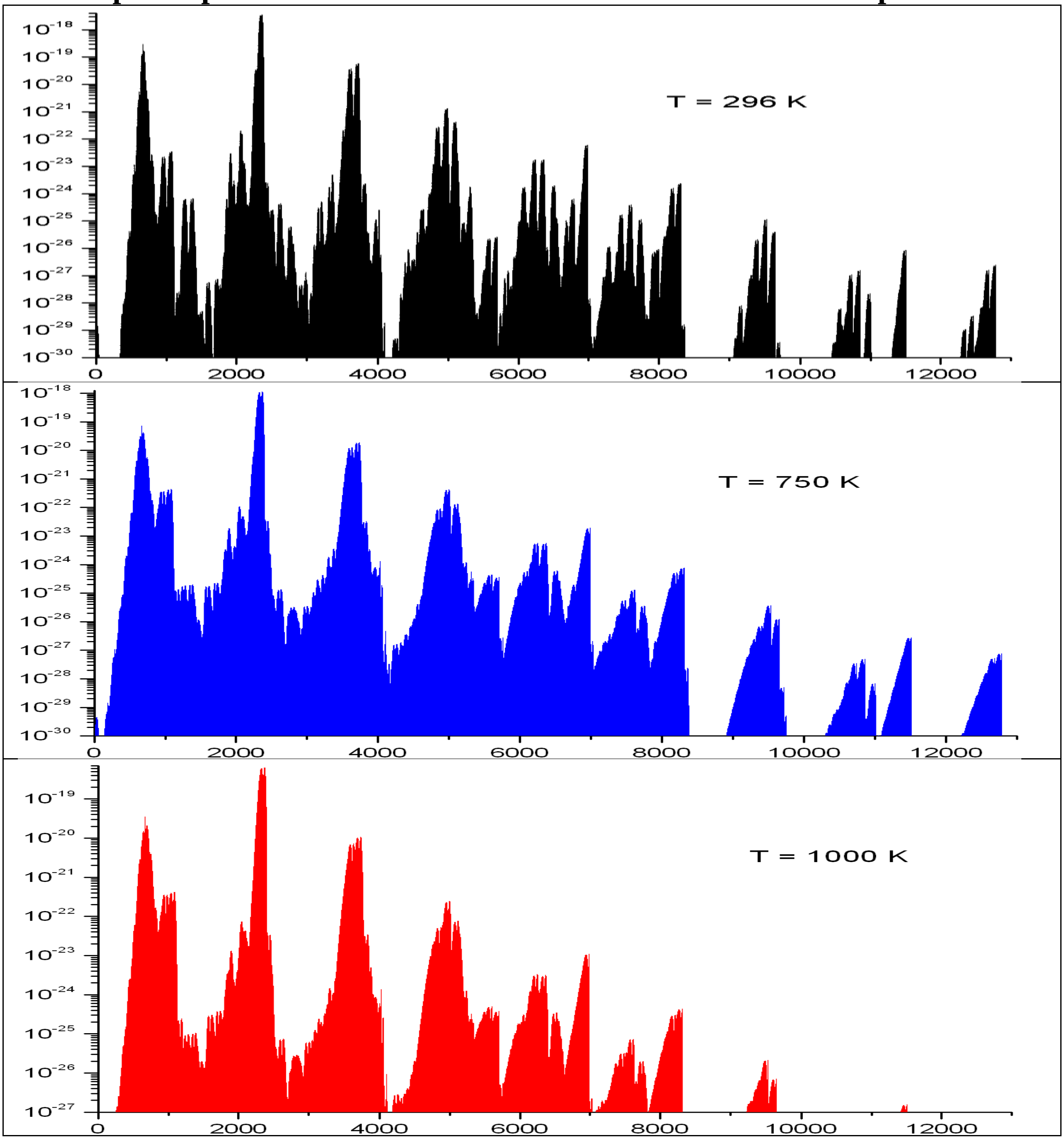
isotopologue	entries	ν_{min}	ν_{max}	s_{min}	s_{max}
$^{12}C^{16}O_2$	5881459	145.8	12784.1	3.47E-51	3.52E-18
$^{13}C^{16}O_2$	1732514	260.7	12462.0	9.28E-48	3.74E-20
$^{16}O^{12}C^{18}O$	2283608	5.9	11422.6	1.55E-46	6.87E-21
$^{16}O^{12}C^{17}O$	604898	10.6	8270.1	2.65E-45	1.26E-21
$^{16}O^{13}C^{18}O$	522204	354.3	6744.2	2.04E-43	7.81E-23
$^{16}O^{13}C^{17}O$	36179	546.6	6768.6	1.29E-41	1.40E-23
$^{12}C^{18}O_2$	132746	392.6	8162.9	3.27E-42	1.33E-23

Distribution of CDSD-HITEMP

CDSD-HITEMP is distributed as a set of 20 zipped ascii files sorted by vacuum wavenumber ν

file	ν_{min} (cm^{-1})	ν_{max} (cm^{-1})
cdsd_01	0	500
cdsd_02	500	625
cdsd_03	625	750
cdsd_04	750	1000
cdsd_05	1000	1500
cdsd_06	1500	2000
cdsd_07	2000	2125
cdsd_08	2125	2250
cdsd_09	2250	2500
cdsd_10	2500	3000
cdsd_11	3000	3250
cdsd_12	3250	3500
cdsd_13	3500	3750
cdsd_14	3750	4000
cdsd_15	4000	4500
cdsd_16	4500	5000
cdsd_17	5000	5500
cdsd_18	5500	6000
cdsd_19	6000	6500
cdsd_20	6500	13000

Graphical presentation of CDSD-HITEMP for 3 different temperatures

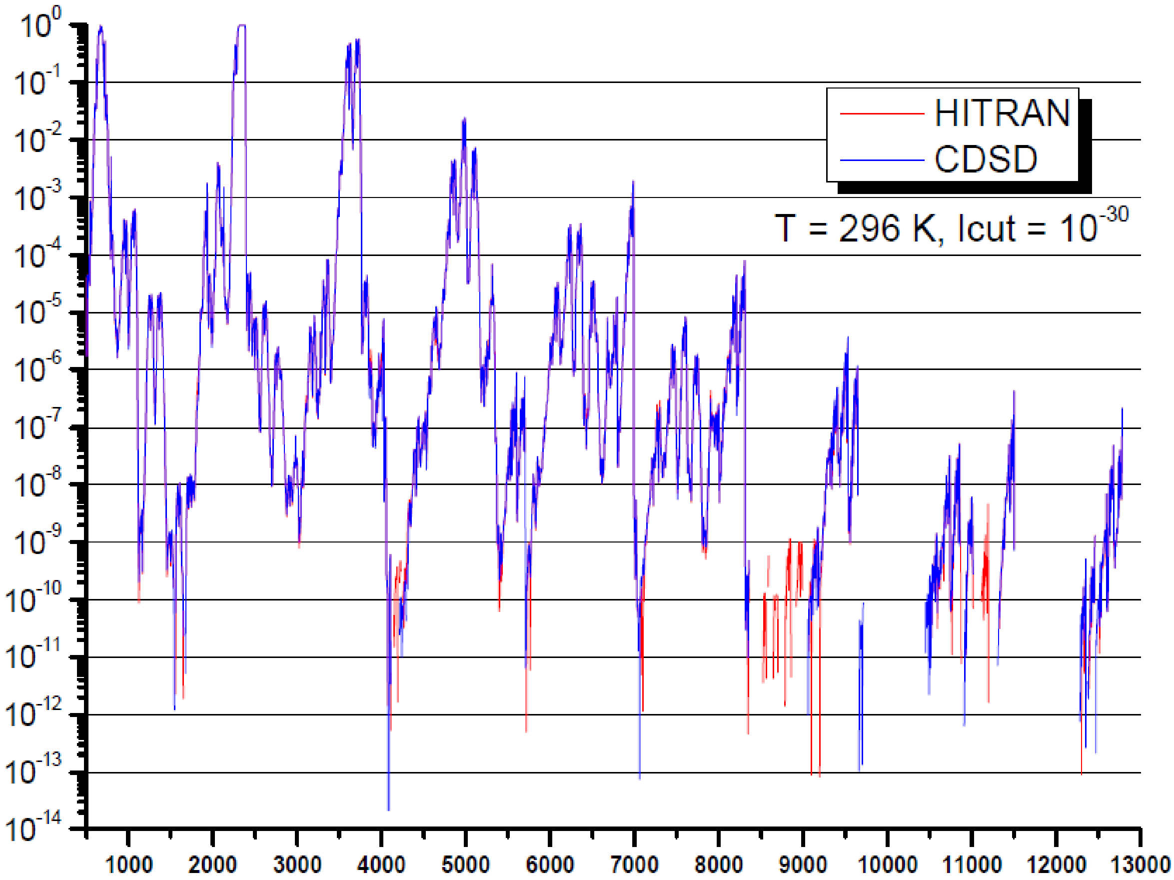


CDSD-HITEMP versus HITRAN-2008, HOT-CO_2 and HITEMP databanks

In order to compare CDSD-HITEMP with other databanks we simulated medium resolution absorption spectra of pure CO_2 with different temperatures and intensity cutoffs under the following conditions:

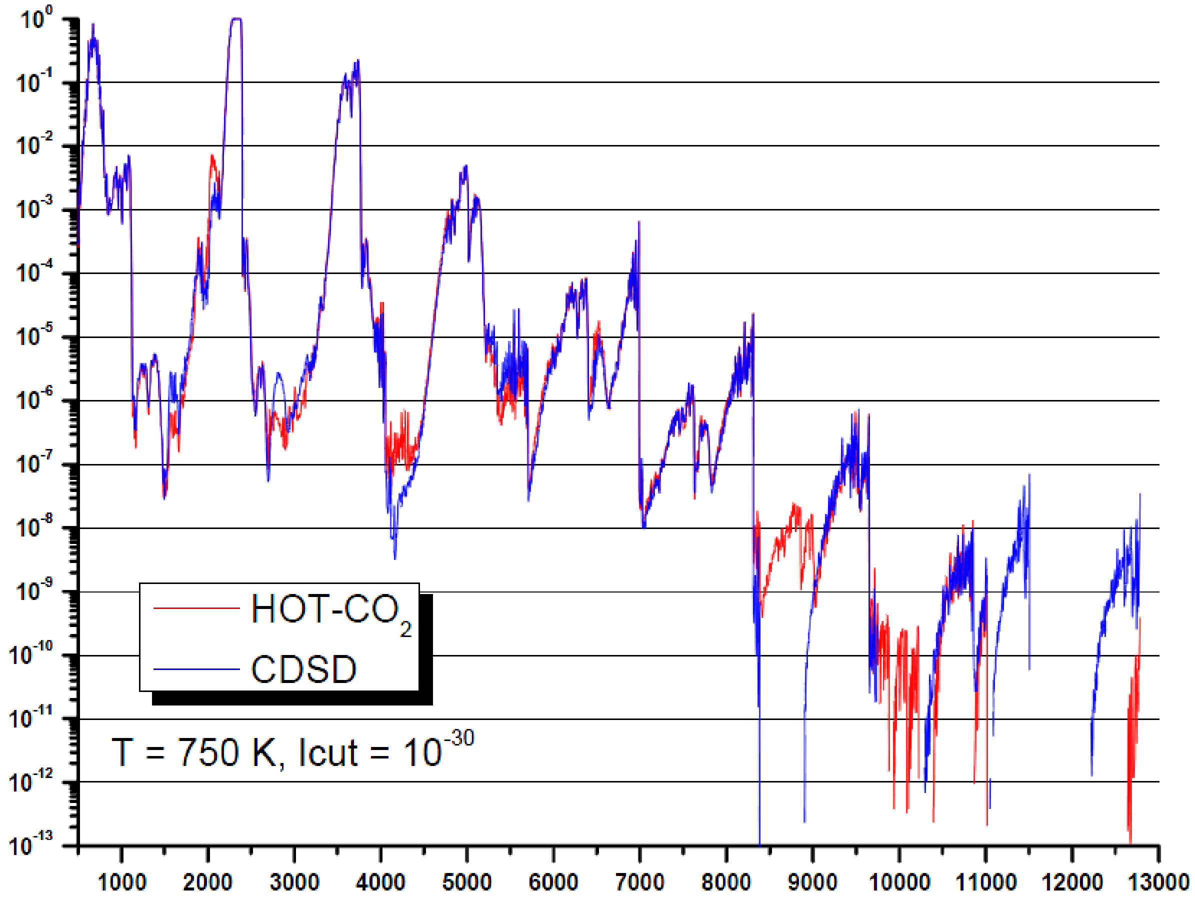
Frequency range (cm^{-1})	500 - 13000
Pressure (atm)	1
Pathlength (cm)	1
Type of apparatus function	rectangle
Width of apparatus function (cm^{-1})	1
Contour type	Lorentz
Wing length (cm^{-1})	2
Number of frequency steps	3000

CDSD-HITEMP versus HITRAN-2008 [3]



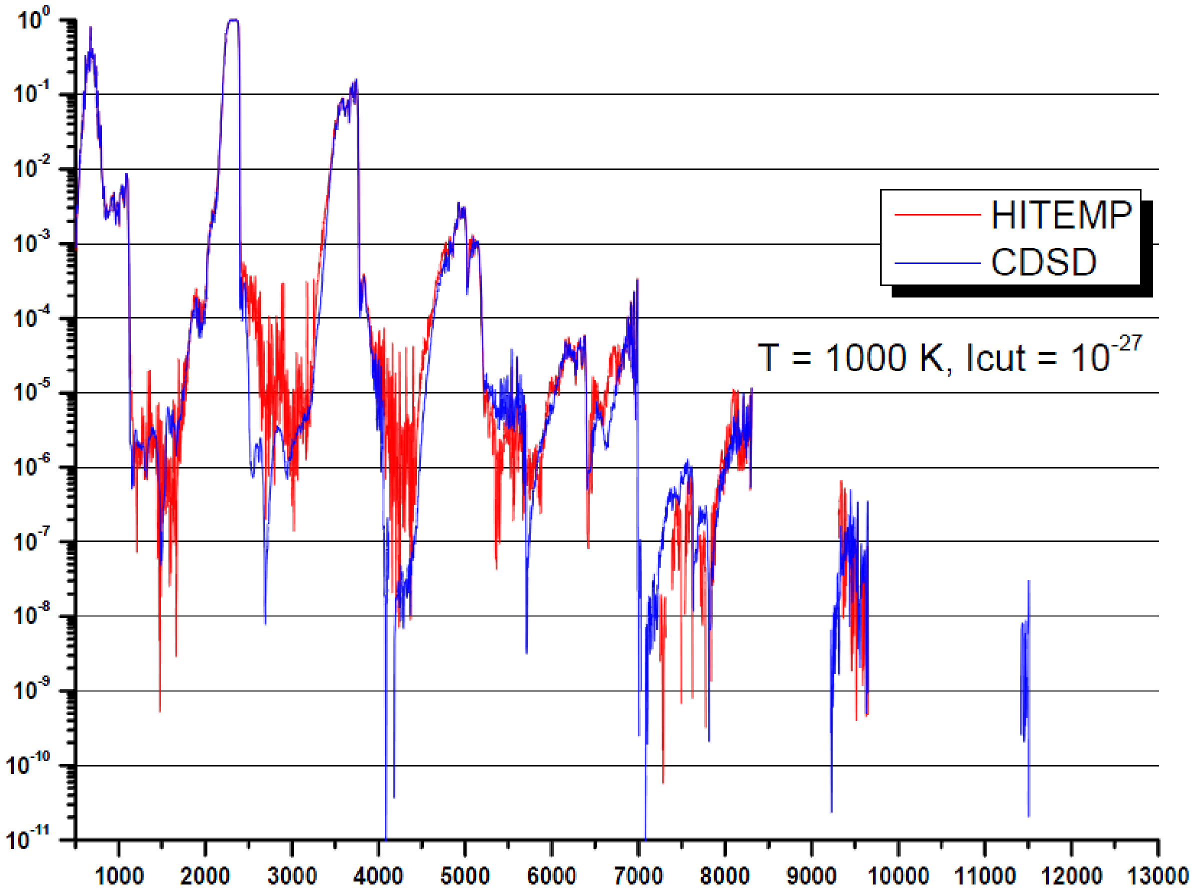
CDSD-HITEMP versus HOT-CO2

HOT-CO2 is a calculated database created by Wattson to study Venus' atmosphere. Reference temperature of the database is 750 K and intensity cutoff is 10^{-30} $cm^{-1}/(cm^{-2}$ molecule)) at 750 K [9]. The database covers the 500 – 12500 cm^{-1} spectral range and includes data for $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$, and $^{16}O^{13}C^{18}O$ isotopologues.



CDSD-HITEMP versus HITEMP-1995

HITEMP-1995 is a previous version of the HITEMP database [10]. Reference temperature of the database is 296 K and intensity cutoff is ~10^{-27} $cm^{-1}/(cm^{-2}$ molecule)) at T = 1000 K. The database consists of 1032269 entries of 8 isotopologues and covers the 500 – 9648 cm^{-1} spectral range.



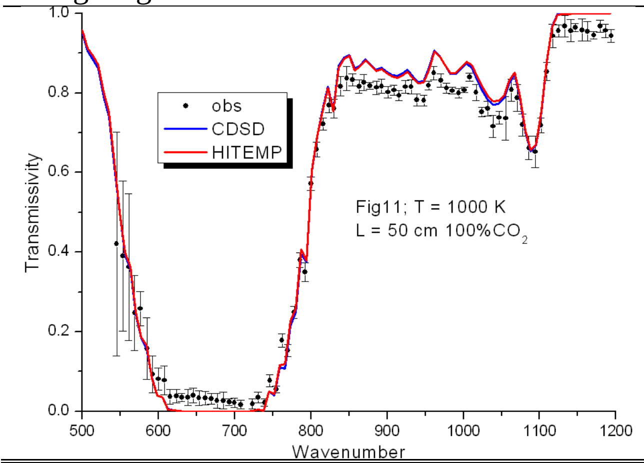
HITEMP
CDSD
T = 1000 K, Icut = 10^-27
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10^-8
10^-9
10^-10
10^-11
1000 2000 3000 4000 5000 6000 7000 8000 9000 10000 11000 12000 13000

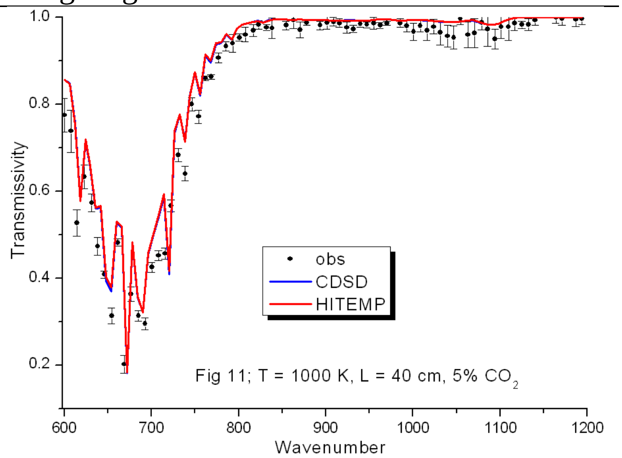
Validation of CDSD-HITEMP using medium and low resolution high-temperature spectra

i) 15 μm region

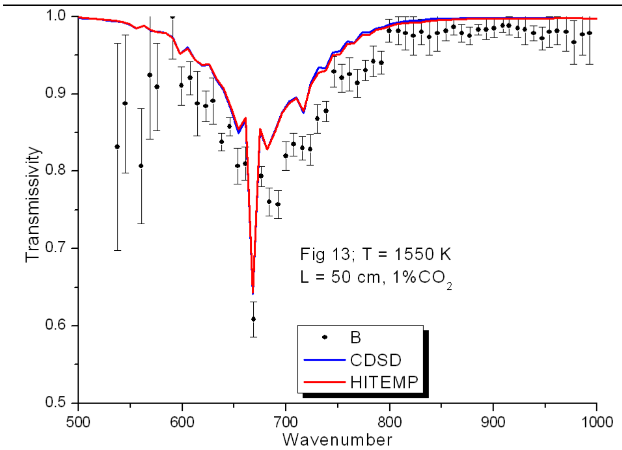
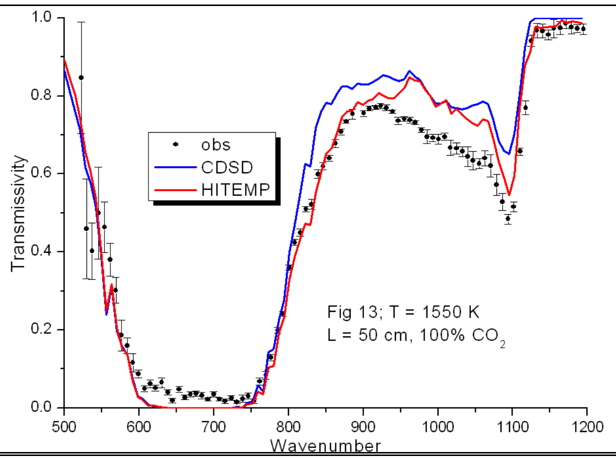
Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K [11]. For each region we give a plot of digitized observed transmittance taken from [11] and simulated transmittances using CDSD-HITEMP and HITEMP [10] data. Transmittances were calculated by a line-by-line code.

Temperature 1000 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1000 K Pressure 1 atm Pathlength 40 cm CO_2 concentration 5% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}

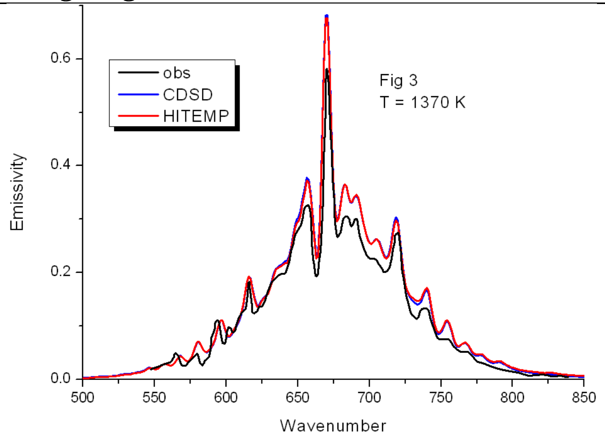
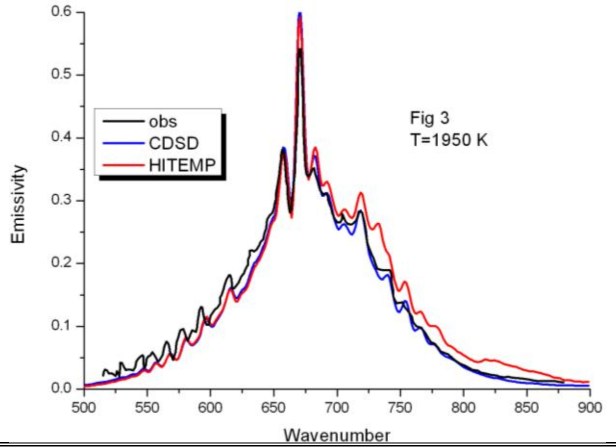




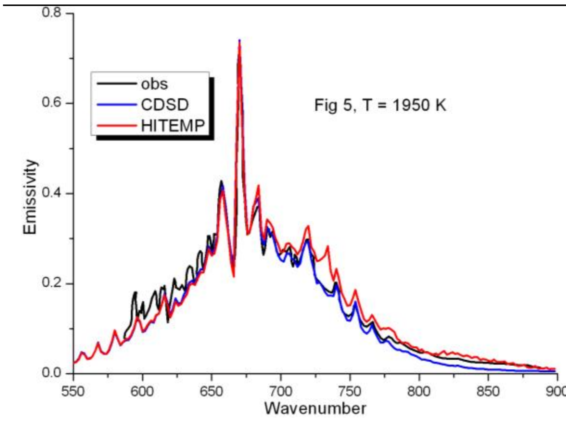
Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 1% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}

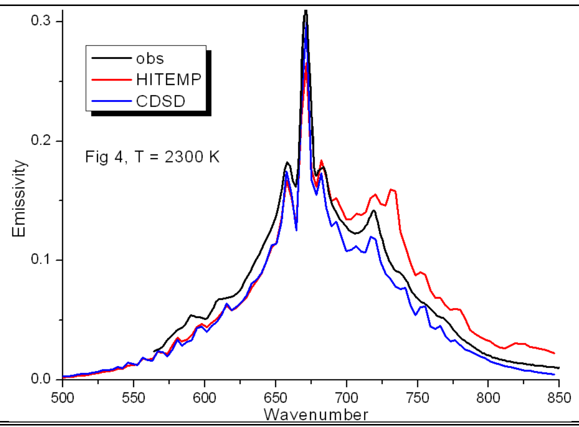
	

Low-resolution emission spectra from [12]

Temperature 1370 K Pressure 1 atm Pathlength 3.12 cm CO_2 concentration 36% ILS function form: triangle ILS full width at half maximum: 5 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1950 K Pressure 1 atm Pathlength 3.12 cm CO_2 concentration 53% ILS function form: triangle ILS full width at half maximum: 5 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}
	

Temperature 1950 K Pressure 1 atm Pathlength 3.12 cm CO_2 concentration 53% ILS function form: triangle ILS full width at half maximum: 2 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 2300 K Pressure 1 atm Pathlength 1.67 cm CO_2 concentration 49% ILS function form: triangle ILS full width at half maximum: 5 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}

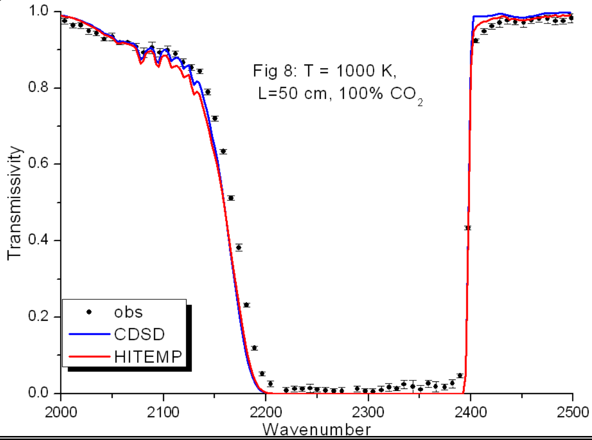




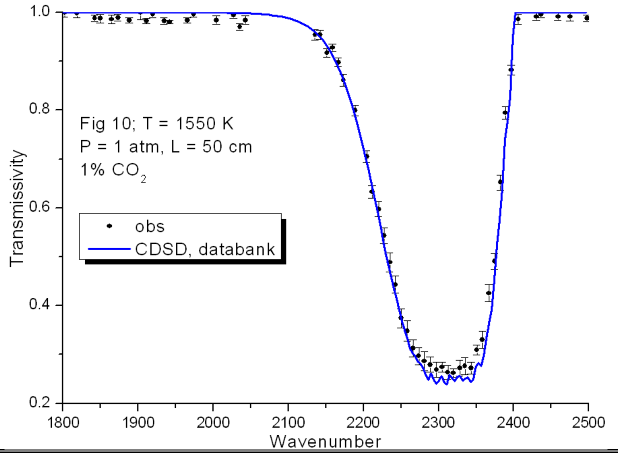
ii) 4.3 µm region

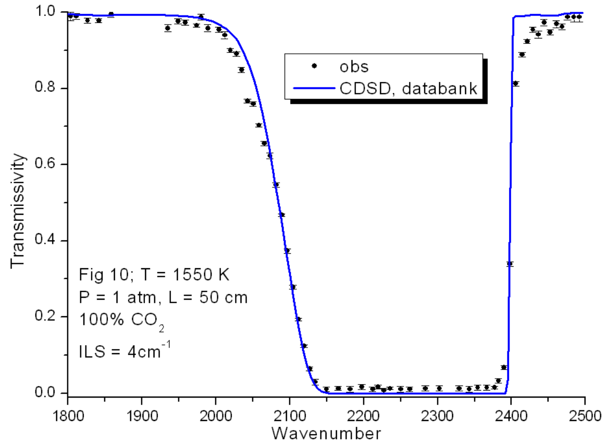
Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K [11]. For each region we give a plot of digitized observed transmittance taken from [11] and simulated transmittances using CDSD-HITEMP and HITEMP [10] data. Transmittances were calculated by a line-by-line code.

Temperature 1000 K
Pressure 1 atm
Pathlength 50 cm
CO_2 concentration 100%
ILS function form: triangle
ILS full width at half maximum: 4 cm^{-1}
Lorentz contour
Wing length: 2 cm^{-1}



Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 1% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}

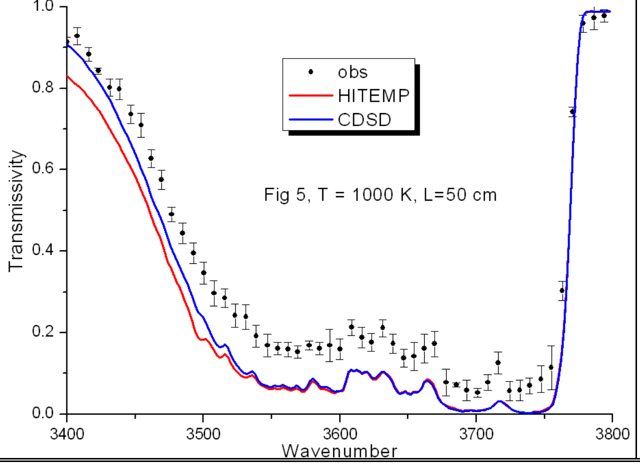


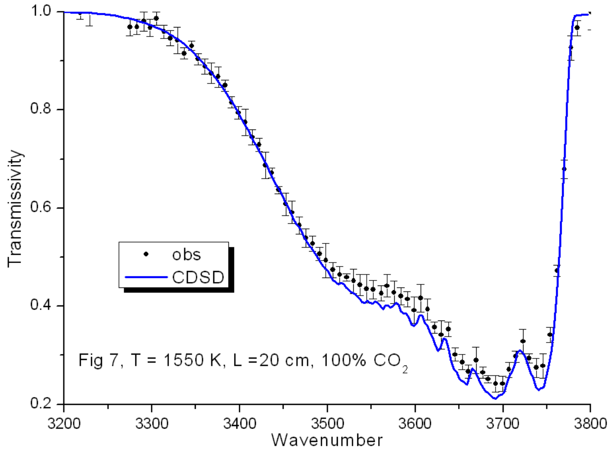


iii) 2.7 µm region

Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K [11]. For each region we give a plot of digitized observed transmittance taken from [11] and simulated transmittances using CDSD-HITEMP and HITEMP [10] data. Transmittances were calculated by a line-by-line code.

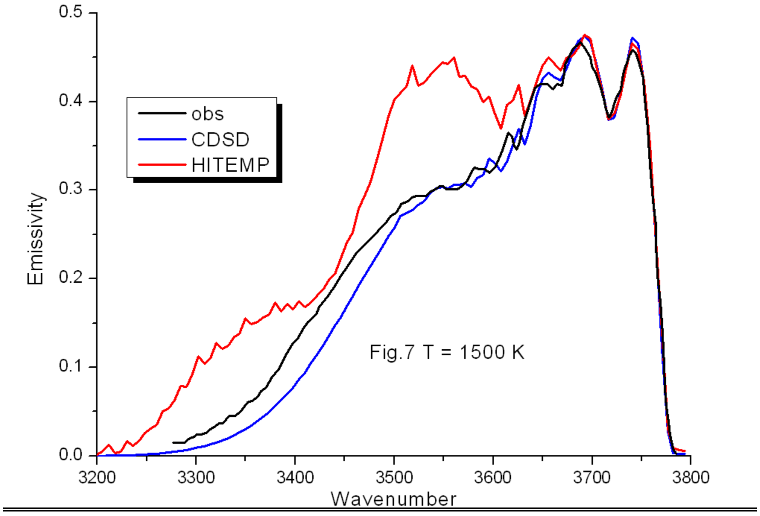
Temperature 1000 K	Temperature 1550 K
Pressure 1 atm	Pressure 1 atm
Pathlength 50 cm	Pathlength 50 cm
CO_2 concentration 100%	CO_2 concentration 100%
ILS function form: triangle	ILS function form: triangle
ILS full width at half maximum: 4 cm^{-1}	ILS full width at half maximum: 4 cm^{-1}
Lorentz contour	Lorentz contour
Wing length: 2 cm^{-1}	Wing length: 2 cm^{-1}





Medium resolution spectrum from [13].

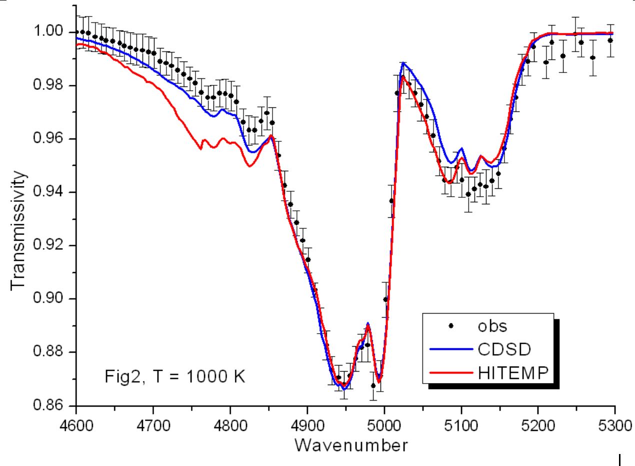
Temperature 1500 K
Pressure 1 atm
Pathlength 7.75 cm
CO_2 concentration 100%
ILS function form: triangle
ILS full width at half maximum: 3 cm^{-1}
Lorentz contour
Wing length: 2 cm^{-1}

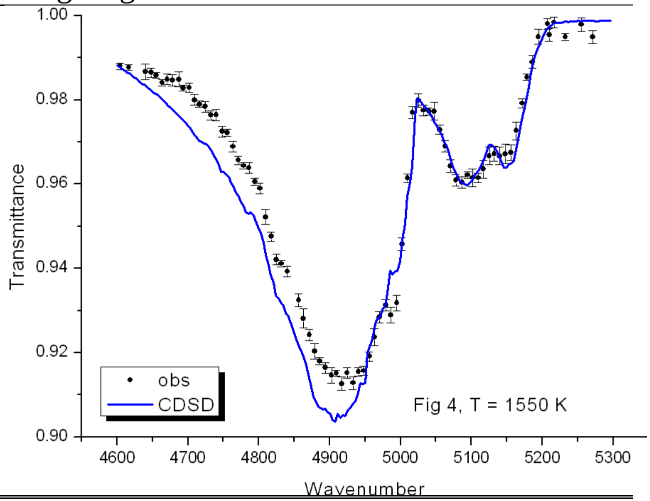


iv) *2.0 μm region*

Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K [11]. For each region we give a plot of digitized observed transmittance taken from [11] and simulated transmittances using CDSD-HITEMP and HITEMP [10] data. Transmittances were calculated by a line-by-line code.

Temperature 1000 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}





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