Readme for **CDSD-HITEMP**

CDSD-HITEMP is a version of the Carbon Dioxide Spectroscopic Databank (CDSD) adapted for the 296 - 2000 K temperature interval. CDSD-HITEMP is also included into 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 can be used for temperatures from 296 K to 2000 K

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

1. an 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. a 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. an 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 similar to the HITRAN-2008 database [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].

Line intensities
All line intensities are **calculated** values based on global fits of measured positions using the effective operator approach [4,6]. Isotopic abundances are the same as in the HITRAN database.

Pressure broadening parameters
Air-broadened halfwidths γ_{air}, self-broadened halfwidths γ_{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 δ_{air} were **calculated** using a FORTRAN function Shift_CO2_air [8].

Format of the databank

The CDSD databank format is mostly compatible with the current HITRAN format [3]. However, there are a number of extra numerical fields which contain additional information specific to CDSD. These fields are given in blue.

Each databank entry has the following fields:

field number	parameter	field length	Fortran descriptor	meaning	type	units and comments
1	Mol	2	I2	Molecule molecule	integer	2 for CO_2
2	I_a	1	I1	Isotopologue number	integer	1-626, 2-636, etc.
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	γ_{air}	5	F5.4	air-broadened half-width	real	$cm^{-1}atm^{-1}$ at 296 K
7	γ_{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 γ_{air}	real	
10	δ_{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 γ_{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	line source	integer	296 – CDSD-296 750 – CDSD-Venus 1000 – CDSD-1000

Uncertainty and reference indices as well as upper- and lower-state statistical weights are not used.

Isotopic composition of CDSD-HITEMP

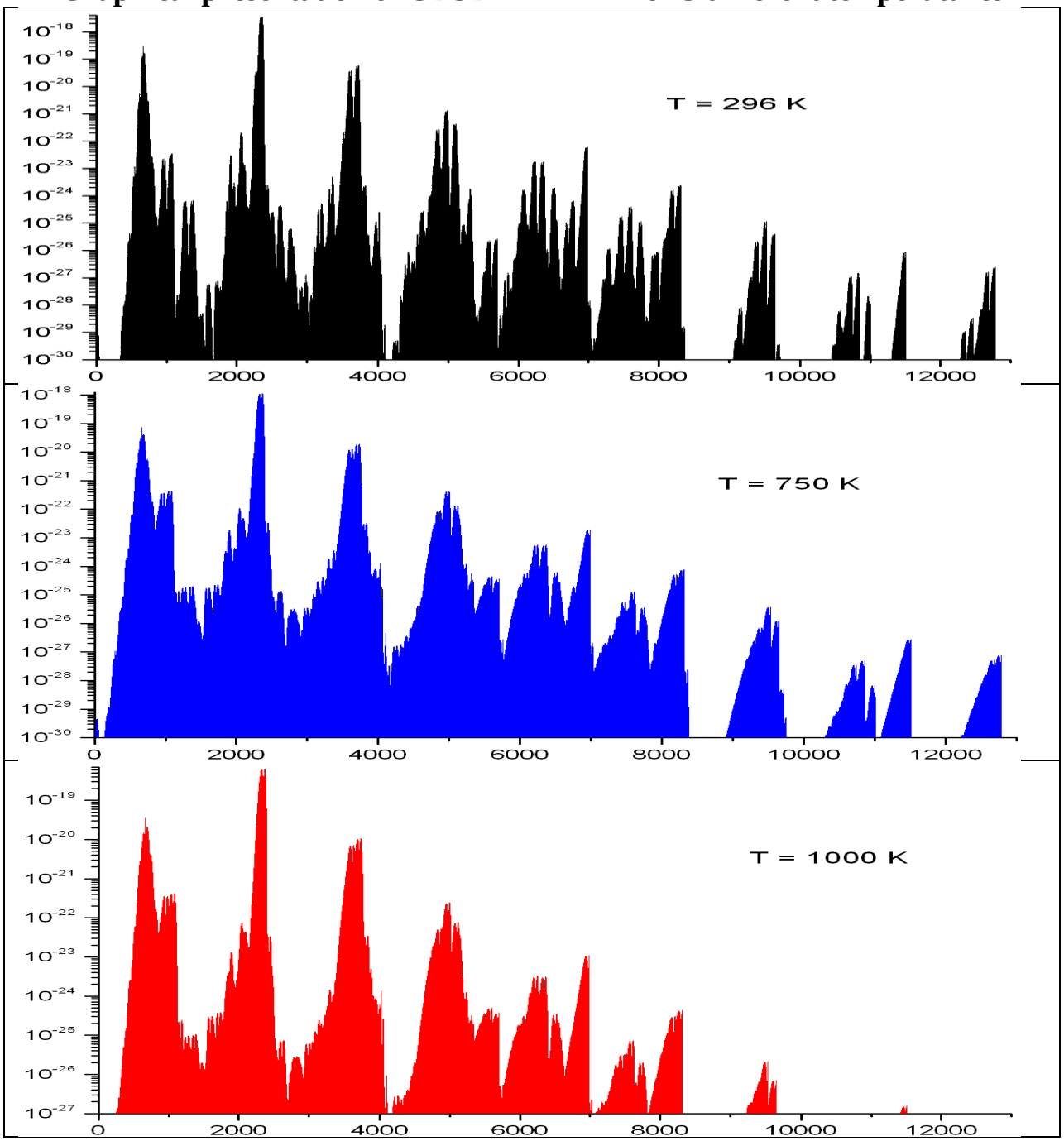
isotopologue	entries	ν_{min}	ν_{max}	s_{min}	s_{max}
$^{12}C^{16}O_2$	5881459	145.8	12784.1	3.47E-51	3.52E-18
$^{13}C^{16}O_2$	1732514	260.7	12462.0	9.28E-48	3.74E-20
$^{16}O^{12}C^{18}O$	2283608	5.9	11422.6	1.55E-46	6.87E-21
$^{16}O^{12}C^{17}O$	604898	10.6	8270.1	2.65E-45	1.26E-21
$^{16}O^{13}C^{18}O$	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 the wavenumber *v*

file	v_{min} (cm^{-1})	v_{max} (cm^{-1})
cdsd_hitemp_0_500	0	500
cdsd_hitemp_500_625	500	625
cdsd_hitemp_625_750	625	750
cdsd_hitemp_750_1000	750	1000
cdsd_hitemp_1000_1500	1000	1500
cdsd_hitemp_1500_2000	1500	2000
cdsd_hitemp_2000_2125	2000	2125
cdsd_hitemp_2125_2250	2125	2250
cdsd_hitemp_2250_2500	2250	2500
cdsd_hitemp_2500_3000	2500	3000
cdsd_hitemp_3000_3250	3000	3250
cdsd_hitemp_3250_3500	3250	3500
cdsd_hitemp_3500_3750	3500	3750
cdsd_hitemp_3750_4000	3750	4000
cdsd_hitemp_4000_4500	4000	4500
cdsd_hitemp_4500_5000	4500	5000
cdsd_hitemp_5000_5500	5000	5500
cdsd_hitemp_5500_6000	5500	6000
cdsd_hitemp_6000_6500	6000	6500
cdsd_hitemp_6500_13000	6500	13000

Graphical presentation of CDSD-HITEMP for 3 different temperatures

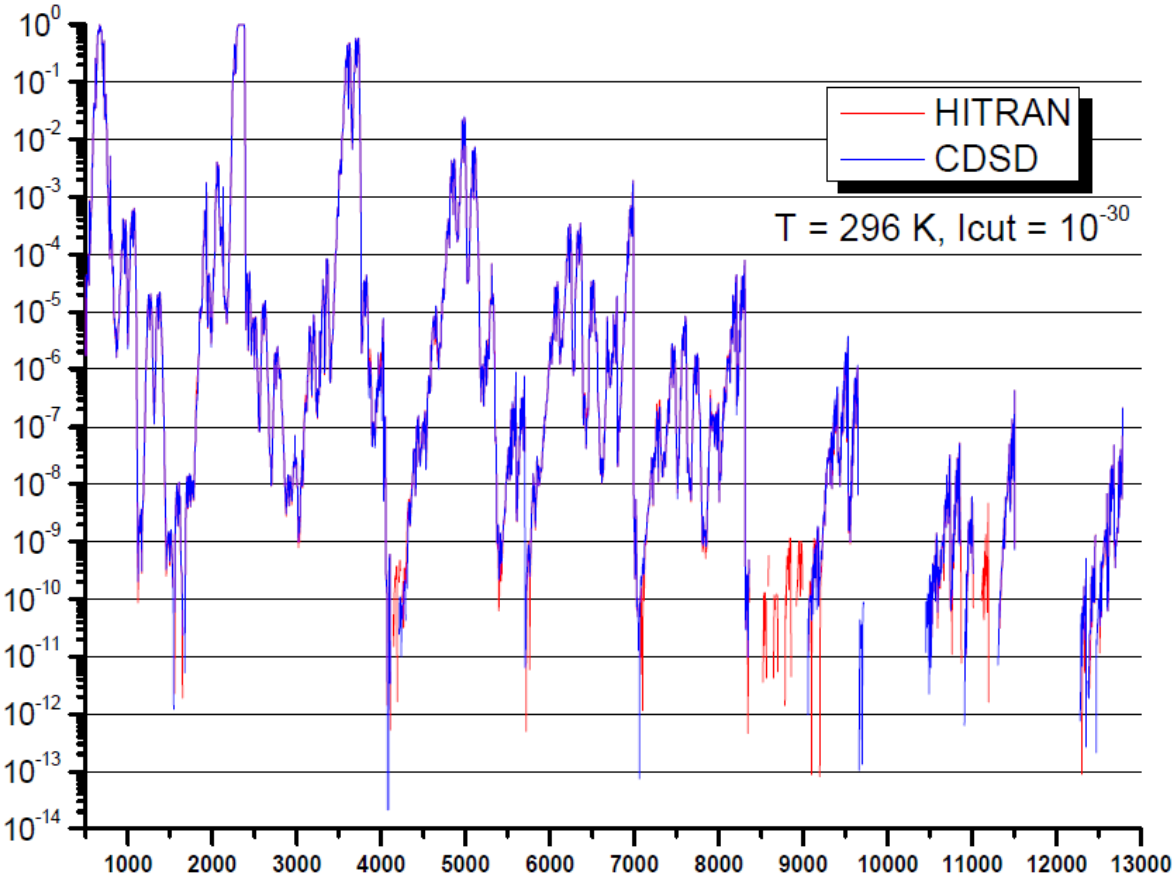


CDSD-HITEMP versus HITRAN-2008, HOT-CO_2 and HITEMP databanks

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:

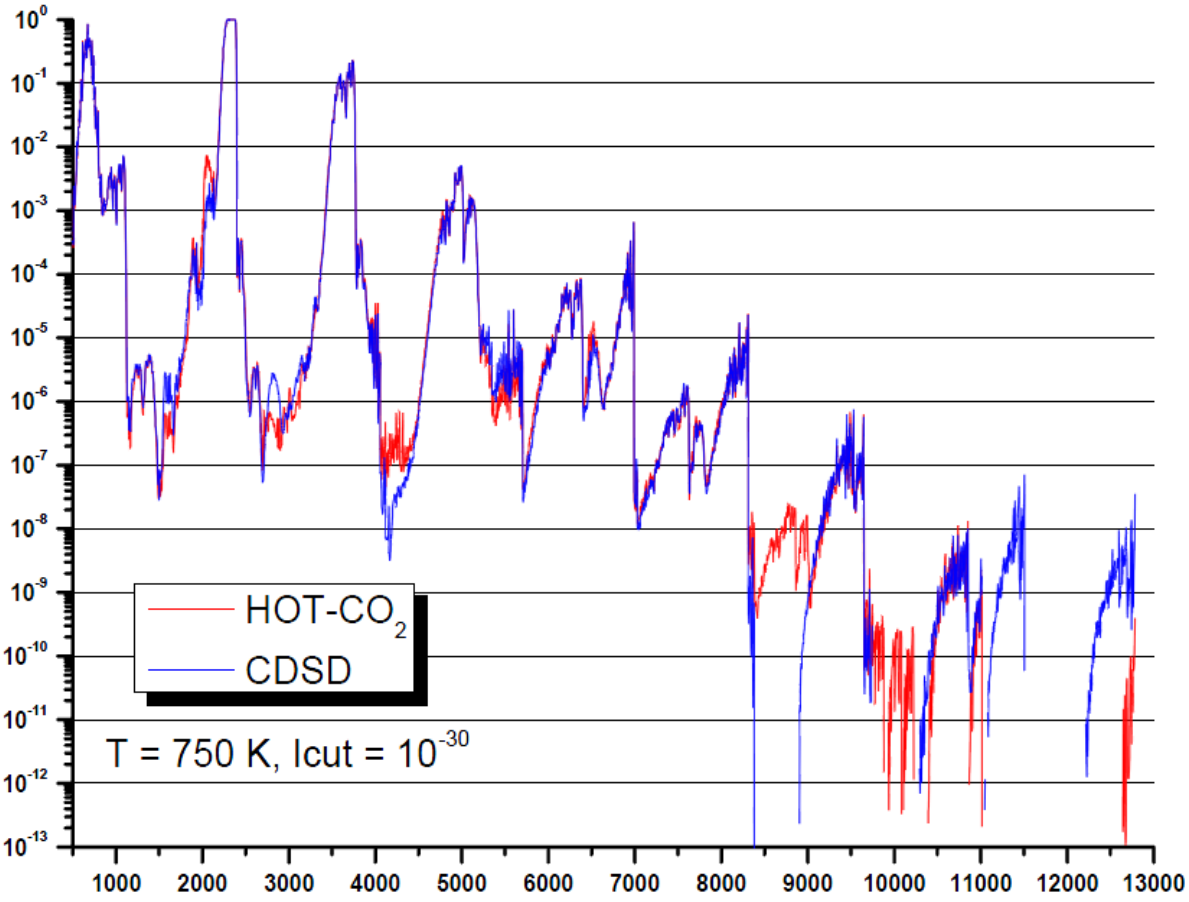
Frequency range (cm^{-1})	500 - 13000
Pressure (atm)	1
Pathlength (cm)	1
Type of apparatus function	rectangle
Width of apparatus function (cm^{-1})	1
Contour type	Lorentz
Wing length (cm^{-1})	2
Number of frequency steps	3000

CDSD-HITEMP versus HITRAN-2008 [3]



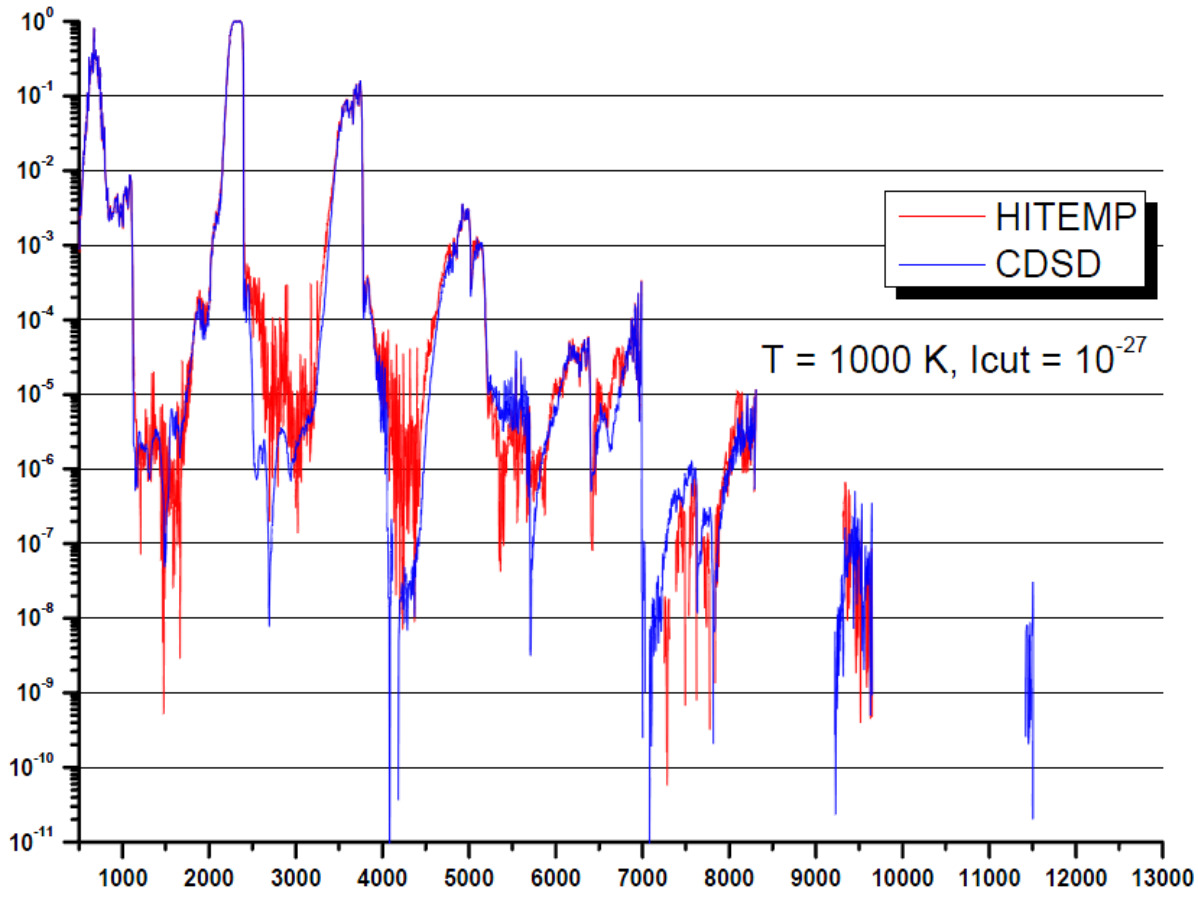
CDSD-HITEMP versus HOT-CO2

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

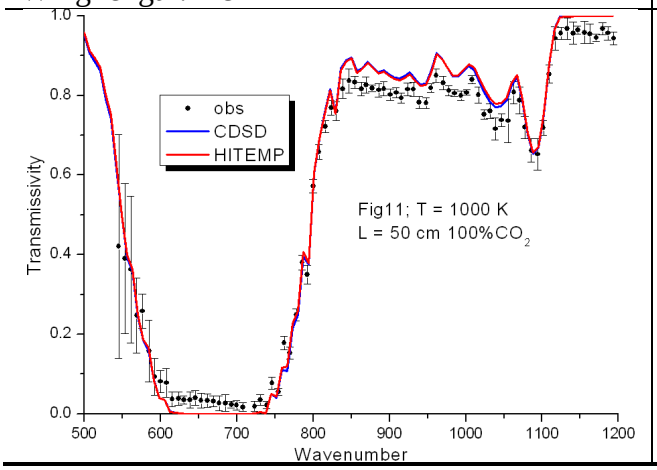
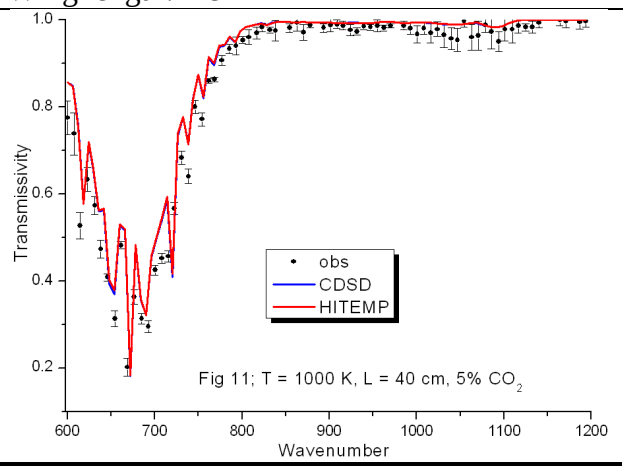
HITEMP-1995 is a previous version of the HITEMP database [10]. Reference temperature of the database is 296 K and intensity cutoff is ~10^{-27} $cm^{-1}/(cm^{-2}$ molecule)) at T = 1000 K. The database consists of 1032269 entries of 8 isotopologues and covers the 500 – 9648 cm^{-1} spectral range.


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

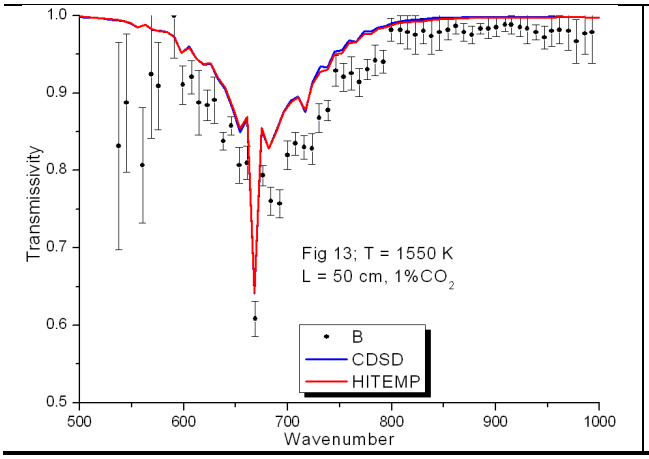
Validation of CDSD-HITEMP using medium and low resolution high-temperature spectra

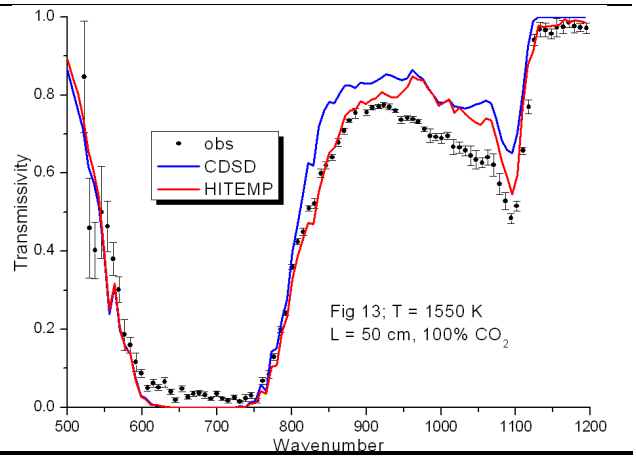
i) 15 μm region

Medium resolution CO2 high-temperature spectra for T = 1000 and 1550. 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.

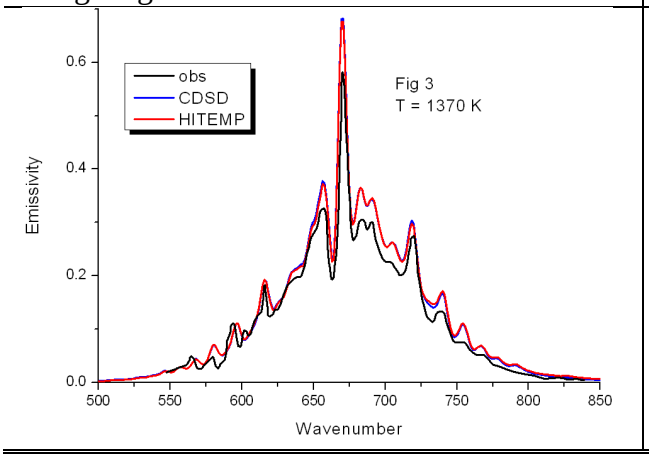
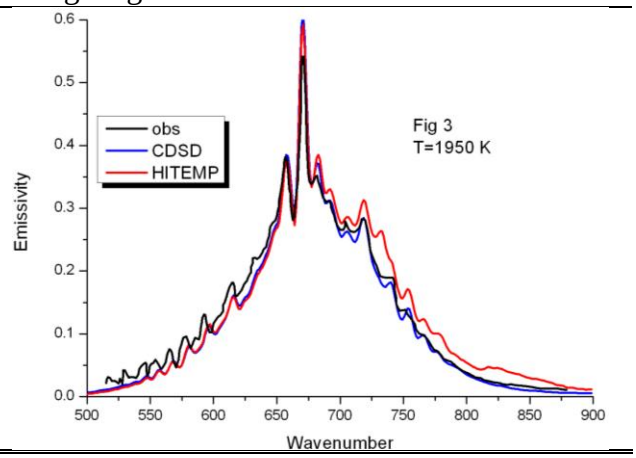
Temperature 1000 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1000 K Pressure 1 atm Pathlength 40 cm CO_2 concentration 5% ILS function form: triangle ILS full width at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

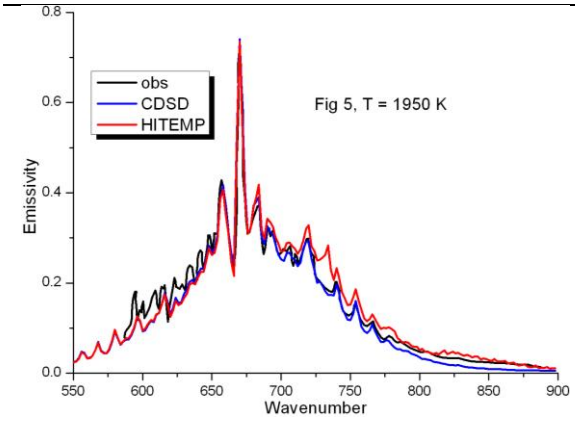


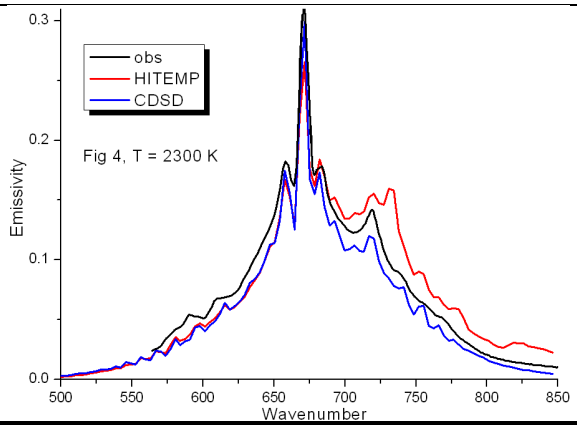


Low-resolution emission spectra from [12].

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}

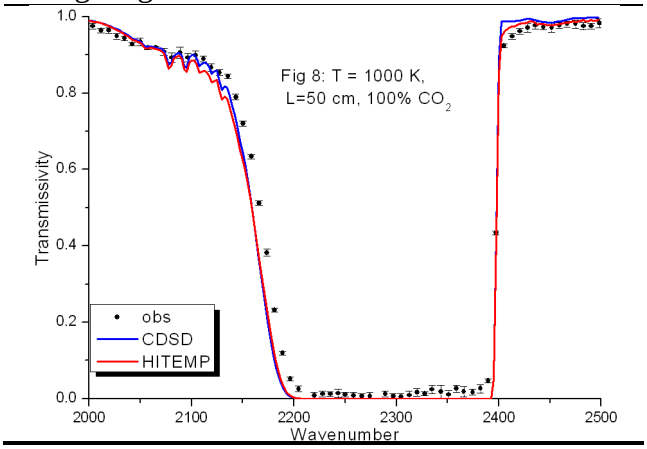




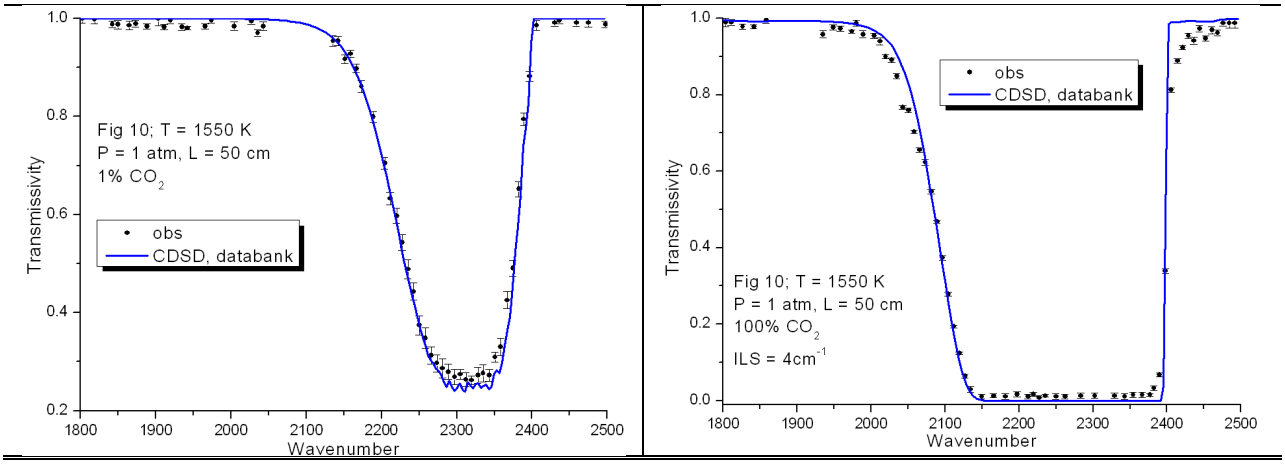
ii) 4.3 μm region

Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K. 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}

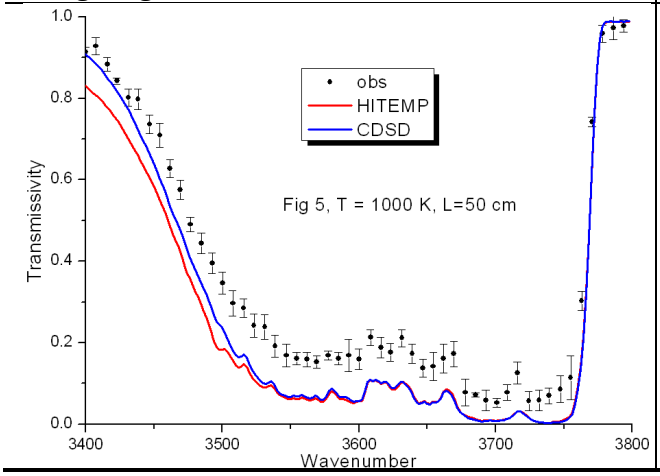
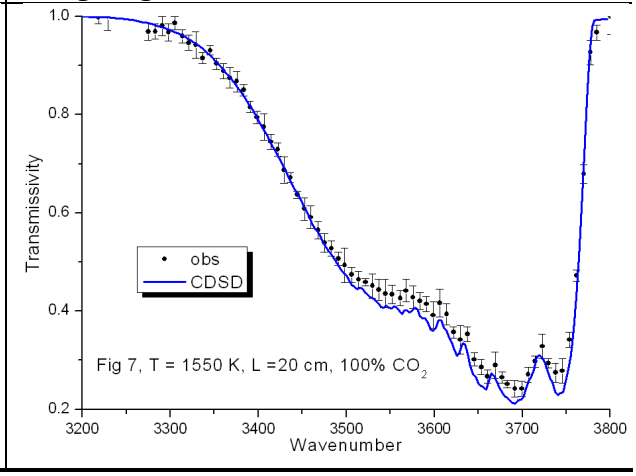


Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 1% ILS function form: triangle ILS full width at half maximum: 4 cm^{-1} Lorentz contour Wing length: 2 cm^{-1}	Temperature 1550 K Pressure 1 atm Pathlength 50 cm CO_2 concentration 100% ILS function form: triangle ILS full width at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



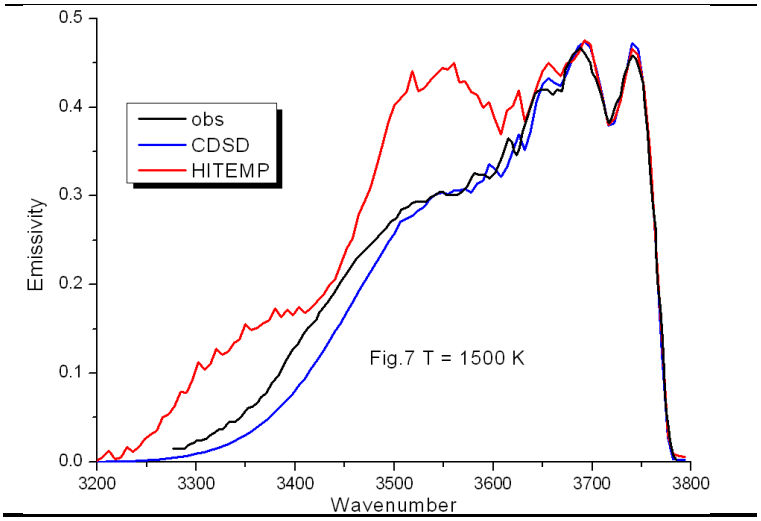
iii) 2.7 μm region

Medium resolution CO2 high-temperature spectra for T = 1000 and 1550 K. 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}
	

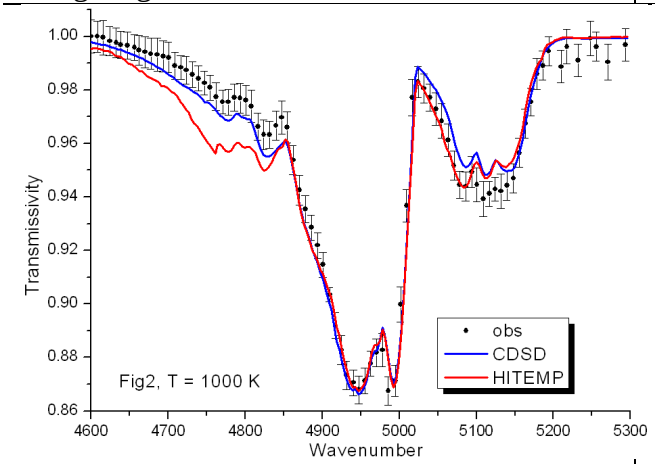
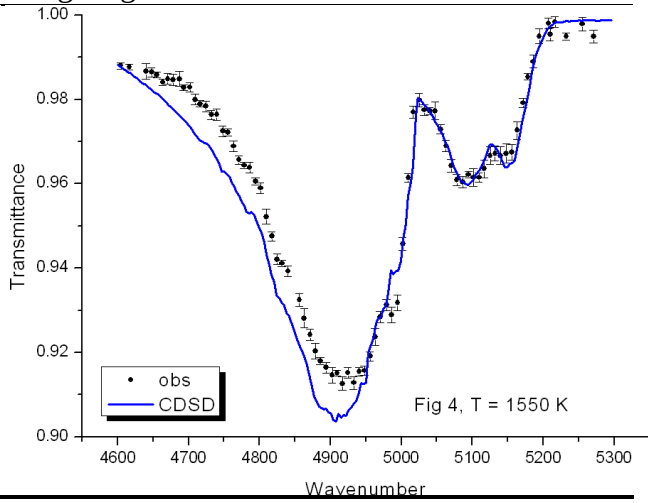
Medium resolution spectrum from [13].

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. 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}
	

References

1. L.S. Rothman, I.E. Gordon, R.J. Barber, H. Dothe, R.R. Gamache, A. Goldman, V.I. Perevalov, S.A. Tashkun, J. Tennyson HITEMP, the High-Temperature Molecular Spectroscopic Database, JQSRT **111**, (2010) 2139–2150
2. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, A.D. Bykov and N.N. Lavrentieva CDSD-1000, the high-temperature carbon dioxide spectroscopic databank JQSRT **82**, (2003) 165-196
3. L.S. Rothman, I.E. Gordon, A. Barbe, D.Chris Benner, P.F. Bernath, M. Birk, V. Boudon, L.R. Brown, A. Campargue, J.-P. Champion, K. Chance, L.H. Coudert, V. Dana, V.M. Devi, S. Fally, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, N. Lacome, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, S. Mikhailenko, N. Moazzen-Ahmadi, O. Naumenko, A. Nikitin, J. Orphal, A. Predoi-Cross, V. Perevalov, A. Perrin, C.P. Rinsland, M. Rotger, M. Šimečková, M.A.H. Smith, S. Tashkun, J. Tennyson, R.A. Toth, A.C. Vandaele, J. Vander Auwera The HITRAN 2008 Molecular Spectroscopic Database, JQSRT, **110** (2009) 533–572
4. J.-L. Teffo, O.N.Sulakshina, V.I. Perevalov Effective Hamiltonian for Rovibrational Energies and Line Intensities of Carbon Dioxide, JMS, **156** (1992) 48-64
5. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, L.S. Rothman, Vl.G. Tyuterev Global fitting of $^{12}C^{16}O_2$ vibrational–rotational line positions using the effective Hamiltonian approach JQSRT, **60** (1998) 785-801
6. S.A. Tashkun, V.I. Perevalov, J.-L. Teffo, VI.G. Tyuterev Global fit of $^{12}C^{16}O_2$ vibrational–rotational line intensities using the effective operator approach JQSRT, **62**, (1999) 571-598
7. A.D. Bykov, N.N. Lavrentieva, L.N. Sinitsa Calculation of CO_2 broadening and shift coefficients for high-temperature databases, Atmos. Oceanic Opt. **13** (2000) 1015-1019
8. J.-M. Hartmann A simple empirical model for the collisional spectral shift of air-broadened CO_2 lines, JQSRT **110**, (2009) 2019–2026
9. J.B. Pollack, J.B. Dalton, D. Grinspoon, R.B. Wattson, R. Freedman, D. Crisp, D.A. Allen, B. Bezard, C. DeBergh, L.P. Giver, Q. Ma, R. Tipping Near-infrared light from Venus' nightside: a spectroscopic analysis, Icarus, **103**, (1993) 1-42
10. L.S. Rothman, R.B. Wattson, R.R. Gamache, J. Schroeder, A. McCann HITRAN, HAWKS and HITEMP High-Temperature Molecular Database. Proc Soc Photo-Optical Instrumentation Engineers **2471** (1995) 105-111
11. S.P. Bharadwaj, M.F. Modest Medium resolution transmission measurements of CO_2 at high temperature - an update. JQSRT **103** (2007) 146-55
12. C.B. Ludwig, C.C. Ferriso, L. Acton High-Temperature Spectral Emissivities and Total Intensities of the 15-μ Band System of CO_2 JOSA **56** (1966) 1685-1692
13. D. Scutary, L. Rosenmann, J. Taine Approximate intensities of CO_2 hot bands at 2.7, 4.3, and 12 μm for high temperature and medium resolution applications JQSRT **52**, (1994) 765–781