New analysis of the CRDS spectrum of the six $^{16}O/^{18}O$ isopotologues of ozone up to 7920 cm^{-1}

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Theoretical model : C_S / C_{2V} species

Nuclear spin statistics:

C_{2V} species (666, 888, 686, 868) : nuclear spin statistical weight = 0

Only one rovibrational level exists for each $[J, K_a]$ value

C_S species (668, 886) : $[J, K_a, K_c = J-K_a]$ and $[J, K_a, K_c = J+1-K_a]$ levels have the same nuclear spin statistical weight

Twice more energy levels and **twice more** A-type transitions ($K_a = 0$) than for C_{2V} species

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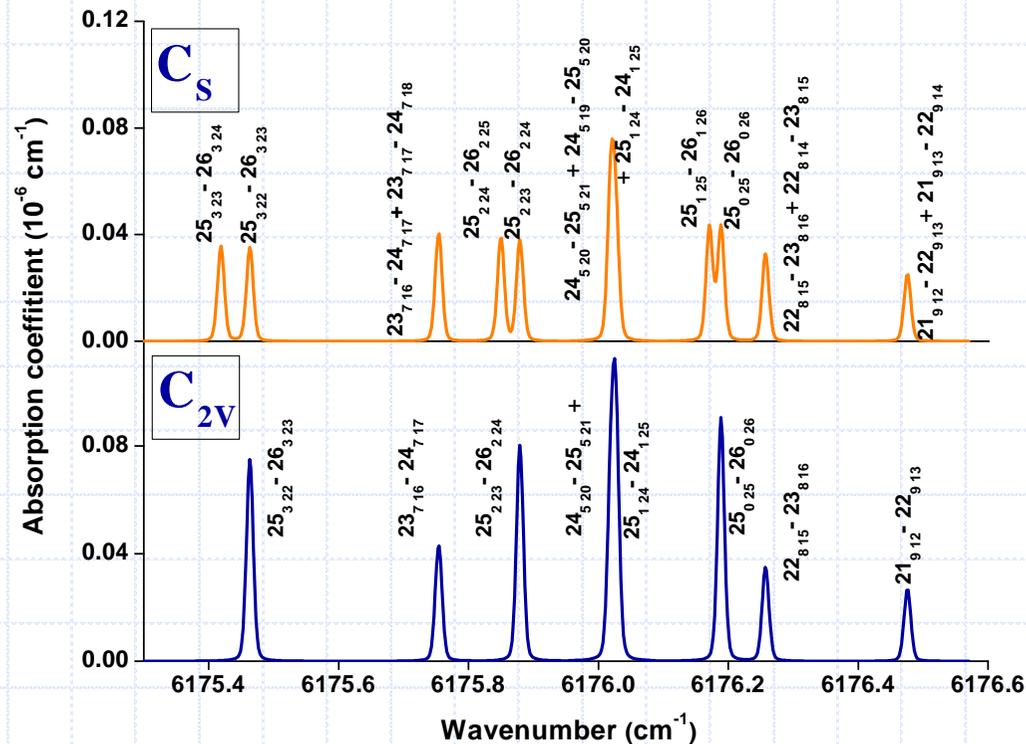
Resonance interactions

V-diagonal blocks of the effective rovibrational Hamiltonian (Watson-type form):

C_{2V} and C_S species

$$^{eff}H^{VV} = E^{VV} + \left[A - \frac{1}{2}(B+C)\right]J_z^2 + \frac{1}{2}(B+C)\,\mathbf{J}^2 + \frac{1}{2}(B-C)J_{xy}^2 - \Delta_K J_z^4 - \Delta_{JK}J_z^2\,\mathbf{J}^2 - \Delta_J\left(\mathbf{J}^2\right)^2$$

$$- \delta_K\left\{J_z^2, J_{xy}^2\right\} - 2\delta_J J_{xy}^2\,\mathbf{J}^2 + H_K J_z^6 + H_{KJ}J_z^4\,\mathbf{J}^2 + H_{JK}J_z^2\left(\mathbf{J}^2\right)^2 + H_J\left(\mathbf{J}^2\right)^3$$

$$+ h_K\left\{J_z^4, J_{xy}^2\right\} + h_{KJ}\left\{J_z^2, J_{xy}^2\right\}\,\mathbf{J}^2 + 2h_J J_{xy}^2\left(\mathbf{J}^2\right)^2 + L_K J_z^8 + ...$$

where $\{A,B\} \equiv AB + BA$ and $J_{xy}^2 \equiv J_x^2 - J_y^2$

Allowed rovibrational resonance interactions:

C_{2V} species

$$\boxed{^{eff}H^{VV'}_{Coriolis}} = C_{001}(J_+ - J_-) + C_{011}\left(J_+(J_z + 1/2) + (J_z + 1/2)J_-\right) + C_{021}\left(J_+(J_z + 1/2)^2 - (J_z + 1/2)^2 J_-\right)$$

$$+ C_{201}\,\mathbf{J}^2(J_+ - J_-) + C_{003}\left(J_+^3 - J_-^3\right) + C_{031}\left(J_+(J_z + 1/2)^3 - (J_z + 1/2)^3 J_-\right)$$

$$+ C_{211}\,\mathbf{J}^2\left(J_+(J_z + 1/2) + (J_z + 1/2)J_-\right) + ...$$

$$\boxed{^{eff}H^{VV'}_{Anharm}} = F_{000} + F_{200}\,\mathbf{J}^2 + F_{020}J_z^2 + F_{002}\left(J_+^2 + J_-^2\right) + F_{022}\left[J_+^2(J_z + 1)^2 + (J_z + 1)^2 J_-^2\right] +$$

$$+ F_{202}\mathbf{J}^2\left(J_+^2 + J_-^2\right) + ...$$

where $J_\pm = J_x \mp iJ_y$

C_S species   **Coriolis and Anharmonic resonance interactions can occur simultaneously**

Dipole selection rules

C$_{2V}$ species

K_a = **even** ; **A-type** transitions with selection rules $J = 0, \pm 1$; dominant intensities

for $K_a = 0$ lines

$$^{(V^u)(V^l)}\tilde{\mu}_Z^{(A)} = d_1^A \varphi_z + d_2^A \left\{\varphi_z, \mathbf{J}^2\right\} + d_3^A \left\{\varphi_z, J_z^2\right\} + d_4^A \frac{1}{2}\left[\left\{\varphi_x, iJ_y\right\} - \left\{i\varphi_y, J_x\right\}\right] + ...$$

K_a = **odd** ; **B-type** transitions with selection rules $J = 0, \pm 1$; dominant intensities

for $K_a = 1$ lines

$$^{(V^u)(V^l)}\tilde{\mu}_Z^{(B)} = d_1^B \varphi_x + d_2^B \left\{\varphi_x, \mathbf{J}^2\right\} + d_3^B \left\{\varphi_x, J_z^2\right\} + d_4^B \left\{i\varphi_y, J_z\right\} + d_5^B \left\{\varphi_z, iJ_y\right\} + ...$$

C$_S$ species

both $^{(V^u)(V^l)}\tilde{\mu}_Z^{(A)}$ and $^{(V^u)(V^l)}\tilde{\mu}_Z^{(B)}$ components are non vanishing for all vibrational states

Hybrid character for rovibrational bands, containing both **A-type** and **B-type** transitions.

Results of the $2\nu_1+2\nu_2+3\nu_3\_2$ band analysis of $^{16}O^{16}O^{18}O$ near 6320 cm^{-1}

(i) Spectroscopic parameters (in cm^{-1})			(iii) Statistics for the line positions	
State	dark	(223)_2	Vibrational state	(223)_2
E^{VV}	6319.712$_1$ (20) [a]	6324.9509$_2$ (84)	Band centre (cm^{-1})	6325.213 [b]
$A-(B+C)/2$	3.19739$_9$ (52)	3.02627$_3$ (15)	J max	27
$(B+C)/2$	0.372150$_0$ (22)	0.3737885$_5$ (72)	K_a max	10
$(B-C)/2$	0.0258 [f]	0.023397$_6$ (13)	Number of transitions	505
κ ×10^3	g	0.2447$_1$ (38)	Number of levels	325
$_{JK}$ ×10^4	g	-0.1131$_8$ (48)	rms (10^{-3} cm^{-1})	5.37
$_J$ ×10^6	g	0.324$_9$ (13)	(iv) Statistics for the intensities	
δ_J ×10^6	g	0.119$_2$ (12)	J max	26
δ_K ×10^5	g	0.84$_0$ (20)	K_a max	7
H_K ×10^6	g	0.165$_2$ (23)	Number of transitions	67
H_{KJ} ×10^7	g	-0.692$_8$ (76)	rms (%)	14.7
Resonance coupling terms:			S_v =3.07×10^{-24} cm/molecule at 296 K [c] (809 lines)	
$A_{000}^{(dark)(223)}$		1.2023 (18)		
$A_{020}^{(dark)(223)}$		-0.01011$_2$ (56)		
$C_{011}^{(dark)(223)}$ ×10^2		0.930$_7$ (17)		
(ii) Dipole transition moment parameter (in Debye)				
$d_1^{(A)}$ ×10^4		0.4885$_1$ (69)		

[f]-fixed to the values predicted from PES
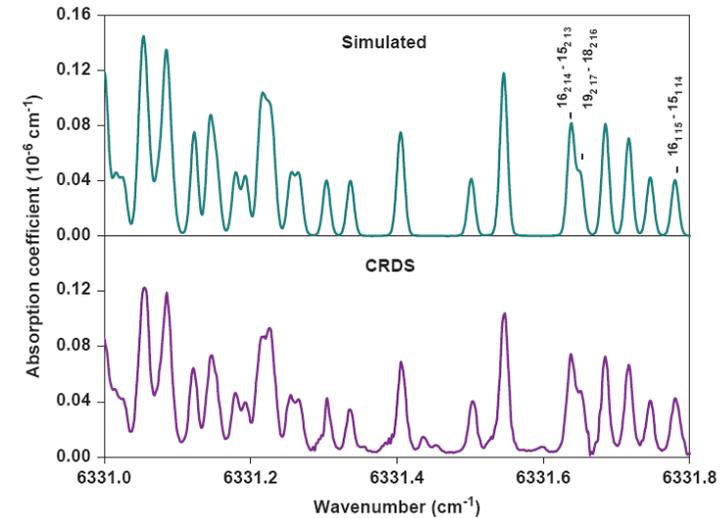
Comparison of the experimental and calculated spectra of $^{16}O^{16}O^{18}O$ in the R-branch region of the $2_1+2_2+3_3\_2$ band near 6331 cm^{-1}.
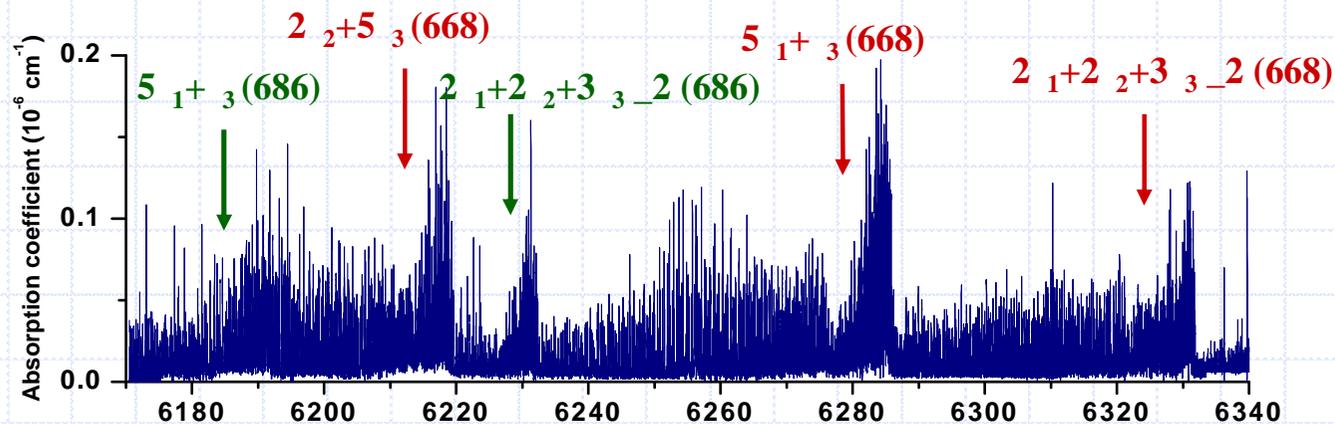
Overview of the CRDS spectrum in the range 6170-6340 cm^{-1}: Contribution of the M50 isotopologue $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$

Results of the $2\nu_1+2\nu_2+3\nu_3\_2$ band analysis of $^{16}O^{16}O^{18}O$
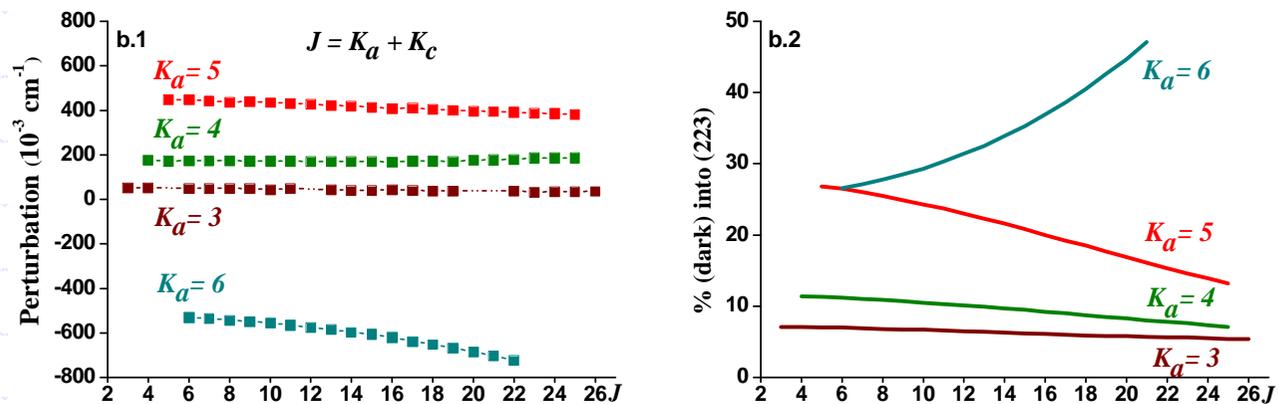
Simultaneous Coriolis and anharmonic interactions between the (223)_2 state and the õdarkö state centred at 6320 cm^{-1}

(a.1): observed perturbations for $K_a = 1$ series due to the Coriolis resonance;
(a.2): mixing coefficients corresponding to the Coriolis resonance;
(b.1): observed perturbations for different K_a series due to the anharmonic resonance;
(b.2): mixing coefficients corresponding to the anharmonic resonance.

Simultaneous analysis of the $2\nu_2+5\nu_3$ and $5\nu_1+\nu_3$ bands of $^{16}O^{18}O^{16}O$

(i) Spectroscopic EH parameters (in cm^{-1})

State		(025)	(501)	(124) *
E^{VV}		6151.3855$_0$ (13)	6182.3007$_0$ (14)	6189.599$_3$ (22)
$A-(B+C)/2$		2.79211$_6$ (13)	2.802906$_5$ (79)	2.76127$_8$ (55)
$(B+C)/2$		0.3931193$_6$ (79)	0.401574$_0$ (81)	0.391196$_4$ (33)
$(B-C)/2$		0.028059$_9$ (16)	0.025656$_0$ (19)	0.02303$_5$ (19)
κ	$\times 10^3$	0.2469$_4$ (34)	0.1885$_4$ (10)	g
$_{JK}$	$\times 10^5$	-0.278$_3$ (11)	-0.179$_0$ (21)	g
$_J$	$\times 10^6$	0.513$_1$ (14)	0.353$_9$ (20)	g
δ_K	$\times 10^4$	0.123$_2$ (18)	0.194$_4$ (45)	g
δ_J	$\times 10^6$	0.133$_5$ (11)	g	g
H_K	$\times 10^6$	0.385$_9$ (23)	g	g

Resonance coupling terms:

$C_{001}^{(dark4)(501)}$	-0.03674$_0$ (25)
$C_{001}^{(dark4)(025)}$	-0.07358$_8$ (19)

(ii) Dipole transition moment parameter (in Debye)

		$2\nu_2+5\nu_3$	$5\nu_1+\nu_3$
d_1	$\times 10^4$	0.5402$_9$ (54)	0.4921$_0$ (84)
d_2	$\times 10^7$	-0.427$_6$ (75)	
d_3	$\times 10^8$	0.323$_7$ (86)	

(iii) Statistics for the line positions

Vibrational state	(025)	(501)
J max	31	30
K_a max	10	9
Number of transitions	416	353
Number of levels	220	194
rms (10^{-3} cm^{-1})	7.87	

(iv) Statistics for the intensities

J max	28	29
K_a max	10	7
Number of transitions	294	41
rms (%)	21.0	20.6
S_v (cm/molecule)^a	4.69×10^{-24}	3.79×10^{-24}
	(625 lines)	(558 lines)

* Assignment from new ab initio PES:
Tyuterev Vl.G., Kochanov R.V., Tashkun S.A., Holka F. and Szalay P.G., *New analytical model for the ozone electronic ground state potential surface and accurate ab initio vibrational predictions at high energy range* // J.Chem.Phys, *in press*, v 139 (2013)
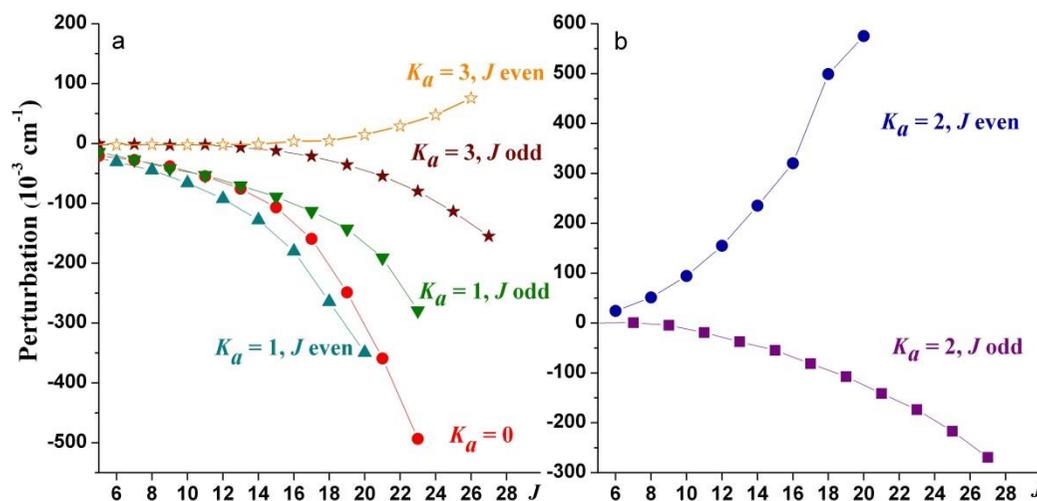
Final agreement of the CRDS spectrum with the calculation in the range 6170-6330 cm^{-1}

Simulated spectrum

$2_2+5_3(668)$

$5_1+_3(668)$

$2_1+2_2+3_3\_2(668)$

$5_1+_3(686)$

$2_1+2_2+3_3\_2(686)$

CRDS

Absorption coefficient (10^{-6} cm^{-1})

0.2

0.1

0.0

0.2

0.1

0.0

6180   6200   6220   6240   6260   6280   6300   6320

W avenumber (cm^{-1})

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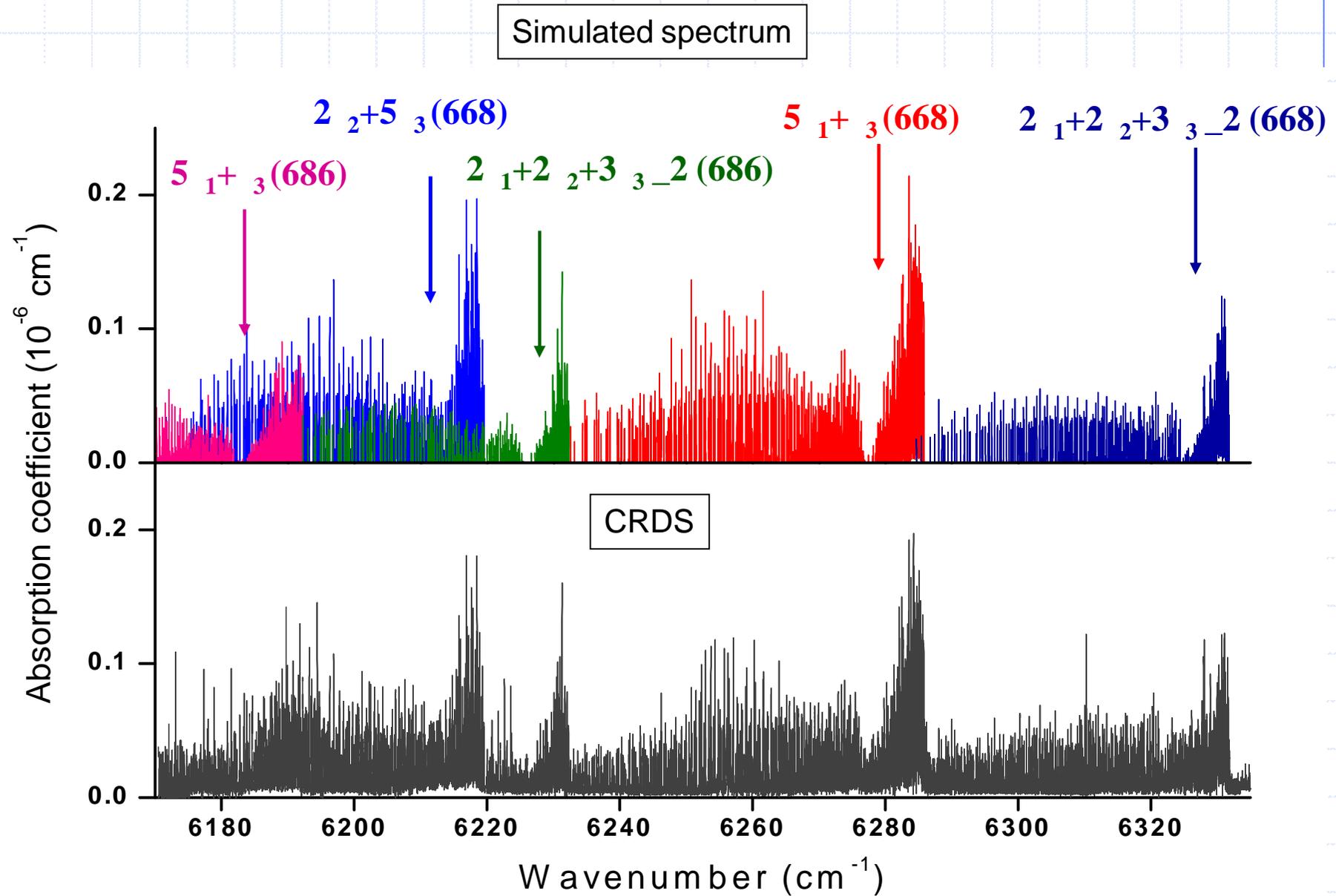
$2\nu_1+5\nu_3$ band of $^{16}O^{18}O^{18}O$ near 6630 cm^{-1}

(i) Spectroscopic EH parameters (in cm^{-1})				
State	**dark1**	**dark2**	**(205)**	**dark3**
E^{VV}	6586.420$_4$ (75)	6595.40$_3$ (25)	6628.1462$_0$ (52)	6634.4607$_0$ (57)
$A-(B+C)/2$	2.8628$_4$ (14)	2.6422$_5$ (35)	2.797188$_4$ (43)	3.0458 [f]
$(B+C)/2$	0.3728$_4$ (11)	0.37128$_9$ (11)	0.3678088$_5$ (39)	0.3688 [f]
$(B-C)/2$	0.0259 [f]	0.0250 [f]	0.025419$_0$ (12)	0.0274 [f]
$\kappa \times 10^3$	g	g	0.12442$_3$ (88)	g
$JK \times 10^5$	g	g	-0.5703$_9$ (83)	g
$\delta_K \times 10^4$	g	g	-0.171$_3$ (15)	g
$\delta_J \times 10^6$	g	g	0.106$_6$ (14)	g
$H_K \times 10^6$	g	g	-0.204$_1$ (47)	g

Resonance coupling terms:

$C^{(dark1)(205)}_{011} \times 10^2$	0.4101$_7$ (86)	$C^{(dark2)(205)}_{011} \times 10^2$	0.3436$_7$ (50)
$C^{(dark1)(205)}_{003} \times 10^5$	0.83$_7$ (22)	$C^{(dark3)(205)}_{011} \times 10^2$	0.623$_1$ (13)

(ii) Dipole transition moment parameter (in Debye)

$d_1^{(A)} \times 10^4$	0.28 [e]

(iii) Statistics for the line positions	
Vibrational state	**(205)**
Band centre (cm^{-1})	6628.146
J max	24
K_a max	12
Number of transitions	633
Number of levels	368
rms (10^{-3} cm^{-1})	4.03
$S_v =1.14\times10^{-24}$ cm/molecule at 296 K (988 lines)	

[f]-fixed to the values predicted from PES (*); [e]-estimated value

*Tyuterev Vl G, Kochanov R V, Taskhun S A, Proceedings of HighRus Conference, St. Petersbourg, July 2012. http://symp.iao.ru/en/hrms/17/proceedings

Simulated spectrum of the $2\nu_1+5\nu_3$ band

CRDS

(205) state of 688, symmetry A" (Kc=odd)

K_a	0	1	2	3	4	5	6	7	8	9	10	11	12
J													
1													
2		1	2										
3	1			2									
4		2	2	1	2								
5	2	2	3	3	1	1							
6		1	2	4	3	2	1						
7	2	2	2	4	3	2		1					
8		1	2	3	2	2	1	1	1				
9	1	1	1	3	2	2	1	2	1				
10		2	1	3	2	2	2	1	1	1			
11	2	2	1	2	2	1	1	4	1	1			
12		1	1	1	2	2	3	2	1	1			
13	2	1	2	3	2	4	2	2	2	2	2	1	
14		3	1	1	2	3	3	3	1	3	1		
15	1	1	2	2	2	2	3	1	3	1	1		
16		2	2		1	2	2	3	1	3	1		
17	1	1	1	1	2	3		1	2	3	2		
18		1	2	1		2			3	3	2		
19	1	1	1	1	1	1			2	1	2		
20		1	1	1	1	1			2	2	1		
21	1	1	1	1	2	2			2	3			
22		1	1		1	1			2	2			
23	1	1			3				1	2			
24					1								
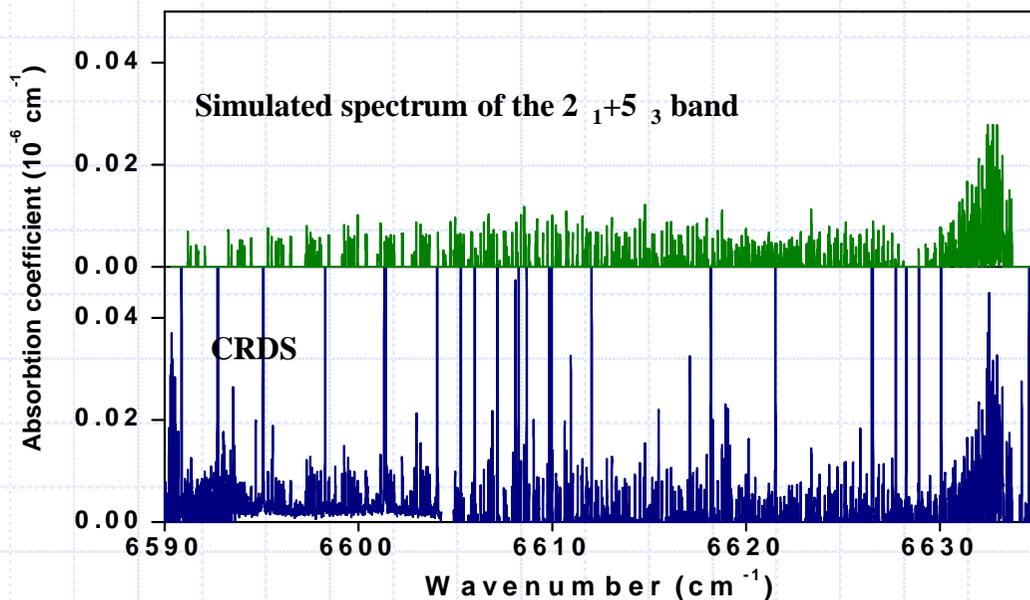
(205) state of 688, symmetry A' (Kc=even)

K_a	0	1	2	3	4	5	6	7	8	9	10	11	12
J													
1		1											
2	2	1	2										
3		2	1	2									
4	2	2	3	1	2								
5		2	3	3	1	1							
6	1	2	2	4	3	2	1						
7		2	1	4	2	2	1	1					
8	1	2	1	3	2	2	1	1	1				
9		1	2	3	2	2		2	1	1			
10	2	1	1	3	3	2	1	3	1	1	1		
11		2	1	1	2	2	1	4	1	1	1		
12	2	1	1	1	2	3	3	2	2	1	1		
13		3	1	3	2	4	2	2	1	2	2	1	
14	2	2	1	1	2	3	2	3	3	3	1		
15		2	1	1	1	2	3	1	3	1	1		
16	1	2	1	1	1	2		3	1	3	1		
17		2	1	1	2	3	1	1	2	3	2		
18		2	1	1	1	2	1		3	1	2		
19		1	1	1	1	1	1		2	2	1		
20	1	1	1	1	2	2	2		2	3	1		
21		1	1	1	2	2	1		2	2			
22	1	1			1	1	1		2	2			
23		1	1		3				1	1			
24			1	1	1								

Example of Comparison of theoretical predictions and experimental values (in cm^{-1}) for the rotational constants of the $^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{16}O$ states

(668)	Band centre			A			B			C		
	Obs.	Calc.[a]	O-C	Obs.	Calc.[a]	(O-C)	Obs	Calc.[a]	(O-C)	Obs	Calc.[a]	(O-C)
(223)_1	6026.084	6026.13	-0.05	3.4472	3.4375	0.0097	0.3974	0.3961	0.0013	0.3487	0.3470	0.0017
(025)	6213.492	6213.56	-0.07	3.3752	3.3714	0.0038	0.3962	0.3944	0.0018	0.3466	0.3455	0.0011
(501)	6276.706	6276.71	0.00	3.4137	3.4035	0.0102	0.4028	0.4019	0.0009	0.3575	0.3556	0.0019
(223)_2	6325.213	6325.38	-0.17	3.4000	3.3936	0.0064	0.3972	0.3953	0.0019	0.3504	0.3500	0.0004

(686)	Band centre			A			B			C		
	Obs.	Calc.[a]	O-C	Obs.	Calc.[a]	(O-C)	Obs	Calc.[a]	(O-C)	Obs	Calc.[a]	(O-C)
(133)/(223)	5983.636	5983.98	-0.35	3.2182	3.2083	0.0099	0.4208	0.4202	0.0006	0.3652	0.3646	0.0006
(025)	6151.385	6151.66	-0.27	3.1852	3.1756	0.0096	0.4212	0.4220	-0.0008	0.3651	0.3659	-0.0008
(501)	6182.301	6182.51	-0.21	3.2045	3.1950	0.0095	0.4272	0.4257	0.0015	0.3759	0.3753	0.0006
(223)_2	6225.259	6225.19	0.06	3.2000	3.1916	0.0084	0.4216	0.4208	0.0008	0.3672	0.3708	-0.0036

Band centers and rotational constants using empirically optimised PES:
Tyuterev VlG, Kochanov RV, Taskhun SA, *Analytical representation for accurate potential energy function of the ozone molecule and extended vibration calculations*. Proceedings of HighRus Conference, St. Petersbourg, July 2012. http://symp.iao.ru/en/hrms/17/proceedings
Assignment is consitent with those obtained from new ab initio PES:
Tyuterev Vl.G., Kochanov R.V., Tashkun S.A., Holka F. and Szalay P.G., *New analytical model for the ozone electronic ground state potential surface and accurate ab initio vibrational predictions at high energy range* // J.Chem.Phys, *in press*, v 139 (2013)

Comparison of theoretical predictions and experimental values (in cm^{-1}) for the rotational constants of the $^{16}O^{18}O^{18}O$ and $^{18}O^{16}O^{18}O$ states

(688)	Band centre			A			B			C		
	Obs.	Calc.^{a}	O-C	Obs.	Calc.^{a}	(O-C)	Obs	Calc.^{a}	(O-C)	Obs	Calc.^{a}	(O-C)
(025)	6054.64	6055.08	-0.44	3.1214	3.1137	0.0077	0.3968	0.3950	0.0018	0.3454	0.3434	0.0020
(223)_2	6168.35	6168.96	-0.61	3.1412	3.1329	0.0083	0.3980	0.3964	0.0016	0.3486	0.3480	0.0006
(205)	6628.14	6628.80	-0.66	3.1650	3.1562	0.0088	0.3932	0.3915	0.0017	0.3424	0.3411	0.0013

(868)	Band centre			A			B			C		
	Obs.	Calc.^{a}	O-C	Obs.	Calc.^{a}	(O-C)	Obs	Calc.^{a}	(O-C)	Obs	Calc.^{a}	(O-C)
(133)/(223)	5964.74	5964.97	-0.23	3.3638	3.3540	0.0098	0.3746	0.3741	0.0005	0.3302	0.3297	0.0005
(501)	6195.36	6195.28	0.08	3.3566	3.3476	0.0090	0.3801	0.3788	0.0013	0.3371	0.3364	0.0007
(223)/(313)	6240.48	6240.43	0.06	3.3133	3.2952	0.0181	0.3736	0.3766	-0.0030	0.3296	0.3332	-0.0036
(205)	6457.44	6457.35	0.09	3.2315	3.2099	0.0216	0.3710	0.3807	-0.0097	0.3282	0.3391	-0.0109

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Tyuterev VlG, Kochanov RV, Taskhun SA, *Analytical representation for accurate potential energy function of the ozone molecule and extended vibration calculations*. Proceedings of HighRus Conference, St. Petersbourg, July 2012. http://symp.iao.ru/en/hrms/17/proceedings

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# Complexity of spectra analysis in the range near dissociation

É**The bands are weak and dense**

É**High density of vibrational levels**

É**Numerous resonances with « dark » states**
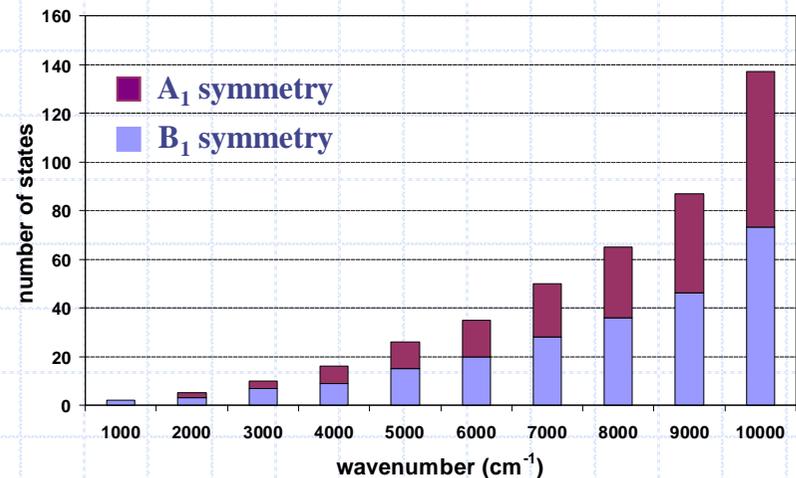
Number of states as a function of the spectral range.
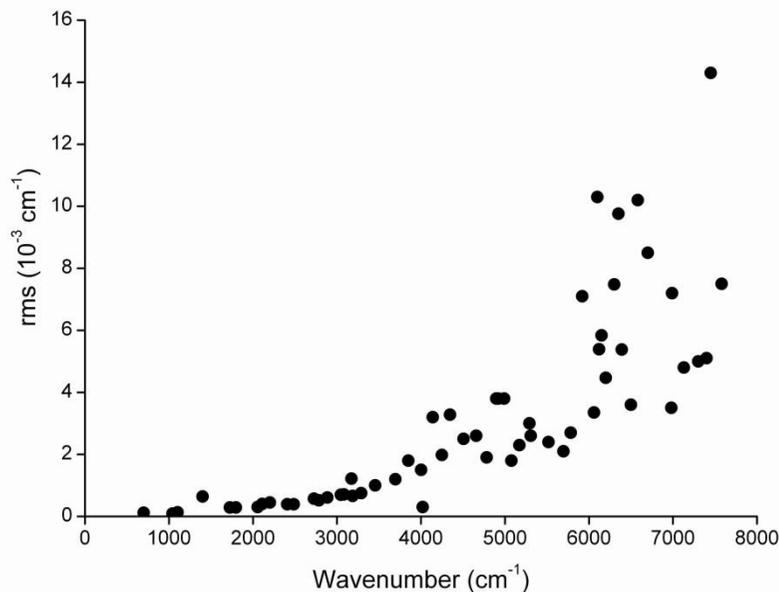
Variation of the rms (Obs.-Calc.) deviations achieved in the fits of line positions versus the band centres in the line-by-line analyses of the $^{16}O_3$ spectra.
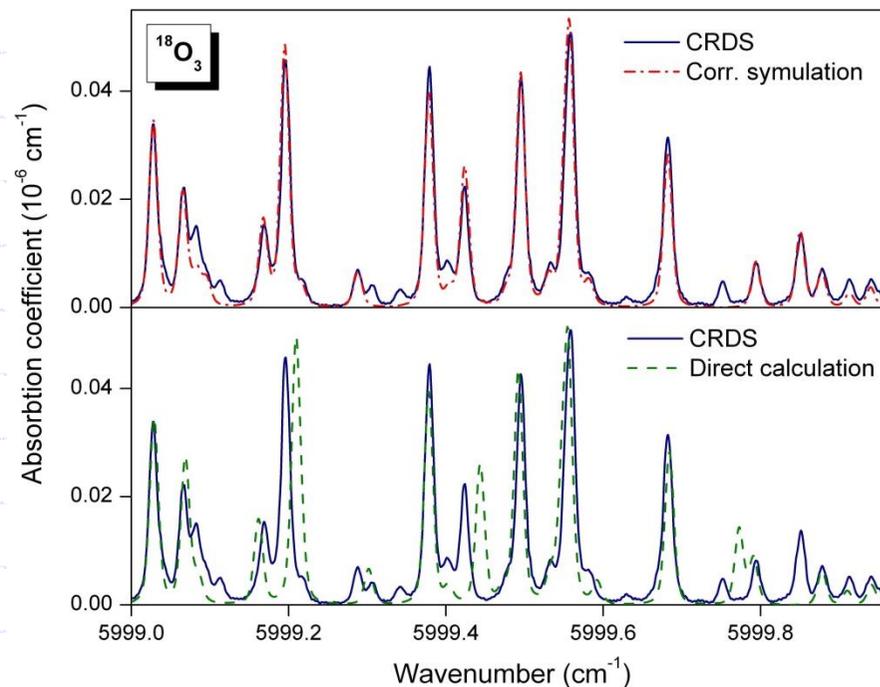
666 new results

* in 10^{-3} cm^{-1}

Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
CRDS									
133	37B	5919.160	5919.114	433	264	38	0	7.5	0.046
411	38B	5947.070	5946.296	294	179	34	0	8.5	0.774
034	58A	6046.076	6044.711	135	77	43	1	14.8	1.365
105	39B	6063.922	6063.118	531	265	43		3.3	0.804
510	59A	6100.216	6099.285	22	17	31	1	10.2	0.931
133	41B	6124.287	6124.998	507	338	44		6.1	-0.711
232	60A	6154.702	6155.528	479	227	49		6.6	-0.826
331	42B	6198.534	6197.503	115	80	25	0	4.5	1.043
025	44B	6305.047	6303.590	734	368	40		7.5	-0.543
124	65A	6343.983	6343.946	46	31	42		20.7	0.037
501	45B	6355.722	6354.702	506	271	35	1	9.7	1.020
430	66A	6365.264	6365.588	53	36	31			-0.324
223	46B	6386.996	6388.120	596	284	37		5.4	-1.124
044	69A	6506.129	6505.560	304	147	49	0	3.6	0.569
421	50B	6567.841	6567.979	270	169	36	2	10.2	-0.138
205	51B	6586.966	6588.945	419	220	35			-1.979
143	53B	6716.539	6717.496			37			-0.957
520	76A	6751.246	6751.218	836	511	33	3	8.5	0.028
242	77A	6764.789	6765.487			46			-0.698
035	57B	6895.487	6895.133	508	248	33	0	10.2	0.354
511	59B	6981.870	6980.684	161	126	25	0	3.7	1.186
233	60B	6990.068	6990.224	231	168	25	1	7.2	-0.156
125	64B	7130.813	7133.306	289	171	33	4	4.8	-2.493
153	67B	7286.580	7288.175	213	135	25	1	5.0	-1.595
601	71B	7394.801	7393.589	213	126	31	1	5.1	1.212
351	72B	7446.067	7445.558	144	96	23	2	14.3	0.509
045	73B	7452.322	7452.810	88	39	23			-0.488
351	76B	7578.828	7577.974	146	93	30	3	7.5	0.854
243_2	80B	7686.114	7687.224	198	92	30	2	13.6	-1.110
271	82B	7739.623	7741.147	135	83	26	3	7.9	-1.524
405	86B	7860.077	7863.318	210	121	26	1	13.7	-3.241
Tot				8816	4982	26			

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668 new results

* in 10^{-3} cm^{-1}

Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
				CRDS					
223_1	100Aø	6026.084	6026.132	551	366	24	1	5.0	-0.048
025	107Aø	6213.492	6213.564	498	292	29	0	7.5	-0.072
501	111Aø	6276.706	6276.706	601	390	32	2	10.2	0.000
223_2	114Aø	6325.213	6325.377	505	325	27	1	5.4	-0.164
610 ?	126Aø	6566.635	6566.992	352	247	33	1	4.4	-0.357
502 ?	128Aø	6613.688	6613.519	211	156	21	0	6.3	0.169
035 ?	137Aø	6784.839	6784.872	399	241	23	2	3.8	-0.033
Tot				**5772**	**4018**		**13**		

686 new results

Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
				CRDS					
223_1	40B	5983.636	5983.981	356	190	27	3	4.9	-0.345
025	43B	6151.385	6151.656	416	220	31	1	7.9	-0.271
501	45B	6182.300	6182.510	353	194	30			-0.210
223_2	46B	6225.299	6225.195	183	116	22	2	13.1	0.104
Tot				**1673**	**972**		**7**		

688 new results

| Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
				CRDS					
025	107Aø	6054.647	6054.917	746	389	29	2	6.0	-0.270
223_2	112Aø	6168.355	6168.759	471	289	25	1	5.4	-0.404
205	135Aø	6628.146	6628.424	632	244	24	3	4.0	-0.278
Tot				1849	922		6		

* in 10^{-3} cm^{-1}

868 new results

Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
				CRDS					
223_1	41B	5964.753	5964.974	315	168	25	2	6.7	-0.221
501	46B	6195.369	6195.282	344	191	27	2	6.9	0.087
313	48B	6240.484	6240.429	289	159	27	1	10.5	0.055
205	51B	6457.448	6457.352	454	244	33	2	5.8	0.096
143	54B	6535.823	6536.070	324	194	30	1	4.2	-0.247
035	57B	6713.422	6713.434	188	118	28	1	3.1	-0.012
Tot				2645	1603		15		

888 new results

Label $v_1v_2v_3$	N global	E obs (cm^{-1})	Pred *ab initio*	Nb tran	Nb lev	J_{max}	Nb dark	*rms* *	O-C
CRDS									
025	44B	5982.657	5984.439	507	283	35			1.782
430	65A	6011.487	6011.836	32	21	37			0.349
501	45B	6012.227	6013.048	566	313	38	1	9.5	0.821
214	66A	6048.271	6047.101	184	92	38			-1.170
115	46B	6073.575	6072.132	599	307	35			-1.443
016	71A	6244.102	6245.001	89	49	42			0.899
205	51B	6273.575	6270.604	659	330	37	2	6.3	-2.971
304	73A	6297.404	6296.358	131	104	43			-1.046
233	54B	6392.891	6392.213	344	191	33	2	9.3	-0.678
035	58B	6555.813	6556.786	574	310	37			0.973
134	82A	6593.628	6592.661	352	162	48	2	18.4	-0.967
511	59B	6610.079	6611.039	255	164	35			0.960
233	60B	6643.808	6642.897	364	233	34			-0.911
125	64B	6797.736	6796.461	389	213	30	2	7.3	-1.275
431	66B	6826.395	6825.511	183	109	25	1	3.7	-0.884
305	71B	7012.075	7009.092	252	158	29	2	9.2	-2.983
017	73B	7101.159	7101.475	206	128	28	0	9.9	0.316
045	74B	7115.051	7115.370	133	101	27			0.319
441	86B	7505.893	7503.402	75	48	23	0	16.4	-2.491
163	90B	7632.176	7629.530	222	131	30	1	9.5	-2.646
027	96B	7752.035	7752.696	136	79	26	2	9.5	-0.673
0111	101B	7910.411	7908.838	80	58	21	1	8.1	-1.573
Tot				6785	3852		19		
All six Isotopes				27540	16349				

* in 10^{-3} cm^{-1}

% of recent results from CRDS

666
Total : 89 "bright" levels

32.5%

67.5%

668
Total : 32 "bright" levels

21.8%

78.2%

686
Total : 20 "bright" levels

25.0%

75.0%

886
Total : 19 "bright" levels

16.0%

84.0%

868
Total : 26 "bright" levels

23.0%

77.0%

888
Total : 49 "bright" levels

44.9%

55.1%
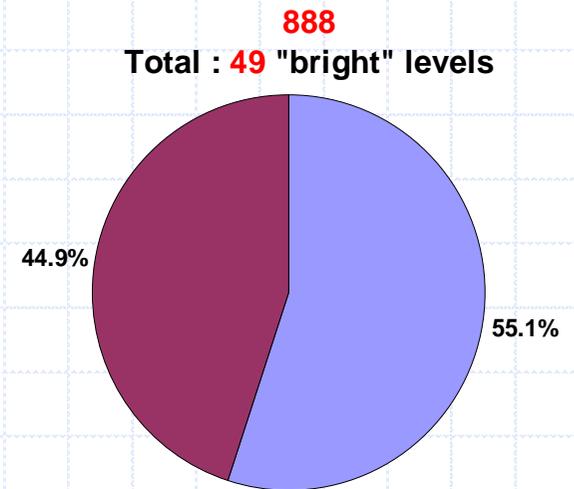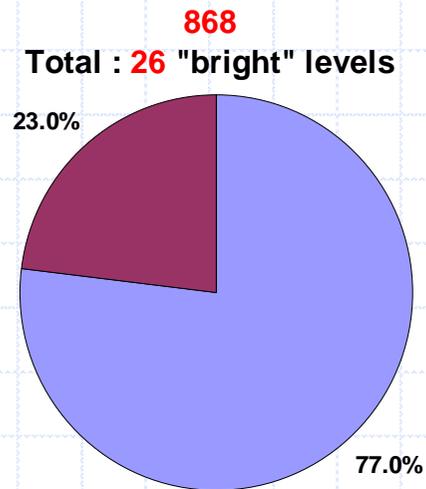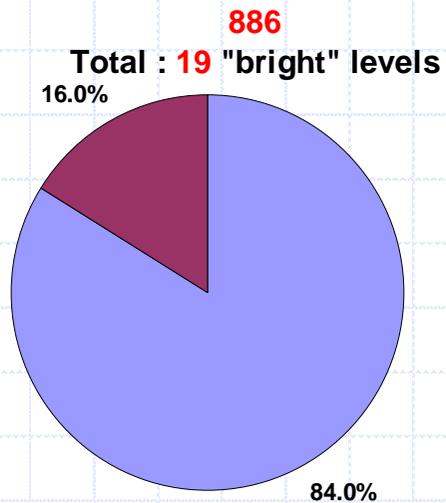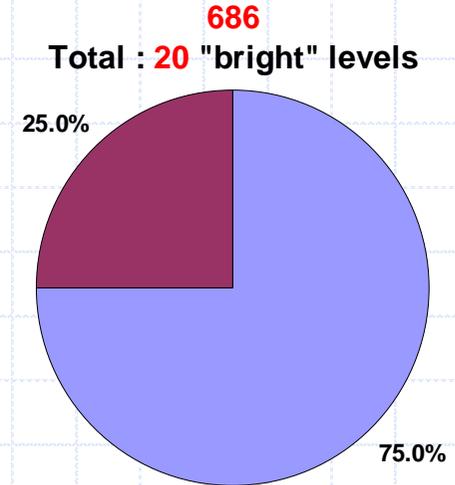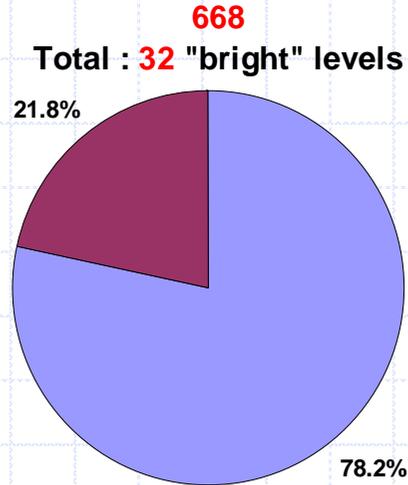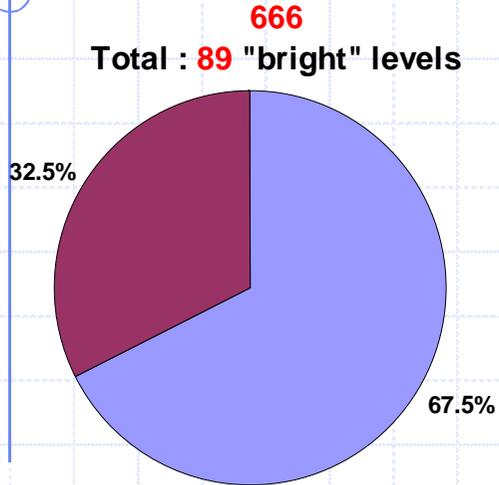
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Summary of the number of vibrational states involved in the analyses

666	668	686	886	868	888	TOT
89	30	19	15	23	51	227
41	20	10	10	24	31	136
						363

Specific case of $^{16}O_3$

210 vibrational levels predicted up to 8000 cm^{-1}

Number of analyzed bright levels :89

Number of darks levels 42 tot:131

Percentage : 62% total; 91 % up to 4000 cm^{-1}

Information

All these results , added to older ones are included in the S&MPO (Spectral and molecular properties of ozone).

Two recent publications :

Ozone spectroscopy in the electronic ground state: High resolution spectra analyses and update of line parameters since 2003 , J.Q.S.R.T   130 (2013) 172-190, A.Barbe, S.Mikhailenko, E.Starikova, M-R De Backer,D. Mondelain *et al*

S&MPO . An information system for ozone spectroscopy on the web. J.Q.S.R.T   145 (2014) 169-196 Y.Babikov,S.Mikhailenko, A.Barbe, Vl.G Tyuterev

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