

DESCRIPTION OF VIBRATIONAL QUANTUM NUMBER IMPLEMENTATIONS IN FIELDS E1 and E2 for GEISA-2015

V_j: quantum number associated with the normal mode of vibration j

$\sum xV_j$: combination vibrational state

l_j: vibrational angular momentum quantum number associated with the degenerate bending mode j

l: absolute value of the sum of the vibrational angular momentum quantum number l_j.

GROUND for identification of fundamental vibrational state of some specific molecules, i.e.:

HNO₃, C₂H₆, CH₃D, C₂H₄, C₃H₈, CH₃Cl, HCOOH, SF₆, C₃H₄, ClONO₂, CH₃Br, CH₃OH, C₆H₆, CH₃CN

GREY LINE if no quantum identification of vibrational levels

Molecule in GEISA-2015:

H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂, NO, SO₂, NO₂, NH₃, PH₃, HNO₃, OH, HF, HCl, HBr, HI, ClO, OCS, H₂CO, C₂H₆, CH₃D, C₂H₂, C₂H₄, GeH₄, HCN, C₃H₈, C₂N₂, C₄H₂, HC₃N, HOCl, N₂, CH₃Cl, H₂O₂, H₂S, HCOOH, COF₂, SF₆, C₃H₄, HO₂, ClONO₂, CH₃Br, CH₃OH, NO⁺, HNC, C₆H₆, C₂HD, CF₄, CH₃CN, HDO, SO₃

References:

[1] Tashkun et al., JQSRT 152 (2015) 45–73

[2] Barbe et al., JQSRT 130 (2013) 172–190

[3] Brown et al., JQSRT 130 (2013) 201–219

[4] Down et al., JQSRT 130 (2013) 260–272

[5] Gomez et al., JQSRT 111 (2010) 2256–2264

[6] Perrin et al. JMS 171 (1995) 358–373

H₂O Molecule 1

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																				❖		❖		❖

E2: lower state vibrational identification

																				❖		❖		❖
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CO₂ Molecule 2

V1,V2,l2,V3,r

r: ranking index[1]

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																	❖		❖		❖		❖	❖

E2: lower state vibrational identification

																	❖		❖		❖		❖	❖
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O₃ Molecule 3

V1,V2,V3_r

r: ranking index [2]

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																				❖	❖	❖	-	❖

E2: lower state vibrational identification

																				❖	❖	❖	-	❖
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N₂O Molecule 4

V1,V2,l2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																					❖	❖	❖	❖

E2: lower state vibrational identification

																					❖	❖	❖	❖
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CO Molecule 5

V1

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																								❖

E2: lower state vibrational identification

																								❖
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CH₄ Molecule 6

V1,V2,V3,V4,n,C

n: multiplicity index; *C*: vibrational symmetry [3]

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
														❖	❖	❖	❖	❖	❖	❖				

E2: lower state vibrational identification

														❖	❖	❖	❖	❖	❖	❖				

O₂ Molecule 7

X,V1

X electronic state of the molecule

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																							❖	❖

E2: lower state vibrational identification

																								❖	❖
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NO Molecule 8

X,i,V1

X electronic state of the molecule; i=1/2 or 3/2

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																	❖	❖	❖	❖			❖	❖

E2: lower state vibrational identification

																	❖	❖	❖	❖			❖	❖
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SO₂ Molecule 9

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																				❖	❖	❖		

E2: lower state vibrational identification

																				❖	❖	❖
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NO₂ Molecule 10

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																						❖	❖	❖

E2: lower state vibrational identification

																						❖	❖	❖
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NH₃ Molecule 11

V1,V2,V3,V4,I3,I4,I,Gvib

Gvib : Vibrational symmetry [4]

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
											❖	❖	❖	❖		❖	❖		❖		❖	❖	❖	

E2: lower state vibrational identification

											❖	❖	❖	❖		❖	❖		❖		❖	❖	❖	
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PH₃ Molecule 12

V1,V2,V3,V4

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																					❖	❖	❖	❖

E2: lower state vibrational identification

																					❖	❖	❖	❖
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HNO₃ Molecule 13

$$\sum xV_j$$

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																				❖	❖	❖	❖	❖
																			G	R	O	U	N	D

E2: lower state vibrational identification

																							❖	❖	❖			
																							G	R	O	U	N	D

OH Molecule 14

X_iV₁

X electronic state of the molecule; i=1/2 or 3/2

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																	❖	❖	❖	❖				❖	❖

E2: lower state vibrational identification

																	❖	❖	❖	❖				❖	❖
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HF Molecule 15

V1

E1: upper state vibrational identification

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

	❖
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E2: lower state vibrational identification

	❖
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HCl Molecule 16

V1

E1: upper state vibrational identification

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

	❖
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E2: lower state vibrational identification

	❖
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HBr Molecule 17

V1

E1: upper state vibrational identification

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

	❖
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E2: lower state vibrational identification

	❖
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HI Molecule 18

V1

E1: upper state vibrational identification

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

	❖
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E2: lower state vibrational identification

	❖
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ClO Molecule 19

X,i,V1

X electronic state of the molecule; i=1/2 or 3/2

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																	❖	❖	❖	❖			❖	❖

E2: lower state vibrational identification

																	❖	❖	❖	❖			❖	❖
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OCS Molecule 20

V1,V2,l2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																						❖	❖	❖	❖

E2: lower state vibrational identification

																						❖	❖	❖	❖
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H₂CO Molecule 21

V1,V2,V3,V4,V5,V6

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																			❖	❖	❖	❖	❖	❖

E2: lower state vibrational identification

																			❖	❖	❖	❖	❖	❖
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C₂H₆ Molecule 22

$\sum xV_j$

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25				
															❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖
																			G	R	O	U	N	D				

E2: lower state vibrational identification

																					❖	❖	❖	
																			G	R	O	U	N	D

HC₃N Molecule 31

V1,V2,V3,V4,V5,V6,V7,I5,I6,I7,S

S: Vibrational symmetry

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
					❖		❖		❖		❖		❖		❖		❖	❖	❖	❖	❖	❖	❖	❖

E2: lower state vibrational identification

					❖		❖		❖		❖		❖		❖		❖	❖	❖	❖	❖	❖	❖	❖
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HOCl Molecule 32

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																							❖	❖	❖

E2: lower state vibrational identification

																								❖	❖	❖
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N₂ Molecule 33

V_j

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																								❖

E2: lower state vibrational identification

																								❖
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CH₃Cl Molecule 34

∑ xV_j

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																			❖	❖	❖	❖	❖	❖
																			G	R	O	U	N	D

E2: lower state vibrational identification

																			G	R	O	U	N	D
--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	---	---	---	---	---	---

H₂O₂ Molecule 35

V1,V2,V3,n4,t4,V5,V6

n4,t4: torsional quantum numbers [6]

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
														❖		❖		❖	❖	❖		❖		❖

E2: lower state vibrational identification

														❖		❖		❖	❖	❖		❖		❖
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H₂S Molecule 36

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																							❖	❖	❖

E2: lower state vibrational identification

																							❖	❖	❖
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HCOOH Molecule 37

$$\sum xV_j$$

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																				❖	❖	❖	❖	❖	
																				G	R	O	U	N	D

E2: lower state vibrational identification

																				G	R	O	U	N	D
--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	---	---	---	---	---	---

COF₂ Molecule 38

$$V_1, V_2, V_3, V_4, V_5, V_6$$

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																				❖	❖	❖	❖	❖	❖

E2: lower state vibrational identification

																				❖	❖	❖	❖	❖	❖
--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	---	---	---	---	---	---

HO₂ Molecule 41

V1,V2,V3

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																						❖	❖	❖

E2: lower state vibrational identification

																						❖	❖	❖
--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	---	---	---

ClONO₂ Molecule 42

$\sum xV_j$

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																				❖	❖	❖	❖	❖	
																				G	R	O	U	N	D

E2: lower state vibrational identification

																						❖	❖		
																				G	R	O	U	N	D

CH₃Br Molecule 43

V_j

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
																							❖	❖

E2: lower state vibrational identification

																				G	R	O	U	N	D
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CH₃OH Molecule 44

∑ xV_j

E1: upper state vibrational identification

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
																		❖	❖	❖	❖	❖	❖	❖	
																				G	R	O	U	N	D

E2: lower state vibrational identification

																						❖	❖	❖	❖
																				G	R	O	U	N	D

