DESCRIPTION OF VIBRATIONAL QUANTUM NUMBER IMPLEMENTATIONS IN FIELDS E1 and E2 for GEISA-2020

Vj*:* quantum number associated with the normal mode of vibration j
∑ **xVj**: combination vibrational state
lj: 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 lj .

GROUND for identification of fundamental vibrational state of some specific molecules, i.e.:
HNO_3, C_2H_6, CH_3D, C_2H_4, C_3H_8, CH_3Cl, HCOOH, SF_6, C_3H_4, $ClONO_2$, CH_3Br, CH_3OH, C_6H_6, CH_3CN, …
GREY LINE if no quantum identification of vibrational levels

Molecule in GEISA-2015:
H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NO, SO_2, NO_2, NH_3, PH_3, HNO_3, OH, HF, HCl, HBr, HI, ClO, OCS, H_2CO, C_2H_6, CH_3D, C_2H_2, C_2H_4, GeH_4, HCN, C_3H_8, C_2N_2, C_4H_2, HC_3N, HOCl, N_2, CH_3Cl, H_2O_2, H_2S, HCOOH, COF_2, SF_6, C_3H_4, HO_2, $ClONO_2$, CH_3Br, CH_3OH, NO+, HNC, C_6H_6, C_2HD, CF_4, CH_3CN, HDO, SO_3

New molecule in GEISA-2020:
HONO, COFCl, CH_3I, CH_3F, RUO_4, $H_2C_3H_2$

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

H_2O 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

																				❖		❖		❖

CO_2 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

																	❖		❖		❖		❖	❖

O_3 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

																				❖	❖	❖	-	❖

N_2O 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

																					❖	❖	❖	❖

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

																								❖

CH_4 Molecule 6

V1,V2,V3,V4,n,C ***n:*** *multiplicity index;* ***C****:* vibrational s*ymmetry [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

														❖		❖		❖		❖		❖	❖	❖

O_2 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

																							❖	❖

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

																	❖	❖	❖	❖			❖	❖

SO_2 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

																				❖		❖		❖

NO_2 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

																						❖	❖	❖

NH_3 Molecule 11

V1,V2,V3,V4,l3,l4,l,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

											❖	❖	❖	❖		❖	❖		❖		❖	❖	❖	

PH_3 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

																					❖	❖	❖	❖

HNO_3 Molecule 13

$\sum$ xVj

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,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

																							❖

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
																								❖

E2: lower state vibrational identification

																								❖

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
																								❖

E2: lower state vibrational identification

																								❖

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
																								❖

E2: lower state vibrational identification

																								❖

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
																								❖

E2: lower state vibrational identification

																								❖

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

																	❖	❖	❖	❖			❖	❖

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

																					❖	❖	❖	❖

H_2CO 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

																			❖	❖	❖	❖	❖	❖

C_2H_6 Molecule 22

$\sum$ xVj

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

CH_3D Molecule 23

$\sum$ **xVj**

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

C_2H_2 Molecule 24

V1,V2,V3,V4,V5,l,+/-,r,p *+/-: Symmetry type for $\sum$ levels (l=0)* ***r:*** *ranking index;* ***p****: vibrational level u or g parity [5]*

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

																❖	❖	❖	❖	❖	❖	❖		❖

C_2H_4 Molecule 25

$$\sum xVj$$

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

GeH_4 Molecule 26

V1,V2,l2,V3,l3,V4,l4,l

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

																❖	❖	❖	❖	❖	❖	❖	❖

HCN Molecule 27

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

																		❖	❖	❖	❖	❖		❖

C_3H_8 Molecule 28

Vy

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

C_2N_2 Molecule 29

V1,V2,V3,V4,V5,l4 ,l5

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

									❖		❖		❖		❖		❖			❖	❖		❖	❖

C_4H_2 Molecule 30

V3,V4,V5,V6,V7,V8,V9,l6,l7,l8,l9

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

										❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖	❖

HC_3N Molecule 31

V1,V2,V3,V4,V5,V6,V7,l5,l6,l7,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

					❖		❖		❖		❖		❖		❖		❖	❖	❖	❖	❖	❖	❖	❖

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

																						❖	❖	❖

N_2 Molecule 33

Vj

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

																								❖

CH_3Cl Molecule 34

$\sum$ xVj

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

H_2O_2 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

														❖		❖		❖	❖	❖		❖		❖

H_2S 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

																						❖	❖	❖

HCOOH Molecule 37

$\sum$ xVj

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

COF_2 Molecule 38

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

																			❖	❖	❖	❖	❖	❖

SF_6 Molecule 39

∑ xVj,S,p *S: vibrational symmetry; **p**: parity g or u*

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

C_3H_4 Molecule 40

Vj or Vj HOT L=x or As1As2Vj HOT L=x *s1 or s2: +/-*

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

HO_2 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

																						❖	❖	❖

$ClONO_2$ Molecule 42

$\sum$ **xVj**

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

CH_3Br Molecule 43

Vj

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

CH_3OH Molecule 44

$\sum$ xVj

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

NO+ Molecule 45

Vj

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

																								❖

HNC Molecule 46

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

																		❖	❖	❖		❖		❖

C_6H_6 Molecule 47

Vj

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

C_2HD Molecule 48

V1,V2,V3,V4,V5,l4,l5,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

										❖		❖		❖		❖		❖	❖	❖	❖	❖	❖	❖

CF_4 Molecule 49

V1,V2,V3,V4,n,C ***n:*** *multiplicity index;* ***C:*** 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

																	❖	❖	❖	❖		❖	❖	❖

CH_3CN Molecule 50

Vj

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

HDO Molecule 51

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

																				❖		❖		❖

SO_3 Molecule 52

V1,V2,V3,V4,V5,V6,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

												❖		❖		❖		❖		❖		❖	❖	❖

HONO Molecule 53

Cis or Trans Vj ***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

																		G	R	O	U	N	D

COFCl Molecule 54

$\sum$ xVj

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

CH_3I Molecule 55

Vj

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
																							V	6

E2: lower state vibrational identification

																			G	R	O	U	N	D

CH_3F Molecule 56

Vj

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
																							V	6

E2: lower state vibrational identification

																			G	R	O	U	N	D

RUO_4 Molecule 57

V1,V2,V3,V4,n,C

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

														❖		❖		❖		❖		❖	❖	❖

$H_2C_3H_2$ Molecule 58

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
