TABLE B.3. Peak positions and associated vibrational modes for the VN_3H^q defect in diamond from first-principals density functional simulations of IR spectra from selected studies.

Frequency (cm^{-1})	Defect	Mode (x)	H/Ah	*S*	Functional	Cell	Basis set	Comment	Ref.
VN_3H: C-H bending frequencies (observed C-H bending frequency is 1405 cm^{-1})									
1296	VN_3H	C-H_b	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 40 (C/N) 5 core atoms incl. MP2 sampling	[1]
1297	VN_3H	C-H_b	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) 5 core atoms incl. MP2 sampling	[1]
1333	VN_3H	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1360	VN_3H	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[3]
1361	VN_3H	C-H_b	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[1]
1365	VN_3H	C-H_b	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
1366	VN_3H	C-H_b	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[1]
1367	VN_3H	C-H_b	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
1384	VN_3H	C-H_b	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. Γ point sampling	[1]
1411	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms	[4]

								MP 2x2x2 mesh	
1415	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[4]
1416	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[4]
1442	VN_3H	C-H_b	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling C-H mode coupling Anharmonicity by VCI	[5]
1446	VN_3H	C-H_b	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling C-H mode coupling Anharmonicity by VSCF	[5]
1447	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[4]
1448	VN_3H	C-H_b	H	-	B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
1452	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[4]
1454	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[4]
1459	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[4]
1461	VN_3H	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]

1461	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
1463	VN_3H	C-H_b	H	-	B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
1476	VN_3H	C-H_b	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling No C-H mode coupling Anharmonicity by VCI	[5]

VN_3H: C-H stretching frequencies (observed C-H stretching frequency is 3107 cm^{-1})

2207	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	^{13}C-D isotopes Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
2221	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	^{12}C-D isotopes Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
3018	VN_3H	C-H_s	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) 5 core atoms incl. MP2 sampling	[1]
3025	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	^{13}C-H isotopes Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
3028	VN_3H	C-H_s	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
3034	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[1]
3037	VN_3H	C-H_s	H	0	LDA*	64	Gaussian	Basis set: 40 (C/N)	[1]

							(*atom centered*)	All atoms incl. MP2 sampling	
3039	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 40 (C/N) 5 core atoms incl. MP2 sampling	[1]
3054	VN_3H	C-H_s	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling C-H mode coupling Anharmonicity by VSCF	[5]
3094	VN_3H	C-H_s	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling C-H mode coupling Anharmonicity by VCI	[5]
3120	VN_3H	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[3]
3122	VN_3H	C-H_s	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling No C-H mode coupling Anharmonicity by VCI	[5]
3125	VN_3H	C-H_s	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[1]
3133	VN_3H	C-H_s (a)	Ah	-	B3LYP	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3196	VN_3H	C-H_s	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. Γ point sampling	[1]
3249	VN_3H	C-H_s	H	-	B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
3250	VN_3H	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H)	[2]

								MP8 sampling	
3250	VN_3H	C-H_s	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
3250	VN_3H	C-H_s	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[4]
3251	VN_3H	C-H_s	H	-	B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[5]
3262	VN_3H	C-H_s	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[4]

The defect electrical charge *q* (*e.g.* VNH^q), and the harmonic (H) or anharmonic (Ah) calculated frequencies are only included if explicitly specified in the corresponding reference.

Where more than one H-atom is present, both symmetric (C-H_{sy}) and anti-symmetric (C-H_{asy}) stretching modes are expected and reported only if explicitly specified in the corresponding reference.

Isotopes ^{12}C, ^{1}H and ^{14}N is assumed unless otherwise specified.

Total spin quantum number = *S*; *S* = 0 (singlet), *S* = 1 (triplet), *S* = 3/2 (quartet), *S* = 1/2 (doublet), *S* = 2 (quadruplet).

Monkhorst-Pack sampling scheme denoted as MP*n*, where a mesh of *n* x *n* x *n* points (*k*) is used to sample the Brillouin Zone. Point symmetry of a given defect may reduce *k*.

AIMPRO* (*ab initio* modelling PROgram), ***Crystal*** and **Quantum ESPRESSO*** density-functional modelling programs indicated in **Functional** column.

Note that many bands have calculated intensities significantly less than the intensity of the 3107cm^{-1} band and are unlikely to be observed in experimental data.

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