Table B.2. Peak positions and associated vibrational modes for H-related defects in diamond from first-principals density functional simulations of IR spectra from selected studies listed by type of defect.

Frequency (cm^{-1})	Defect	Mode (x)	H/Ah	*S*	Functional	Cell	Basis set	Comment	Ref.
Interstitial hydrogen defects: H_1 and H_2									
1598	D_1^+	C-H_s (b)	H	-	LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[1]
1797	D_1^+	C-H_s (a)	H	-	LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[1]
1952	D_1^-	C-H_s	H	-	LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[1]
2084	D_1^0	C-H_s	H	-	LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[1]
2086	H_1^+	C-H_s (b)	H	-	LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[1]
2456	H_1^+	C-H_s (a)	H	-	LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[1]
2571	H_2	C-H_{sy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[2]
2584	H_2	C-H_{sy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = H (AB site) MP 2x2x2 mesh	[2]
2693	H_2	C-H_{sy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[2]
2712	H_2	C-H_{asy}	H	-	LDA*	64	Gaussian	H_1 = D (BC site)	[2]

								(*atom centered*)	H_2 = D (AB site) MP 2x2x2 mesh
2730	H_1^-	C-H_s	H	-	LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[1]
2900	H_1	C-H_s	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) MP 2x2x2 mesh	[2]
2919	H_1^0	C-H_s	H	-	LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[1]
3511	H_2	C-H_{sy}	H	-	LDF*	64	Gaussian	H_1 = H (BC site) H_2 = H (AB site) Atom and bond centered basis sets	[1]
3520	H_2	C-H_{sy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) H_2 = H (AB site) MP 2x2x2 mesh	[2]
3584	H_2	C-H_{asy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[2]
3720	H_2	C-H_{asy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = H (AB site) MP 2x2x2 mesh	[2]
3741	H_2	C-H_{asy}	H	-	LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) H_2 = H (AB site) MP 2x2x2 mesh	[2]
3882	H_2	C-H_{asy}	H	-	LDF*	64	Gaussian	H_1 = H (BC site) H_2 = D (AB site) Atom and bond centered basis sets	[1]
Vacancy – hydrogen defects: VH_y, y = 1-4 C-H bending, y = 1									
1349	VH_1	C-H_b	H	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]

1350	VH_1^-	C-H_b	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1370	VH_1^+	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1420	VH_1	C-H_b (b)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1487	VH_1	C-H_b (a)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
					C-H stretching, y = 1				
2450	VH_1^0	C-H_s	H	3/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2450	VH_1^0	C-H_s	H	3/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2470	VH_1^{-3}	C-H_s	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2483	VH_1	C-H_s	Ah	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
2483	VH_1	C-H_s	Ah	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
2540	VH_1^{-3}	C-H_s	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2580	VH_1^+	C-H_s	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2710	VH_1^{-2}	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2750	VH_1^{-2}	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2764	VH_1	C-H_s	H	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
2818	VH_1	C-H_s	H	2	B3LYP**	64	Gaussian	Basis set: 6-21G (C/N)	[6]

							(*all electron*)	6-31G$^{(*)}$ (H) Γ point sampling	
2893	VH_1	C-H_s	Ah	1/2	PBE**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
2928	VH_1^-	C-H_s	H	-	LDA*	64	Gaussian (*atom centered*)	MP 2x2x2 mesh	[2]
2946	VH_1	C-H_s	Ah	1/2	HSE06**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
2952	VH_1	C-H_s	Ah	1/2	PBE0**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
2970	VH_1^-	C-H_s	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2981	VH_1	C-H_s	Ah	1/2	LDA**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3000	VH_1^-	C-H_s	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3010	VH_1^-	C-H_s	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3015	VH_1	C-H_s	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3015	VH_1	C-H_s	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3040	VH_1^0	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3114	VH_1^0	C-H_s	H	-	LDA*	64	Gaussian (*atom centered*)	MP 2x2x2 mesh	[2]
3130	VH_1^0	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3153	VH_1	C-H_s	H	1/2	PBE**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H)	[6]

								Γ point sampling	
3174	VH_1	C-H_s	H	1/2	HSE06**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3176	VH_1	C-H_s	H	1/2	PBE0**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3188	VH_1	C-H_s	H	1/2	LDA**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3193	VH_1	C-H_s	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3210	VH_1^+	C-H_s	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3231	VH_1	C-H_s	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3310	VH_1^+	C-H_s	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3428	VH_1	C-H_s	Ah	1/2	HF**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
3568	VH_1	C-H_s	H	1/2	HF**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[6]
					C-H bending, y = 2				
1350	VH_2^0	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1353	VH_2	C-H_b (c)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1358	VH_2	C-H_b (c)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]

1360	VH_2	C-H_b (b)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1461	VH_2	C-H_b (b)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1520	VH_2^+	C-H_b	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1540	VH_2^0	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1550	VH_2^0	C-H_b	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1590	VH_2^-	C-H_b	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1616	VH_2	C-H_b (a)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1627	VH_2	C-H_b (a)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1680	VH_2^{-2}	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
					C-H stretching, y = 2				
2770	VH_2^{-2}	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3040	VH_2^0	C-H_{asy}	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3050	VH_2^{-2}	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3060	VH_2^0	C-H_{asy}	H	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3100	VH_2^+	C-H_{asy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3118	VH_2^-	C-H_{asy}	H	-	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3120	VH_2^-	C-H_{asy}	H	1/2	PBE*	1000	Gaussian	Γ point sampling	[4]

							(*atom centered*)		
3253	VH_2	C-H_{asy}	Ah	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3275	VH_2	C-H_{asy}	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3310	VH_2^0	C-H_{sy}	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3330	VH_2^-	C-H_{sy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3337	VH_2^0	C-H_{sy}	H	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3339	VH_2^-	C-H_{sy}	H	-	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3350	VH_2^0	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3356	VH_2^0	C-H_{asy}	H	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3370	VH_2^+	C-H_{sy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3378	VH_2	C-H_{asy}	Ah	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3426	VH_2	C-H_{asy}	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3477	VH_2	C-H_{sy}	Ah	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3520	VH_2^0	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3525	VH_2^0	C-H_{sy}	H	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3526	VH_2	C-H_{sy}	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]

3552	VH_2	C-H_{sy}	Ah	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3606	VH_2	C-H_{sy}	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
					C-H bending, y = 3				
1400	VH_3^+	C-H_b (c)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1410	VH_3^0	C-H_b (b)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1430	VH_3^+	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1440	VH_3^+	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1450	VH_3^0	C-H_b (a)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1489	VH_3	C-H_b (b)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1520	VH_3^-	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1538	VH_3	C-H_b (a)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1560	VH_3^-	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
					C-H stretching, y = 3				
3120	VH_3^-	C-H_{asy} (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3420	VH_3^+	C-H_{asy} (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3430	VH_3^-	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]

3450	VH_3^+	C-H_{asy} (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3450	VH_3^0	C-H_{asy} (b)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3460	VH_3^0	C-H_{asy} (a)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3651	VH_3	C-H_{asy}	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3653	VH_3	C-H_{asy}	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3700	VH_3^+	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3710	VH_3^0	C-H_{sy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3908	VH_3	C-H_{sy}	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3953	VH_3	C-H_{sy}	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
					C-H bending, $y = 4$				
412	VH_4	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[8]
422	VH_4	C-H_b (c)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[8]
494	VH_4	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[8]
496	VH_4	C-H_b (c)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[8]

749	VH_4	C-H_b (c)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[8]
750	VH_4	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[8]
853	VH_4	C-H_b (c)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
861	VH_4	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
1320	VH_4	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
1322	VH_4	C-H_b (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
1331	VH_4	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[8]
1333	VH_4	C-H_b (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[8]
1380	VH_4	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1387	VH_4	C-H_b (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
1389	VH_4	C-H_b (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[8]
1390	VH_4	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1398	VH_4	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms	[8]

								MP 4x4x4 mesh	
1399	VH_4	C-H_b (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[8]
1400	VH_4	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1423	VH_4	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[8]
1428	VH_4	C-H_b (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[8]
1478	VH_4	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[8]
1484	VH_4	C-H_b (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[8]
1486	VH_4	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[8]
1488	VH_4	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
1492	VH_4	C-H_b (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[8]
					C-H stretching, $y = 4$				
3853	VH_4	C-H_s (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
3868	VH_4	C-H_s (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]

3974	VH_4	C-H_s (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[8]
3974	VH_4	C-H_{asy}	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
3989	VH_4	C-H_s (b)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[8]
4037	VH_4	C-H_{asy}	Ah	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
4120	VH_4	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
4199	VH_4	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
4221	VH_4	C-H_s (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
4276	VH_4	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[8]
4276	VH_4	C-H_{sy}	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]
4298	VH_4	C-H_s (a)	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[8]
4434	VH_4	C-H_{sy}	Ah	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[3]

Nitrogen – hydrogen defects: NH_y, y = 1

C-H bending

972	NH_1	C-H_b	H	-	LDF*	64	Gaussian	^{12}C-D isotopes	[1]

								Atom and bond centered basis sets	
1400	NH_1	C-H_b	H	-	LDF*	64	Gaussian	Atom and bond centered basis sets	[1]
1404	NH_1	C-H_s	H	-	LDA*	64	Gaussian (*atom centered*)	2-fold degenerate MP 2x2x2 mesh	[2]
1586	NH_1	C-H_b	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[9]
1590	NH_1	C-H_b	H	1	B3LYP**	216	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[9]
					C-H stretching				
2414	NH_1	C-H_s	H	-	LDF*	64	Gaussian	^{12}C-D isotopes	[1]
								Atom and bond centered basis sets	
3309	NH_1	C-H_s	H	-	LDA*	64	Gaussian (*atom centered*)	MP 2x2x2 mesh	[2]
3318	NH_1	C-H_s	H	-	LDF*	64	Gaussian	^{13}C-H isotopes	[1]
								Atom and bond centered basis sets	
3324	NH_1	C-H_s	H	-	LDF*	64	Gaussian	Atom and bond centered basis sets	[1]
3408	NH_1	C-H_s	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[9]
3471	NH_1	C-H_s	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[9]

Vacancy - nitrogen – hydrogen defects: VN_xH_y, x = 1-4, *y* = 1-3

C-H bending, *x* = 1, *y* = 1

1310	VNH^0	C-H_b	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1330	VNH^+	C-H_b	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1340	VNH^-	C-H_b	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]

1400	VNH^{-2}	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1414	VNH	C-H_b (b)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1421	VNH	C-H_b (a)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1422	VNH	C-H_b (b)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1430	VNH^0	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1431	VNH^0	C-H_b	H	-	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[11]
1452	VNH^-	C-H_b	H	-	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[11]
1501	VNH	C-H_b (a)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
				C-H stretching, x = 1, y = 1					
1973	VNH^0	C-H_s	H	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[12]
1986	VNH^0	C-H_s	H	1	LDA*	64	Gaussian	^{12}C-D isotopes $MP2^3$ sampling	[12]
2026	VNH^+	C-H_s	H	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[12]
2038	VNH^+	C-H_s	H	1	LDA*	64	Gaussian	^{12}C-D isotopes $MP2^3$ sampling	[12]
2067	VNH^-	C-H_s	H	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[12]
2080	VNH^-	C-H_s	H	1	LDA*	64	Gaussian	^{12}C-D isotopes $MP2^3$ sampling	[12]
2550	VNH^{-2}	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]

2689	VNH^0	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[12]
2697	VNH^0	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	$MP2^3$ sampling	[12]
2763	VNH^+	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[12]
2771	VNH^+	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	$MP2^3$ sampling	[12]
2819	VNH^-	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[12]
2827	VNH^-	$C\text{-}H_s$	H	1	LDA*	64	Gaussian	$MP2^3$ sampling	[12]
2850	VNH^0	$C\text{-}H_{sy}$	H	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2858	VNH^0	$C\text{-}H_s$	H	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
2866	VNH^-	$C\text{-}H_s$	H	-	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[11]
2894	VNH	$C\text{-}H_s$ (a)	Ah	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
2930	VNH^-	$C\text{-}H_{sy}$	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2941	VNH^-	$C\text{-}H_s$	H	-	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
2950	VNH^+	$C\text{-}H_{sy}$	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3069	VNH	$C\text{-}H_s$ (a)	Ah	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3096	VNH	$C\text{-}H_s$ (a)	H	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3122	VNH^0	$C\text{-}H_s$	H	-	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[11]
3180	VNH^0	$C\text{-}H_{sy}$	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]

3190	VNH^0	C-H_s	H	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[7]
3224	VNH	C-H_s (a)	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
					C-H bending, x = 1, y = 2				
476	VNH_2	C-H_b (d)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1330	VNH_2^-	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1372	VNH_2	C-H_b (c)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1391	VNH_2	C-H_b (b)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1550	VNH_2^+	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1580	VNH_2^0	C-H_b	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1653	VNH_2	C-H_b (a)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1680	VNH_2^-	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
					C-H stretching, x = 1, y = 2				
2850	VNH_2^-	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3100	VNH_2^-	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3200	VNH_2^+	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3230	VNH_2^0	C-H_{asy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]

3402	VNH_2	C-H_s (b)	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3410	VNH_2^+	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3417	VNH_2	C-H_s (b)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3420	VNH_2^0	C-H_{sy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3580	VNH_2	C-H_s (a)	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3615	VNH_2	C-H_s (a)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
				C-H bending, x = 1, y = 3					
446	VNH_3	C-H_b (d)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
451	VNH_3	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[10]
1460	VNH_3	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1480	VNH_3	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1529	VNH_3	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1584	VNH_3	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[10]

C-H stretching, $x = 1$, $y = 3$

3570	VNH_3	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3704	VNH_3	C-H_s (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[10]
3725	VNH_3	C-H_s (b)	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[10]
3790	VNH_3	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3943	VNH_3	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
4000	VNH_3	C-H_s (a)	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]

C-H bending, $x = 2$, $y = 1$

1310	VN_2H^+	C-H_b (b)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1330	VN_2H^0	C-H_b (b)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1340	VN_2H^0	C-H_b (a)	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1350	VN_2H^+	C-H_b (a)	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1424	VN_2H	C-H_b (b)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1470	VN_2H^-	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1479	VN_2H	C-H_b (a)	H	1/2	B3LYP**	64	Gaussian	Basis set: 6-21G (C/N)	[10]

							(*all electron*)	6-31G (H) MP8 sampling	
				C-H stretching, x = 2, y = 1					
2630	VN_2H^-	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
2700	VN_2H^-	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Basis set: 8-31G (C) 4-31G (N), 3-21G (H) Γ point sampling	[13]
3040	VN_2H^0	C-H_{sy}	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3050	VN_2H^0	C-H_s	H	1/2	PBE*	1000	Gaussian (*atom centered*)	Basis set: 8-31G (C) 4-31G (N), 3-21G (H) Γ point sampling	[13]
3050	VN_2H^+	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3065	VN_2H	C-H_s (a)	Ah	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3213	VN_2H	C-H_s (a)	H	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
				C-H bending, x = 3, y = 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	[11]
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	[11]
1333	VN_3H	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1360	VN_3H	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1361	VN_3H	C-H_b	H	0	LDA*	64	Gaussian	Basis set: 40 (C/N)	[11]

							(*atom centered*)	All atoms incl. MP2 sampling	
1365	VN_3H	C-H_b	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[11]
1366	VN_3H	C-H_b	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[11]
1367	VN_3H	C-H_b	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[11]
1384	VN_3H	C-H_b	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. Γ point sampling	[11]
1411	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
1415	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
1416	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
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	[14]
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	[14]
1447	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[8]

1448	VN_3H	C-H_b	H	-	B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
1452	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[8]
1454	VN_3H	C-H_b	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[8]
1459	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[8]
1461	VN_3H	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1461	VN_3H	C-H_b	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
1463	VN_3H	C-H_b	H	-	B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
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	[14]
C-H stretching, $x = 3$, $y = 1$									
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	[11]
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	[11]

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	[11]
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	[11]
3028	VN_3H	C-H_s	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[11]
3034	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[11]
3037	VN_3H	C-H_s	H	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[11]
3039	VN_3H	C-H_s	H	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 40 (C/N) 5 core atoms incl. MP2 sampling	[11]
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	[14]
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	[14]
3120	VN_3H	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
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	[14]

3125	VN_3H	C-H_s	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[11]
3133	VN_3H	C-H_s (a)	Ah	-	B3LYP	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3196	VN_3H	C-H_s	H	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. Γ point sampling	[11]
3249	VN_3H	C-H_s	H	-	B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
3250	VN_3H	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3250	VN_3H	C-H_s	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
3250	VN_3H	C-H_s	H	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[8]
3251	VN_3H	C-H_s	H	-	B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[14]
3262	VN_3H	C-H_s	H	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[8]
C-H bending, $x = 4$, $y = 1$									
1394	VN_4H	C-H_b	H	-	LDA***	68	Planewave	Model 2 position MP 6x6x2 mesh	[15]
1589	VN_4H	C-H_b	H	-	LDA***	68	Planewave	Model 2 position MP 6x6x2 mesh	[15]
C-H stretching, $x = 4$, $y = 1$									
3095	VN_4H	C-H_s	H	-	LDA***	68	Planewave	Model 2 position	[15]

								MP 6x6x2 mesh	
3221	VN_4H	C-H_s	H	-	LDA***	68	Planewave	Model 1 position MP 6x6x2 mesh	[15]
					C-H bending, *x* = 2, *y* = 2				
471	VN_2H_2	C-H_b (d)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1392	VN_2H_2	C-H_b (c)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1398	VN_2H_2	C-H_b (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
1620	VN_2H_2	C-H_b	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
1701	VN_2H_2	C-H_b (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
					C-H stretching, *x* = 2, *y* = 2				
3320	VN_2H_2	C-H_{asy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Gaussian basis set	[4]
3370	$VN_2H_2^0$	C-H_{asy}	H	-	PBE*	1000	Gaussian (*atom centered*)	Basis set: 8-31G (C) 4-31G (N), 3-21G (H) Γ point sampling	[13]
3469	VN_2H_2	C-H_{asy} (b)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3470	VN_2H_2	C-H_s (b)	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3490	VN_2H_2	C-H_{sy}	H	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[4]
3540	$VN_2H_2^0$	C-H_{sy}	H	-	PBE*	1000	Gaussian (*atom centered*)	Basis set: 8-31G (C) 4-31G (N), 3-21G (H)	[13]

								Γ point sampling	
3641	VN_2H_2	C-H_s (a)	Ah	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]
3664	VN_2H_2	C-H_s (a)	H	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[10]

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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