Table B.1. Peak positions and associated vibrational modes for H-related defects in diamond from first-principals density functional simulations of IR spectra from selected studies.

Frequency (cm^{-1})	Defect	Mode (x)	H/Ah	Intensity (km/mol)	*S*	Functional	Cell	Basis set	Comment	Ref.
412	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[1]
422	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[1]
446	VNH_3	C-H_b (d)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
451	VNH_3	C-H_b (c)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[2]
471	VN_2H_2	C-H_b (d)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
476	VNH_2	C-H_b (d)	H	4 (0.6%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
494	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[1]
496	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[1]
749	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[1]
750	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[1]

853	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]
861	VH_4	C-H_b (c)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]
972	NH_1	C-H_b	H	-	-	LDF*	64	Gaussian	^{12}C-D isotopes Atom and bond centered basis sets	[3]
1296	VN_3H	C-H_b	H	-	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 40 (C/N) 5 core atoms incl. MP2 sampling	[4]
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	[4]
1310	VNH^0	C-H_b	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1310	VN_2H^+	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1320	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]
1322	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]
1330	VNH^+	C-H_b	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1330	VNH_2^-	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1330	VN_2H^0	C-H_b (b)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1331	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[1]
1333	VN_3H	C-H_b (b)	H	5 (0.8%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H)	[2]

									MP8 sampling	
1333	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms	[1]
									MP 2x2x2 mesh	
1340	VNH^-	C-H_b	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1340	VN_2H^0	C-H_b (a)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1347	BH_1	C-H_b	H	60	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1348	BH_1	C-H_b	H	60	1	B3LYP**	216	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1349	VH_1	C-H_b	H	99	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1350	VH_1^-	C-H_b	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1350	VH_2^0	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1350	VN_2H^+	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1353	VH_2	C-H_b (c)	H	2	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1358	VH_2	C-H_b (c)	H	61	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1360	VN_3H	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1360	VH_2	C-H_b (b)	H	70	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1361	VN_3H	C-H_b	H	-	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[4]
1365	VN_3H	C-H_b	H	-	0	LDA*	216	Gaussian	Basis set: 28 (C) 40 (N)	[4]

								(*atom centered*)	All atoms incl. MP2 sampling	
1366	VN_3H	C-H_b	H	-	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[4]
1367	VN_3H	C-H_b	H	-	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[4]
1370	VH_1^+	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1372	VNH_2	C-H_b (c)	H	23 (4%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1380	VH_4	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1382	VH_4	C-H_b (a)	H	233 (38%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first only defect atoms MP 4x4x4 mesh	[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	[4]
1387	VH_4	C-H_b (a)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]
1389	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[1]
1390	VH_4	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1391	VNH_2	C-H_b (b)	H	87 (14%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1392	VN_2H_2	C-H_b (c)	H	8 (1%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1394	VN_4H	C-H_b	H	-	-	LDA***	68	Planewave	Model 1 position	[8]

									MP 6x6x2 mesh	
1398	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[1]
1398	VN_2H_2	C-H_b (b)	H	114 (18%)	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1399	VH_4	C-H_b (b)	H	0 (0%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[1]
1400	NH_1	C-H_b	H	-	-	LDF*	64	Gaussian	Atom and bond centered basis sets	[3]
1400	VNH^{-2}	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1400	VH_3^{+}	C-H_b (c)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1400	VH_4	C-H_b (b)	H	0	-	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1404	NH_1	C-H_s	H	-	-	LDA*	64	Gaussian (*atom centered*)	2-fold degenerate MP 2x2x2 mesh	[9]
1407	BH_1	C-H_b	H	115	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1410	VH_3^{0}	C-H_b (b)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1411	BH_1	C-H_b	H	115	1	B3LYP**	216	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1411	VN_3H	C-H_b	H	240 (39%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]
1414	VNH	C-H_b (b)	H	74 (12%)	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1415	VN_3H	C-H_b	H	249 (41%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]

1420	VH_1	C-H_b (b)	H	32	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1421	VNH	C-H_b (a)	H	58 (9%)	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1422	VNH	C-H_b (b)	H	81 (13%)	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1423	VH_4	C-H_b (a)	H	285 (46%)	-	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[1]
1424	VN_2H	C-H_b (b)	H	39 (6%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1428	VH_4	C-H_b (a)	H	292 (48%)	-	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[1]
1430	VNH^0	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1430	VH_3^+	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1431	VNH^0	C-H_b	H	-		LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[4]
1440	VH_3^+	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[10]
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	[10]

1447	VN_3H	C-H_b	H	206 (34%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[1]
1448	VN_3H	C-H_b	H	16 (32%)		B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
1450	VH_3^0	C-H_b (a)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1452	VNH^-	C-H_b	H	-		LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[4]
1452	VN_3H	C-H_b	H	213 (34%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[1]
1454	VN_3H	C-H_b	H	194 (31%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[1]
1459	VN_3H	C-H_b	H	202 (33%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[1]
1460	VNH_3	C-H_b (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1461	VN_3H	C-H_b (a)	H	205 (33%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1461	VN_3H	C-H_b	H	16 (32%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
1461	VH_2	C-H_b (b)	H	361	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1463	VN_3H	C-H_b	H	16 (32%)		B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
1470	VN_2H^-	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1476	VN_3H	C-H_b	Ah	-		B3LYP**	64	Gaussian	Basis set: 6-21G (C/N)	[10]

								(*all electron*)	6-31G (H) Γ point sampling No C-H mode coupling Anharmonicity by VCI	
1478	VH_4	C-H_b (a)	H	244 (39%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 4x4x4 mesh	[1]
1479	VN_2H	C-H_b (a)	H	42 (7%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1480	VNH_3	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1484	VH_4	C-H_b (a)	H	252 (41%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 12 neighboring atoms MP 2x2x2 mesh	[1]
1486	VH_4	C-H_b (a)	H	233 (38%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 4x4x4 mesh	[1]
1487	VH_1	C-H_b (a)	H	12	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1488	VH_4	C-H_b (a)	H	231		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1489	VH_3	C-H_b (b)	H	77	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1492	VH_4	C-H_b (a)	H	239 (39%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 24 neighboring atoms MP 2x2x2 mesh	[1]
1501	VNH	C-H_b (a)	H	17 (3%)	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1520	VH_2^+	C-H_b	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1520	VH_3^-	C-H_b (b)	H	-	0	PBE*	1000	Gaussian	Γ point sampling	[5]

								(*atom centered*)		
1529	VNH_3	C-H_b (b)	H	189 (30%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1538	VH_3	C-H_b (a)	H	104	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1540	VH_2^0	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1550	VH_2^0	C-H_b	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1550	VNH_2^+	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1560	VH_3^-	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1580	VNH_2^0	C-H_b	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1584	VNH_3	C-H_b (a)	H	159 (26%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[2]
1586	NH_1	C-H_b	Ah	20	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1589	VN_4H	C-H_b	H	-		LDA***	68	Planewave	Model 2 position MP 6x6x2 mesh	[8]
1590	NH_1	C-H_b	Ah	20	1	B3LYP**	216	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1590	VH_2^-	C-H_b	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1598	D_1^+	C-H_s (b)	H	-		LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[3]
1616	VH_2	C-H_b (a)	H	21	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]

1620	VN_2H_2	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1627	VH_2	C-H_b (a)	H	284	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
1653	VNH_2	C-H_b (a)	H	50 (8%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1680	VH_2^{-2}	C-H_b	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1680	VNH_2^-	C-H_b (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
1701	VN_2H_2	C-H_b (a)	H	153 (25%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
1797	D_1^+	C-H_s (a)	H	-		LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[3]
1804	BH_1	C-H_b	H	250	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1866	BH_1	C-H_b	H	275	1	B3LYP**	216	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
1952	D_1^-	C-H_s	H	-		LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[3]
1973	VNH^0	C-H_s	H	-	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[11]
1986	VNH^0	C-H_s	H	-	1	LDA*	64	Gaussian	^{12}C-D isotopes $MP2^3$ sampling	[11]
2026	VNH^+	C-H_s	H	-	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[11]
2038	VNH^+	C-H_s	H	-	1	LDA*	64	Gaussian	^{12}C-D isotopes $MP2^3$ sampling	[11]
2067	VNH^-	C-H_s	H	-	1	LDA*	64	Gaussian	^{13}C-D isotopes $MP2^3$ sampling	[11]
2080	VNH^-	C-H_s	H	-	1	LDA*	64	Gaussian	^{12}C-D isotopes	[11]

									$MP2^3$ sampling	
2084	D_1^0	C-H_s	H		-		LDF*	64	Gaussian	H_1 = D (BC site) Atom and bond centered basis sets	[3]
2086	H_1^+	C-H_s (b)	H		-		LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[3]
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	[4]
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	[4]
2414	NH_1	C-H_s	H		-		LDF*	64	Gaussian	^{12}C-D isotopes Atom and bond centered basis sets	[3]
2450	VH_1^0	C-H_s	H		-	3/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2450	VH_1^0	C-H_s	H		-	3/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
2456	H_1^+	C-H_s (a)	H		-		LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[3]
2470	VH_1^{-3}	C-H_s	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[13]
2483	VH_1	C-H_s	Ah	253		2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
2540	VH_1^{-3}	C-H_s	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]

2550	VNH^{-2}	$C\text{-}H_{sy}$	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2571	H_2	$C\text{-}H_{sy}$	H		-		LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[9]
2580	VH_1^+	$C\text{-}H_s$	H		-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
2584	H_2	$C\text{-}H_{sy}$	H		-		LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = H (AB site) MP 2x2x2 mesh	[9]
2630	VN_2H^-	$C\text{-}H_{sy}$	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2689	VNH^0	$C\text{-}H_s$	H		-	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[11]
2693	H_2	$C\text{-}H_{sy}$	H		-		LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[9]
2697	VNH^0	$C\text{-}H_s$	H		-	1	LDA*	64	Gaussian	$MP2^3$ sampling	[11]
2700	VN_2H^-	$C\text{-}H_s$	H		-	1/2	PBE*	1000	Gaussian (*atom centered*)	Basis set: 8-31G (C) 4-31G (N), 3-21G (H) Γ point sampling	[14]
2710	VH_1^{-2}	$C\text{-}H_s$	H		-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
2712	H_2	$C\text{-}H_{asy}$	H		-		LDA*	64	Gaussian (*atom centered*)	H_1 = D (BC site) H_2 = D (AB site) MP 2x2x2 mesh	[9]
2730	H_1^-	$C\text{-}H_s$	H		-		LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[3]
2750	VH_1^{-2}	$C\text{-}H_s$	H		-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2763	VNH^+	$C\text{-}H_s$	H		-	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[11]
2764	VH_1	$C\text{-}H_s$	H	253		2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H)	[7]

									Γ point sampling	
2770	VH_2^{-2}	C-H_{asy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2771	VNH^{+}	C-H_s	H	-	1	LDA*	64	Gaussian	$MP2^3$ sampling	[11]
2818	VH_1	C-H_s	H	-	2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[13]
2819	VNH^{-}	C-H_s	H	-	1	LDA*	64	Gaussian	^{13}C-H isotopes $MP2^3$ sampling	[11]
2827	VNH^{-}	C-H_s	H	-	1	LDA*	64	Gaussian	$MP2^3$ sampling	[11]
2850	VNH^0	C-H_{sy}	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2850	VNH_2^{-}	C-H_{asy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2858	VNH^0	C-H_s	H	-	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
2866	VNH^{-}	C-H_s	H	-		LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 sampling	[4]
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	[13]
2894	VNH	C-H_s (a)	Ah	15 (2%)	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
2900	H_1	C-H_s	H	-		LDA*	64	Gaussian (*atom centered*)	H_1 = H (BC site) MP 2x2x2 mesh	[9]
2919	H_1^0	C-H_s	H	-		LDF*	64	Gaussian	H_1 = H (BC site) Atom and bond centered basis sets	[3]
2928	VH_1^{-}	C-H_s	H	-		LDA*	64	Gaussian (*atom centered*)	MP 2x2x2 mesh	[9]
2930	VNH^{-}	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
2941	VNH^{-}	C-H_s	H	-		GGA*	216	Gaussian	MP 2x2x2 mesh	[15]

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	[13]
2950	VNH^+	C-H_{sy}	H		-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[13]
2970	VH_1^-	C-H_s	H		-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
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	[13]
3000	VH_1^-	C-H_s	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
3010	VH_1^-	C-H_s	H		-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3015	VH_1	C-H_s	Ah	77		1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
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	[13]
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	[4]
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	[4]
3028	VN_3H	C-H_s	H		-	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[4]
3034	VN_3H	C-H_s	H		-	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C) 40 (N) All atoms incl. MP2 sampling	[4]

3037	VN_3H	C-H_s	H	-	0	LDA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[4]
3039	VN_3H	C-H_s	H	-	0	LDA*	216	Gaussian (*atom centered*)	Basis set: 40 (C/N) 5 core atoms incl. MP2 sampling	[4]
3040	VH_2^0	C-H_{asy}	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3040	VN_2H^0	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3040	VH_1^0	C-H_s	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
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	[14]
3050	VH_2^{-2}	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3050	VN_2H^+	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[10]
3060	VH_2^0	C-H_{asy}	H	-	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3065	VN_2H	C-H_s (a)	Ah	122 (20%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3069	VNH	C-H_s (a)	Ah	129 (21%)	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3090	VH_3^-	C-H_{asy} (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[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	[10]

3095	VN_4H	C-H_s	H	-		LDA***	68	Planewave	C-H mode coupling Anharmonicity by VCI Model 2 position MP 6x6x2 mesh	[8]
3096	VNH	C-H_s (a)	H	7 (1%)	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3100	VH_2^+	C-H_{asy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3100	VNH_2^-	C-H_{sy}	H	-	0	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	[9]
3118	VH_2^-	C-H_{asy}	H	-		GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3120	VH_2^-	C-H_{asy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3120	VH_3^-	C-H_{asy} (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3120	VN_3H	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3122	VNH^0	C-H_s	H	-		LDA*	216	Gaussian (*atom centered*)	Basis set: 28 (C/N) MP2 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	[10]
3125	VN_3H	C-H_s	H	-	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. MP2 sampling	[4]
3130	VH_1^0	C-H_s	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3132	VN_3H	C-H_s	Ah	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
3133	VN_3H	C-H_s (a)	Ah	621 (100%)		B3LYP	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H)	[2]

										MP8 sampling	
3153	VH_1	C-H_s	H		-	1/2	PBE**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G$^{(*)}$ (H) Γ point sampling	[13]
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	[13]
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	[13]
3180	VNH^0	C-H_{sy}	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[13]
3190	VNH^0	C-H_s	H		-	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3193	VH_1	C-H_s	H	77		1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3196	VN_3H	C-H_s	H		-	0	GGA*	64	Gaussian (*atom centered*)	Basis set: 40 (C/N) All atoms incl. Γ point sampling	[4]
3200	VNH_2^+	C-H_{asy}	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3210	VH_1^+	C-H_s	H		-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[12]
3213	VN_2H	C-H_s (a)	H	122 (20%)		1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3221	VN_4H	C-H_s	H		-		LDA***	68	Planewave	Model 1 position MP 6x6x2 mesh	[8]
3224	VNH	C-H_s (a)	H	129 (21%)		0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3230	VNH_2^0	C-H_{asy}	H		-	1/2	PBE*	1000	Gaussian	Γ point sampling	[5]

								(*atom centered*)		
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	[13]
3249	VN_3H	C-H_s	H	50 (100%)		B3LYP**	32	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
3250	VN_3H	C-H_s (a)	H	621 (100%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3250	VN_3H	C-H_s	H	50 (100%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
3250	VN_3H	C-H_s	H	619 (100%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]
3251	VN_3H	C-H_s	H	50 (100%)		B3LYP**	128	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[10]
3253	VH_2	C-H_{asy}	Ah	29	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3262	VN_3H	C-H_s	H	608 (100%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]
3271	VN_3H	C-H_s	H	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
3275	VH_2	C-H_{asy}	H	29	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3309	NH_1	C-H_s	H	-		LDA*	64	Gaussian (*atom centered*)	MP 2x2x2 mesh	[9]
3310	VH_1^+	C-H_s	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3310	VH_2^0	C-H_{sy}	H	-	1	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]

3318	NH_1	C-H_s	H	-		LDF*	64	Gaussian	^{13}C-H isotopes Atom and bond centered basis sets	[3]
3320	VN_2H_2	C-H_{asy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Gaussian basis set	[5]
3324	NH_1	C-H_s	H	-		LDF*	64	Gaussian	Atom and bond centered basis sets	[3]
3330	VH_2^-	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3337	VH_2^0	C-H_{sy}	H	-	1	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3339	VH_2^-	C-H_{sy}	H	-		GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3350	VH_2^0	C-H_{asy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3356	VH_2^0	C-H_{asy}	H	-	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
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	[14]
3370	VH_2^+	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3378	VH_2	C-H_{asy}	Ah	395	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3394	BH_1	C-H_s	Ah	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
3402	VNH_2	C-H_s (b)	Ah	88 (14%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3410	VNH_2^+	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3417	VNH_2	C-H_s (b)	H	88 (14%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3408	NH_1	C-H_s	Ah	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]

3420	VNH_2^0	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3420	VH_3^+	C-H_{asy} (b)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3426	VH_2	C-H_{asy}	H	395	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
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	[13]
3430	VH_3^-	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3450	VH_3^+	C-H_{asy} (a)	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3450	VH_3^0	C-H_{asy} (b)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3455	BH_1	C-H_s	H	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
3460	VH_3^0	C-H_{asy} (a)	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3469	VN_2H_2	C-H_{asy} (b)	H	346 (56%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3470	VN_2H_2	C-H_s (b)	Ah	346 (56%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3471	NH_1	C-H_s	H	-	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G Γ point sampling	[6]
3477	VH_2	C-H_{sy}	Ah	2	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3490	VN_2H_2	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3511	H_2	C-H_{sy}	H	-		LDF*	64	Gaussian	H_1 = H (BC site) H_2 = H (AB site) Atom and bond centered	[3]

									basis sets	
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	[9]
3520	VH_2^0	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3525	VH_2^0	C-H_{sy}	H	-	0	GGA*	216	Gaussian	MP 2x2x2 mesh	[15]
3526	VH_2	C-H_{sy}	H	2	1	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
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) Γ point sampling	[14]
3552	VH_2	C-H_{sy}	Ah	571	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
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	[13]
3570	VNH_3	C-H_{asy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3580	VNH_2	C-H_s (a)	Ah	52 (8%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[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	[9]
3606	VH_2	C-H_{sy}	H	571	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3615	VNH_2	C-H_s (a)	H	52 (8%)	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3641	VN_2H_2	C-H_s (a)	Ah	185 (30%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H)	[2]

									MP8 sampling	
3651	VH_3	C-H_{asy}	H	0	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3653	VH_3	C-H_{asy}	Ah	0	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3664	VN_2H_2	C-H_s (a)	H	185 (30%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3700	VH_3^+	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3704	VNH_3	C-H_s (b)	H	189 (30%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[2]
3710	VH_3^0	C-H_{sy}	H	-	1/2	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
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	[9]
3725	VNH_3	C-H_s (b)	Ah	189 (30%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling 2-fold degenerate	[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	[9]
3790	VNH_3	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
3853	VH_4	C-H_s (b)	H	14 (2%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]
3868	VH_4	C-H_s (b)	H	12 (2%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]

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	[3]
3908	VH_3	C-H_{sy}	H	1	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3943	VNH_3	C-H_s (a)	H	56 (9%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
3953	VH_3	C-H_{sy}	Ah	1	1/2	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3974	VH_4	C-H_s (b)	H	4 (0.6%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[1]
3974	VH_4	C-H_{asy}	H	4		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
3989	VH_4	C-H_s (b)	H	3 (0.5%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[1]
4000	VNH_3	C-H_s (a)	Ah	56 (9%)		B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) MP8 sampling	[2]
4037	VH_4	C-H_{asy}	Ah	5	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
4120	VH_4	C-H_{sy}	H	-	0	PBE*	1000	Gaussian (*atom centered*)	Γ point sampling	[5]
4199	VH_4	C-H_s (a)	H	0 (0%)		B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 4x4x4 mesh	[1]
4221	VH_4	C-H_s (a)	H	0 (0%)		B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes only defect atoms MP 2x2x2 mesh	[1]

4276	VH_4	C-H_s (a)	H	0 (0%)	B3LYP**	64	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 4x4x4 mesh	[1]
4276	VH_4	C-H_{sy}	H	0	B3LYP**	64	Gaussian (*all electron*)	Basis set: 6-21G (C/N) 6-31G (H) Γ point sampling	[7]
4298	VH_4	C-H_s (a)	H	0 (0%)	B3LYP**	216	Gaussian (*all electron*)	Freq. calc. includes first 4 neighboring atoms MP 2x2x2 mesh	[1]

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.

Calculated peak intensities are reported in km/mol. In cases where the VN_3H defect is simulated, relative intensities were normalized and reported (as %) in comparison to the VN_3H C-H stretching mode, which is always the most intense peak observed in experiment.

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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