TABLE A.1. Observed peak positions and associated vibrational modes for H-related defects in natural diamonds from this work and selected studies.

Obs. Freq. (cm^{-1})	Assigned Defect	Vibrational Mode	Norm. Intensity (%)	Comment	References	Calc. Freq. (cm^{-1}) defect and reference
1170	[N][H]	C/N-H	–	Type IaAB	[1]	–
1173	[N][H]	C/N-H	–	Type IaAB	[1]	–
1240	–	C/N-H	–	In H-rich brown Type Ib diamond	[2,3]	–
1352	–	–	w	Brown-orange Type IbXY	[4]	**VH^- –** 1350 [5] **VH_2^0 –** 1350 [5] **VN_2H^+ –** 1350 [5] **VH_2 –** 1353 [6]
1358	–	–	w	Brown-orange Type IbXY	[4]	**VN_3H –** 1360 [5] **VH_2 –** 1358, 1360 [6]
1363	–	–	w	Brown-orange Type IbXY	[4]	**VN_3H –** 1361 [7]
1367	–	C-H_b	1.06*	Platelet peak Type IaB, samples *G1-G3*	[3,8] This work	**VN_3H –** 1366, 1367 [7] **VH^+ –** 1370 [5]
1375	–	–	w	Brown-orange Type IbXY	[4]	–
1384	–	C-H_b	–	Type Ib	[9]	**VN_3H –** 1384 [7,10], 1382 [10]
1387	–	–	w	Brown-orange Type IbXY	[4]	**VN_3H –** 1387, 1389 [10]
1388	–	C-H_b	–	Brown Type IaA>>B	[4]	**VN_3H –** 1387, 1389 [10] **VH_4 –** 1390 [5]
1396	–	C-H_b	–	Type Ib	[9]	**VN_4H –** 1394 [11] **VN_3H –** 1398 [10] **VN_2H_2 –** 1398 [12]
1397	–	–	w	Brown-orange Type IbXY	[4]	**VN_3H –** 1398, 1399 [10] **VN_2H_2 –** 1398 [12]
1398	–	C-H_b	1.46*	Type IaB, samples *G1-G3*	**This work**	**VN_3H –** 1398, 1399 [10] **VN_2H_2 –** 1398 [12] **NH –** 1400 [13] **VNH^{-2} –** 1400 [5] **VH_3^+ –** 1400 [5]

						VH_4 – 1400 [6]
1401-1402	**–**	$C\text{-}H_b$	**–**	Type IaB, samples *G1-G3* observed as weak shoulder of 1405 cm^{-1} peak Type Ib	[9] This work	**VN_3H –** 1399 [10,12] **NH –** 1400 [13] **VNH^{-2} –** 1400 [5] **VH_3^+ –** 1400 [5] **VH_4 –** 1400 [6]
1405	VN_3H	$C\text{-}H_b$	20, 15-62*	Type IaA and IaAB Type IaB, samples *G1-G3* Associated with 3107cm^{-1} stretch	[14–18] This work	**NH –** 1404 [19]
1410	**–**	$C\text{-}H_b$	**–**	Type Ib	[9]	**VH_3^0 –** 1410 [5] **VN_3H –** 1411 [10]
1430	**–**	$C\text{-}H_b$	w	Brown-orange Type IbXY	[4]	**VNH^0 –** 1430 [5], 1431 [7] **VH_3^+ –** 1430 [5]
1432	**–**	$C\text{-}H_b$	**–**	Type Ib	[9]	**VNH^0 –** 1430 [5], 1431 [7] **VH_3^+ –** 1430 [5]
1461	**–**	$C\text{-}H_b$	**–**	Type Ib	[9]	**VN_3H –** 1459 [10], 1461 [12], 1461 [20], 1463 [20] **VNH_3 –** 1460 [5]
1470	VN_4H^0	$N\text{-}H_b$	**–**	associated with 3236cm^{-1} peak	[21,22]	**VN_2H^- –** 1470 [5]
1498-1499	**–**	$C\text{-}H_b$	0.41*	Type IaB, samples *G1* and *G2* observed as broad peak. Brown Type IaA>>B	[4] This work	**VNH –** 1501 [12]
1547	**–**	**–**	**–**	In Type IaAB diamond	[17,18,23,24]	**–**
2688	VNH*	C-H	**–**	Yellow Type IaB>A>Ib Orange Type IaA+Ib	[25]	**VNH^0 –** 2689 [26]
2722	**–**	**–**	**–**	Grey/white Type IaB Orange Type IaA+Ib	[25]	**–**
2723	**–**	**–**	0.62*	Type IaB, samples *G1-G3*	**This work**	**–**
2741	**–**	**–**	**–**	Type Ib Type IaA+Ib with X/Y centers	[9]	**–**
2742	**–**	**–**	w	Brown-orange Type IbXY	[4]	**–**
2750	**–**	**–**	**–**	Grey Type IaB and IaA Orange Type IaA+Ib Brown-orange Type IbXY	[4,25]	**VH^{-2} –** 2750 [5]

2770	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2^{-2} –** 2770 [5] **VNH^+ –** 2771 [26]
2784-2786	VN_3H	C-H_b	3.4-4.1, 3.0	Type Ia 2 x 1405cm^{-1} overtone Intensity calculated for 2786 cm^{-1}	[4,9,15,17,18,27,28] This work	–
2786-2787	VN_3H	C-H_b	3.0	Type Ia 2 x 1405cm^{-1} overtone Intensity calculated for 2786 cm^{-1}	[14,15,17,18] This work	–
2793	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2798	–	–	w	Type Ib Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,9,27]	–
2806	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2812-2813	–	–	1.27*	Type IaB, samples *G1-G3* Brown/green/yellow/white/purple Type IaB>A Black/grey/white Type IaB Grey/colorless Type IaA Orange Type IaA+Ib Type IaA+Ib with X/Y centers	[25,27,28] This work	–
2817	VNH/VH*	C-H	w	Type IaA+Ib with X/Y centers	[27]	**VNH^- –** 2819 [26] **VH –** 2818 [29]
2818	VNH/VH*	C-H	w	Brown-orange Type IbXY	[4]	**VNH^- –** 2819 [26] **VH –** 2818 [29]
2831	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2840	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2849_c	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH^0 –** 2850 [5] **VNH_2^- –** 2850 [5]
2852_c	–	–	w	Type IaB, samples *G1-G3* Observed as broad peak. Type Ib	[9] This work	**VNH^0 –** 2850 [5] **VNH_2^- –** 2850 [5]
2854	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
2857	VNH^{0*}	C-H	–		[28,30]	**VNH^0 –** 2858 [31]

2859	VNH^{0}*	C-H	w	Grey Type IaA Type IaA+Ib with X/Y centers	[25,27]	**VNH^{0} –** 2858 [31]
2869	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
2870	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
2873	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2876	–	–	w	Brown-orange Type IbXY	[4]	–
2877	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
2879	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2888	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2889	–	–	w	Brown-orange Type IbXY	[4]	–
2896	–	–	w	Brown-orange Type IbXY	[4]	–
2897	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2904	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
2906	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
2911	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
2912	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
2920_{c}	VN_4H^{0}	$N\text{-}H_{b}$	w	Type IaB, samples *G1-G3* Observed as broad peak. 2 x 1470cm^{-1} overtone in H-rich grey diamond	[17] This work	**H^{0}** – 2919 [13]
2932	VNH*	C-H	w	Type Ib Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,9]	**VNH^{-} –** 2930 [5]
2940	VNH/VH*	C-H	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	**VNH^{-} –** 2941 [31]

2941	VNH/VH*	C-H	w		Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VNH^- –** 2941 [31]
2942	VNH/VH*	C-H	w		Type IaA+Ib with X/Y centers	[27]	**VNH^- –** 2941 [31]
2944	VNH/VH*	C-H		–	Yellow Type IaB>A>Ib Orange Type IaA+Ib	[25]	**VH –** 2946 [29]
2945	VNH/VH*	C-H	w		Type IaA+Ib with X/Y centers	[27]	**VH –** 2946 [29]
2949	VNH/VH*	C-H		–	Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VNH^+ –** 2950 [5]
2964	–	–	s		Type IaA+Ib with X/Y centers	[27]	–
2965	–	–	s		Type Ib Brown-orange Type IbXY	[4,9]	–
2967	–	–	w		Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
2972	$[H_2]$	$C-H_s$		–	Doublet with 3025cm^{-1} olefinic sp^2-C-H stretch	[9,32]	**VH^- –** 2970 [33]
2973	–	–	s		Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
2981	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VH –** 2981 [29]
2982	[N][H]	$N-H_s$		–	Brown, green, and yellow Type IaB>A Black and grey IaB Grey Type IaA Brown-orange Type IbXY	[4,25,34]	**VH –** 2981 [29]
2984	–	–		–	Type Ib	[9]	–
2985	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
2987_c	–	–	w		Brown-orange Type IbXY	[4]	–
2990_c	–	–	w		Type IaB, sample *G2*	**This work**	–
2993_c	–	–	s		Type IaA+Ib with X/Y centers	[27]	–
2994_c	–	–	w		Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
3006	–	–		–	Grey Type IaB and IaA	[25]	–

3013	VH*	C-H_s	–	Type Ib	[9]	**VH –** 3015 [29], 3015 [6]
3014	VH*	C-H_s	s	Type IaA+Ib with X/Y centers	[27]	**VH –** 3015 [29], 3015 [6]
3015	VH*	C-H_s	–	Brown Type IaB>A Brown-orange Type IbXY	[4,25]	**VH –** 3015 [29], 3015 [6]
3023	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3025 [7]
3025-3026	[H_2]	C-H_s	s	Doublet with 3025cm^{-1} olefinic sp^2-C-H stretch Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,9,27,32]	**VN_3H –** 3025 [7], 3028 [7]
3028	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3028 [7]
3030	–	–	–	Grey/white Type IaB	[25]	**VN_3H –** 3028 [7]
3031	–	–	0.37*	Type IaB, sample *G3*	**This work**	–
3032	–	–	s	Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VN_3H –** 3034 [7]
3033	–	–	w	Brown-orange Type IbXY	[4]	–
3035	–	–	0.99*	Type IaB, samples *G1-G3*	**This work**	**VN_3H –** 3034, 3037 [7]
3041	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VN_3H –** 3039 [7] **VH_2^0 –** 3040 [5] **VN_2H^0 –** 3040 [5] **VH^0 –** 3040 [5]
3043	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
3048	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_2H^0 –** 3050 [35] **VH_2^{2-} –** 3050 [5] **VN_2H^+ –** 3050 [5]
3050	[N][H]	N-H_{sy}	0.1-3.7, 1.1	Type IaB, samples *G1* and *G2* Observed as doublet with 3056 cm^{-1} peak Yellow Type IaB>A>Ib Grey Type IaB and IaA White Type IaB>A	[4,8,25,27,28,36,37] This work	**VN_2H^0 –** 3050 [35] **VH_2^{2-} –** 3050 [5] **VN_2H^+ –** 3050 [5] **VN_3H –** 3054 [20]

				Orange Type IaA+Ib Colorless Type IaA Brown Type IaA>>B Type IaA+Ib with X/Y centers Observed in only cuboid and not octahedral sectors by [28]		
3052	–	–	–	–	[36]	**VN_2H^0 –** 3050 [35] **VH_2^{2-} –** 3050 [5] **VN_2H^+ –** 3050 [5] **VN_3H –** 3054 [20]
3054	–	–	s	Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VN_3H –** 3054 [20]
3055	[N][H]	N-H_{sy}	–	Type IaB	[34]	**VN_3H –** 3054 [20]
3056-3057	[N][H]	N-H_{sy}	0.68*	Type IaB, samples *G1* and *G2* Observed as doublet with 3050 cm^{-1} peak Brown/green/yellow Type IaB>A Black and grey IaB Grey Type IaA	[25,34] This work	**VN_3H –** 3054 [20]
3059	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2^0 –** 3060 [31]
3061	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2^0 –** 3060 [31]
3067	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH –** 3069 [12] **VN_2H –** 3065 [12]
3069	VNH*	C-H_s	–	Orange Type IaA+Ib	[25]	**VNH –** 3069 [12]
3072	–	–	s	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
3073	–	–	w	Brown-orange Type IbXY	[4]	–
3075	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3076	–	–	1.07*	Type IaB, samples *G1-G3*	**This work**	–
3079	–	–	w	–	[36]	–
3080	–	–	w	Type IaA+Ib with X/Y centers	[27]	–

3081	–	–	2.09*	Type IaB, samples *G1-G3* Observed as shoulder on 3085 cm^{-1} peak Grey/colorless Type IaA Brown Type IaA>>B Type IaA+Ib with X/Y centers	[4,25,28,36] This work	–
3083	–	–	w	Type Ib Type IaA+Ib with X/Y centers	[9]	–
3084	–	–	w	Brown-orange Type IbXY	[4]	–
3085	–	–	16.11*	Type IaB, samples *G1-G3* Type IaA+Ib with X/Y centers	[27] This work	–
3086	–	–	s	Black/grey/white Type IaB	[25]	–
3088	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_3^- –** 3090 [5]
3090	–	–	w	Type IaB, sample *G1*	**This work**	**VH_3^- –** 3090 [5]
3091	–	–	3.67*	Type IaB, samples *G2* and *G3*	**This work**	**VH_3^- –** 3090 [5]
3092	–	–	–	Grey/colorless Type IaA	[8,25]	–
3093	–	C-H_s	–	Type IaA+Ib with X/Y centers Brown Type IaA>>B	[4,8,27,28]	**VN_3H –** 3094 [20] **VN_4H –** 3095 [11]
3094	–	C-H_s	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	**VN_3H –** 3094 [20] **VN_4H –** 3095 [11] **VNH –** 3096 [12]
3095	–	C-H_s	–	–	[36]	**VN_3H –** 3094 [20] **VN_4H –** 3095 [11] **VNH –** 3096 [12]
3098	VN_3H	C-H_s	1.4, 6.58*	Type IaA and IaAB Type IaB, samples *G1-G3* ^{13}C-H shift of 3107cm^{-1}	[3,15,38] This work	**VNH –** 3096 [12] **VH_2^+ –** 3100 [5] **VNH_2^- –** 3100 [5]
3099	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
3103	–	–	s	Type IaA+Ib with X/Y centers	[27]	–
3104	–	–	w	Brown-orange Type IbXY	[4]	–

3105	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3107	VN_3H	C-H_s	100	Type IaA and IaAB Type IaB, samples *G1-G3* Associated with 1405cm^{-1} bend	[3,14,15,17,18,22,27,39] This work	–
3109	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3114	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH^0 –** 3114 [19]
3116	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2^- –** 3118 [31] **VH^0 –** 3114 [19]
3119	–	–	2.29*	Type IaB, samples *G2* and *G3* Observed as shoulder on 3107 cm^{-1} peak	**This work**	**VH_2^- –** 3118 [31], 3120 [5] **VH_3^- –** 3120 [5] **VN_3H –** 3120 [5]
3120	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2^- –** 3118 [31], 3120 [5] **VH_3^- –** 3120 [5] **VNH^0 –** 3122 [7] **VN_3H –** 3120 [5], 3122 [7]
3122-3124	VNH^0*	C-H_s	–	VNH^- and VNH^0 defects linked to 3123cm^{-1} peak in CVD diamond Yellow Type IaB>A>Ib Grey/colorless Type IaA White/purple Type IaB>A Brown Type IaA>>B Type IaA+Ib with X/Y centers	[4,8,25,27,28,36,40,41]	**VH_2^- –** 3120 [5] **VH_3^- –** 3120 [5] **VNH^0 –** 3122 [7] **VN_3H –** 3120 [5], 3122 [7], 3125 [7]
3125	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3125 [7]
3127	–	–	0.39*	Type IaB, sample *G3*	**This work**	**VN_3H –** 3125 [7]
3129	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH^0 –** 3130 [5]
3133	VN_3H*	C-H_s	–	Grey Type IaB	[3,25]	**VN_3H –** 3133 [12]
3135	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3133 [12]
3137	[N][H]	N-H_s	w	Type Ib Chameleon Type IaA>B>Ib Type IaA+Ib with X/Y centers	[3,27,42]	–
3139	–	–	w	Brown Type IaA>>B Type IaA+Ib with X/Y centers	[4,27,39]	–

3143	VN_3H-C-N	C-H_s	0.30*	C-centers linked to VN_3H defects via one C atoms Type IaB, sample 2507-ira White Type IaB>A	[3,9,43]	–
3144-3146	[N][H]	N-H_s	s	Correlated with 3310cm^{-1} peak Type Ib Yellow Type IaB>A>Ib Black and grey Type IaB Grey/colorless Type IaA Orange Type IaA+Ib Chameleon Type IaA>B>Ib Brown Type IaA>>B Type IaA+Ib with X/Y centers	[3,4,25,27,36,39,42]	–
3150	[N][H]	N-H_{asy}	–	Intensity correlated to 3050cm^{-1}	[37]	–
3151	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH –** 3153 [29]
3152	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH –** 3153 [29]
3153-3154	[N][H]	N-H_{asy}	0.4-4.0, 1.06*	Type IaB, samples *G1* and *G2* Yellow Type IaB>A>Ib Black and grey Type IaB Grey/colorless Type IaA White Type IaB>A Orange Type IaA+Ib Brown Type IaA>>B Type IaA+Ib with X/Y centers Observed in only cuboid and not octahedral sectors by [28]	[4,8,14,25,27,28,39] This work	**VH –** 3153 [29]
3155	–	–	–	–	[14]	**VH –** 3153 [29]
3156	–	–	s	Type Ib Type IaA+Ib with X/Y centers	[9,27]	–
3157	–	–	w	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	–
3159	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3162	–	–	w	Yellow Type IaB>A>Ib Orange Type IaA+Ib	[25,27]	–

					Type IaA+Ib with X/Y centers		
3163	–	–	w		Chameleon Type IaA>B>Ib Type IaA+Ib with X/Y centers	[27,42]	–
3165	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3167	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3168	–	–	w		Brown-orange Type IbXY	[4]	–
3170	–	–	w		Yellow Type IaB>A>Ib Grey IaB and IaA White Type IaB>A Colorless Type IaA Type IaA+Ib with X/Y centers Brown Type IaA>>B	[4,8,25,27]	–
3172	VH*	C-H_s		–	Black Type IaB	[8,25,28]	**VH –** 3174 [29]
3173	VH*	C-H_s	w		Type IaA+Ib with X/Y centers	[27]	**VH –** 3174 [29]
3175	VH*	C-H_s	w		Type IaA+Ib with X/Y centers	[27]	**VH –** 3174, 3176 [29]
3177	VH*	C-H_s	w		Type IaA+Ib with X/Y centers	[27]	**VH –** 3176 [29]
3179	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VNH^0 –** 3180 [5]
3180	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VNH^0 –** 3180 [5]
3181	[N][H]	N-H_s		–	Type Ib Chameleon Type IaA>B>Ib	[3,42]	**VNH^0 –** 3180 [5]
3182	[N][H]	N-H_s	s		Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VNH^0 –** 3180 [5]
3183	–	–	w		Brown-orange Type IbXY	[4]	–
3185	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3187	VNH/VH*	C-H	w		Black Type IaA Type IaA+Ib with X/Y centers	[25,27]	**VH –** 3188 [29]
3188	VNH/VH*	C-H	w		Yellow Type IaB>A>Ib Grey/colorless Type IaA Orange Type IaA+Ib	[8,25,27]	**VH –** 3188 [29] **VNH^0 –** 3190 [31]

				Type IaA+Ib with X/Y centers		
3189	VNH/VH*	C-H	0.73*	Type IaB, sample *G2* Grey Type IaB White Type IaB>A Type IaA+Ib with X/Y centers	[8,25,27,28] This work	**VH –** 3188 [29] **VNH^0 –** 3190 [31]
3190	VNH/VH*	C-H	w	Brown Type IaA>>B	[4]	**VH –** 3188 [29] **VNH^0 –** 3190 [31]
3191	VNH/VH*	C-H	w	Type IaA+Ib with X/Y centers	[27]	**VNH^0 –** 3190 [31] **VH –** 3193 [6]
3195	**–**	**–**	w	Type Ib Type IaA+Ib with X/Y centers	[9,27]	**VH –** 3193 [6] **VN_3H –** 3196 [7]
3196	**–**	**–**	w	Brown-orange Type IbXY	[4]	**VN_3H –** 3196 [7]
3197	**–**	**–**	w	Orange Type IaA+Ib	[25]	**VN_3H –** 3196 [7]
3198	**–**	**–**	w	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3196 [7] **VNH_2^+** - 3200 [5]
3200	**–**	**–**	w	Type IaA+Ib with X/Y centers	[27]	**VNH_2^+** - 3200 [5]
3203	**–**	**–**	s	Type IaA+Ib with X/Y centers	[27]	**–**
3206	**–**	**–**	w	Chameleon Type IaA>B>Ib Type IaA+Ib with X/Y centers	[27,42]	**–**
3208	**–**	**–**	w	Yellow Type IaB>A>Ib Grey/colorless Type IaA Orange Type IaA+Ib	[25]	**VH^+** - 3210 [33]
3209	**–**	**–**	w	Brown Type IaA>>B	[4]	**VH^+** - 3210 [33]
3210	**–**	**–**	s	Type IaA+Ib with X/Y centers	[27]	**VH^+** - 3210 [33]
3211	**–**	**–**	s w	Type Ib Brown-orange Type IbXY	[4,9]	**VH^+** - 3210 [33] **VN_2H –** 3213 [12]
3212	**–**	**–**	w	Type IaA+Ib with X/Y centers	[27]	**VH^+** - 3210 [33] **VN_2H –** 3213 [12]
3214	**–**	**–**	w	Grey Type IaA Orange Type IaA+Ib Chameleon Type IaA>B>Ib Type IaA+Ib with X/Y centers	[25,27,42]	**VN_2H –** 3213 [12]

3215	–	–	w	Brown Type IaA>>B	[4]	**VN_2H –** 3213 [12]
3218	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3219	–	–	w	Brown-orange Type IbXY	[4]	**VN_4H –** 3221 [11]
3222	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VN_4H –** 3221 [11]
3225	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH –** 3224 [12]
3227	–	–	s	Type IaA+Ib with X/Y centers	[27]	–
3230	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH_2^0 –** 3230 [5] **VH –** 3231 [29]
3232	–	–	w	Brown-orange Type IbXY	[4]	**VNH_2^0 –** 3230 [5] **VH –** 3231 [29]
3234	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3236-3237	VN_4H	$N\text{-}H_s$	6.2-17.6	Type IaA and IaAB Type IaB, samples *G1-G3* Associated with 1470cm^{-1} bend	[11,14,15,17,18,22,25,27,39] This work	–
3237-3238	–	–	–	Type IaA+Ib with X/Y centers Brown Type IaA>>B	[4,8,14,27,39]	–
3240	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3243	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3246	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3250	–	–	s	Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3249 [20], 3250 [12], 3250 [20], 3250 [10]
3252	–	$C\text{-}H_s$	–	Type Ib	[9]	**VN_3H –** 3249 [20], 3250 [12], 3250 [20], 3250 [10], 3251 [20] **VH_2 –** 3253 [6]
3253	–	–	s	Type IaA+Ib with X/Y centers Brown-orange Type IbXY	[4,27]	**VH_2 –** 3253 [6] **VN_3H –** 3251 [20]
3255	–	–	0.73*	Type IaB, sample *G2* Brown/green/yellow/white/purple Type IaB>A Black and grey IaB	[25,28,36] This work	–

					Grey Type IaA		
3257	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3258	–	–		–	–	[36]	–
3259	–	–		–	Chameleon Type IaA>B>Ib	[42]	–
3260	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3262 [10]
3262	–	–	w		Yellow Type IaB>A>Ib	[25,27]	**VN_3H –** 3262 [10]
3264	–	–	w		Orange Type IaA+Ib Type IaA+Ib with X/Y centers Type IaA+Ib with X/Y centers	[27]	**VN_3H –** 3262 [10]
3266	–	–	w		Brown-orange Type IbXY	[4]	–
3267	–	–	w		Type Ib	[9,27]	–
3270	–	–	w		Type IaA+Ib with X/Y centers Type IaA+Ib with X/Y centers	[27]	–
3271	–	–		–	Chameleon Type IaA>B>Ib	[42]	–
3272	–	–	s		Type IaA+Ib with X/Y centers	[27]	–
3275	–	–		–	Type Ib	[9,36]	**VH_2 –** 3275 [6]
3276	–	–	w		Type IaA+Ib with X/Y centers	[4,27]	**VH_2 –** 3275 [6]
3282	–	–	w		Brown-orange Type IbXY Chameleon Type IaA>B>Ib	[27,42]	–
3284	–	–	w		Type IaA+Ib with X/Y centers Black Type IaA	[25,27]	–
3286	–	–	w		Type IaA+Ib with X/Y centers Grey Type IaA	[25,27]	–
3288	–	–	w		Type IaA+Ib with X/Y centers Type IaA+Ib with X/Y centers	[27]	–
3290-91	–	–	s		Type IaA+Ib with X/Y centers	[27]	–
3295-3296	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3299	–	–	s		Type IaA+Ib with X/Y centers	[27]	–

3305	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3309	–	–		–	Type Ib Type IaA+Ib with X/Y centers	[9,27,28,36]	**NH –** 3309 [19] **VH^+ –** 3310 [5] **VH_2^0 –** 3310 [5]
3310	[N][H]	N-H_s	s		Correlated with 3144cm^{-1} peak Type Ib Yellow Type IaB>A>Ib Black IaB and IaA Grey/colorless Type IaA White Type IaB>A Orange Type IaA+Ib Brown Type IaA>>B Brown-orange Type IbXY	[3,4,25,36]	**NH –** 3309 [19] **VH^+ –** 3310 [5] **VH_2^0 –** 3310 [5]
3311	–	–	s		Type IaA+Ib with X/Y centers	[27]	**NH –** 3309 [19] **VH^+ –** 3310 [5] **VH_2^0 –** 3310 [5]
3314	–	–	s		Type IaA+Ib with X/Y centers	[27]	–
3323	NH*	C-H_s		–	observed in CVD by [44] and described as N:H–C acetylenic sp^1-C-H stretch	[3,44,45]	**NH –** 3324 [13]
3325	–	–	w		Type IaA+Ib with X/Y centers	[27]	**NH –** 3324 [13]
3328	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VH_2^- –** 3330 [5]
3334	–	–	w		Type IaA+Ib with X/Y centers	[27]	–
3338	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VH_2^0 –** 3337 [31] **VH_2^- –** 3339 [31]
3342	[N][H]	N-H_s	w		Type IaA+Ib	[39]	–
3343	[N][H]	N-H_s	w		Brown-orange Type IbXY	[4]	–
3350	–	–	w		Type IaA+Ib with X/Y centers	[27]	**VH_2^0 –** 3350 [5]
3354	–	–		–	Yellow Type IaB>A>Ib Orange Type IaA+Ib	[25]	**VH_2^0 –** 3356 [31]
3360	–	–	w		Type IaA+Ib with X/Y centers	[27]	–

3363	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3368	–	–	w	Type IaA+Ib with X/Y centers	[27]	**$VN_2H_2^0$** – 3370 [35] **VH_2^+** - 3370 [5]
3370	[N][H]	N-H_s	w	Type IaA+Ib with X/Y centers	[27]	**$VN_2H_2^0$** – 3370 [35] **VH_2^+** - 3370 [5]
3372	[N][H]	N-H_s	–	Type Ib Chameleon Type IaA>B>Ib	[3,42]	**$VN_2H_2^0$** – 3370 [35] **VH_2^+** - 3370 [5]
3377	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VH_2** - 3378 [6]
3382	–	–	w	Type IaA+Ib with X/Y centers	[27]	–
3394	[N][H]	N-H_s	w	Type Ib Brown-orange Type IbXY	[4]	–
3401	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH_2** - 3402 [12]
3410	–	–	w	Type IaA+Ib with X/Y centers	[27]	**VNH_2^+** - 3410 [5]
3418	–	–	–	associated with 1547cm^{-1} bend	[18]	**VNH_2^0 –** 3420 [5] **VH_3^+ –** 3420 [5]
3470	–	C-H_s	–	Yellow Type IaB>A>Ib	[25]	**VN_2H_2 –** 3469 [12], 3470 [12] **NH –** 3471 [46]
3474	–	–	w	Broad band Grey/colorless Type IaA Orange Type IaA+Ib Brown Type IaA>>B	[4,25,39]	–
3480	–	–	w	Brown-orange Type IbXY	[4]	–
3525	–	–	–	Orange Type IaA+Ib	[25]	**VH_2^0 –** 3525 [31] **VH_2 –** 3526 [6]
4157	–	–	–	–	[17]	–
4167	VN_3H^0	C-H_b	0.6	3 x 1405cm^{-1} overtone	[15]	–
4168	VN_3H^0	C-H_b	0.6, 1.48*	3 x 1405cm^{-1} overtone Type IaB, samples *G1-G3*	[15,17,18] This work	–
4169	VN_3H^0	C-H_b	1.48*	3 x 1405cm^{-1} overtone	[15]	–

4224	–	–	–	Brown, green and yellow Type IaB>A and grey IaB	[25]	–
4239	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4240	–	–	–	Brown, green and yellow Type IaB>A and black and grey IaB	[25]	–
4412	–	–	–	Yellow Type IaB>A>Ib Grey Type IaB and IaA	[25]	–
4419	–	–	–	Type Ib	[9]	–
4431	–	–	–	Type Ib	[9]	–
4435	VH_4*	C-H	–	Green and balck Type IaB>A	[25]	**VH_4 –** 4434 [6]
4440	–	–	–	Yellow Type IaB>A>Ib Grey Type IaB	[25]	–
4442	–	–	0.33*	Type IaB, samples *G1-G3*	**This work**	–
4453	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4463	–	–	–	Orange Type IaA+Ib	[25]	–
4464-4465	–	–	0.44*	Type IaB, samples *G1-G3* Yellow Type IaB>A>Ib Grey Type IaB	[25] This work	–
4471	–	–	–	Type Ib	[9]	–
4482	–	–	0.16*	Type IaB, sample *G2*	**This work**	–
4496	VN_3H^0	C-H	7.37*	1405 and 3107cm^{-1} combination band Type IaB, samples *G1-G3* White Type IaB	[4,9,14,25] This work	–
4499	VN_3H^0	C-H	5	1405 and 3107cm^{-1} combination band	[15,17]	–
4522	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4532	–	–	–	Type Ib Yellow Type IaB>A>Ib	[9,25]	–
4535	–	–	–	Orange Type Ib>IaA>B	[25]	–

4545	–	–	–	Chameleon Type IaA>B>Ib	[42]	–
4546	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4572	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4588	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4592	–	–	–	Type Ib	[9]	–
4622	–	–	–	Type Ib	[9]	–
4630	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4668	–	–	–	Yellow Type IaB>A>Ib	[25]	–
4700	–	–	–	Type Ib	[9]	–
4703	VN_4H^0	N-H	–	1470 and 3236cm^{-1} combination band Yellow Type IaB>A>Ib Black and grey Type IaB Grey Type IaA	[17,22,25]	–
4704	VN_4H^0	N-H	0.11*	1470 and 3236cm^{-1} combination band Type IaB, sample *G2*	[17,22]	–
4722	–	–	–	Yellow Type IaB>A>Ib	[25]	–
5068	–	–	–	Type Ib	[9]	–
5555	VN_3H^0	$C\text{-}H_b$	0.04	4 x 1405cm^{-1} overtone	[4,17]	–
5570	VN_3H^0	$C\text{-}H_b$	–	4 x 1405cm^{-1} overtone Green Type IaB>A Grey Type IaB and IaA	[25]	–
5626	–	–	–	Green Type IaB>A Grey Type IaB	[25]	–
5880	VN_3H^0	C-H	0.06	3107 and 2 x 1405cm^{-1} combination band	[17]	–
5888	VN_3H^0	C-H	0.14*	3107 and 2 x 1405cm^{-1} Type IaB, sample *G2*	[4] This work	–

5889	VN_3H^0	C-H		–	3107 and 2 x 1405cm^{-1}	[42]	–
6070	VN_3H^0	C-H_s	0.4		2 x 3107cm^{-1} overtone	[4,17]	–
6212	–	–		–	Chameleon Type IaA>B>Ib	[42]	–
6214	–	–		–	Green/yellow Type IaB>A Black/grey Type IaB Grey/colorless Type IaA	[25,47]	–
6472	–	–		–	Green Type IaB>A Grey Type IaB and IaA	[25]	–
6474	–	–		–	Yellow and black Type IaB	[25]	–
7500	–	–		–	Broad band in H-rich grey diamond	[17]	–
7850	–	–		–	Broad band in H-rich grey diamond	[17]	–
8255	–	–		–	Broad band in H-rich grey diamond	[17]	–
8615	–	–		–	Broad band in H-rich grey diamond	[17]	–
8992	VN_3H^0	C-H	0.4		2 x 3107cm^{-1} and 2 x 1405cm^{-1} combination	[4]	–

In the **assigned defect** and **vibrational mode** columns, assignments are made by the authors based on previous assignments in the literature and similarities with calculated absorption frequencies. Peak-defect assignments made by the authors are marked with an asterisk (*e.g.* VH_4*)

The defect column is left blank where the type of defect (*e.g.* VNH^0) is unknown, in some studies authors present evidence for the general association of H atoms with other impurities (*e.g.* N), this is indicated using square brackets, for example a defect with an unknown configuration but that has been shown to involve some number of H and N atoms is simply indicated by [N][H].

Peak position (absorption frequency, cm^{-1}) may vary slightly depending on the fitting methods used to determine peak centers or other factors such peak shifting due to ^{13}C (or ^{15}N), peaks that are within ±1-2cm^{-1} of each other and that may be representative of the same vibrational mode are highlighted in grey.

Calculated peak positions and associated defects (Tables 2-4. Appendix B) are listed if within ±2cm^{-1} of the observed peak position.

Peak intensities are normalized to the 3107 cm^{-1} peak (100%) in each respective spectrum. Normalized intensities calculated from spectra in this study are indicated with an asterisk (*e.g.* %*). In most cases, peak intensity could only be assessed semi-quantitatively and are labelled as weak (w) or strong (s) (*e.g.* [18]) where they are less than or greater than ~10% the intensity of the most intense H-related peak (often the 3107 cm^{-1} if present).

Peaks at 3343cm^{-1} and 3394cm^{-1} are commonly observed in hydrogen-rich diamonds but also in diamonds that contain no H and do not show any correlation with other H-related peaks. They are not listed here because it is unlikely that they are directly related to *X*-H vibrational modes [26].

Peak positions with a subscripted c (*e.g.* 2920_c) may be due to contamination by grease, glue, or other adhesive materials but are included as they have been associated with an H-related defect in one or more studies.

References associated with each peak position (row) correspond to the study or studies in which the corresponding peak in the infrared has been identified. Where possible, additional details for each peak position (*e.g.* defect configuration and/or vibrational mode) that are not described in the corresponding reference(s) are included.

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