

Chapter 6

Spectral Lines in Diamond-Related Materials: DLC, Lonsdaleite, etc.

In this chapter 84 lines (and bands), which are observed in diamond-related materials (see Sect. 1.2.5), are presented in 8 tables. The entries are assigned to 55 centers. The corresponding defect structure is established for seven centers, is almost certain for 12 centers, and is incomplete or unknown for 36 centers.

Chapter 6 is subdivided into *absorption lines* (Sect. 6.1: 64 **RA** lines in four tables), into *luminescence lines* (Sect. 6.2: 14 **RL** lines in two tables), and into *broad bands* (Sect. 6.3: six **RB** bands in two tables).

6.1 Absorption Lines (RA)

Table 6.1.1.1 Diamond^{79,35}-related materials: absorption lines, far infrared, part 1 (0.04–0.133 eV)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3–6, [Zat01]; Fig. 7, [Zat98]	References
RA0057	57.03	460.0	21.74	...	Si?	SCI?	3.17, 7.30	2 × [Ghe92b]
RA0079	79.35	640.0	156.2	...	Si, H?	SCI?	3.17	[Ghe92b]
RA0085a1	85.17	687.0	14.56	C–H ₂ bend	H	DGB, NGD ; 4 lines a1–a4 (178.5 meV); sp ³ CH ₂ ; C–H ₂ bend, Table 9.3.2.1	3.8, 3.17, 7.173	[Rei98, Ghe92b], [Enc94, Dis87]
RA0087a	86.78	700.0	14.29	C–H ₁ bend	H	PAC ; sp ₁ CH ₁ ; (only in PAC), Table 9.3.2.1, acetylenic C–H ₁	...	[Dis87]
RA0088a1	88.02	710.0	14.09	C–H ₂ bend	H	DGB, NGD ; 4 lines a1–a4 (181.6 meV); olef. sp ² CH ₂ ; C–H ₂ bend, Table 9.3.2.1	3.17, 3.26, 7.5b	[Ghe92b, Fri91a], [Dis87]
RA0091a	90.75	732.0	13.66	...	N?	NDC ; 2 lines a, b (102.9 meV); nitride inclusions	...	[Zat01]
RA0095a1	95.46	770.0	12.99	C–H ₁ bend	H	DGB, NGD ; 2 lines a1, 2 (177.3); arom. sp ² CH ₁ ; Table 9.3.2.1	3.26, 7.5b	[Fri91a, Dis87]
RA0099	99.18	800.0	12.50	...	Si?	SCI ; Si–C interface, 10–100 nm thick, Si–C stretch?	3.17, 7.30	2 × [Ghe92b]

RA0091b	102.9	830.0	12.05	...	N?	NDC; nitride inclusions	...	[Zai01]
RA0104	104.1	840.0	11.90	C-C bend	H	NDC, DLC, PAC; aromatic sp ² , Table 9.3.5	3.29	[Ang65, Dis87]
RA0108a1	107.9	870.0	11.48	C-H ₁ bend	H	DGB, NGD; 2 lines a1, 2 (159.9); olefin.. sp ² CH ₁ ; Table 9.3.2	3.26, 7.5b 3.29	[Fri91a, Ang65, Dis87]
RA0109a	109.1	880.0	11.40	NDC; 3 lines a-c (179.8 meV), carbonate inclusions?	7.9	[Bok86, Zai01]
RA0110	109.7	885.0	11.30	C-C bend	H	DLC, PAC; Table 9.3.5	...	[Dis87]
RA0088a2	114.1	920.0	10.87	C-H ₂ bend	H	DGB; olef. sp ² CH ₂ Table 9.3.2	3.17, 3.18	[Che92b, Jan92]
RA0115a	114.8	926.0	10.80	LON; 5 lines a-e (165.1 meV); lonsdaleite inclusions in polycrystalline diamond	7.27	[Bok86, Zai01]
RA0120	120.3	970.0	10.31	C=C bend	H	NDC, DLC, PAC; olefinic sp ² , Table 9.3.5	3.29	[Ang65, Dis87]
RA0122	121.5	980.0	10.20	...	Si?	SCI	...	[Cel91, Zai01]

(continued)

Table 6.1.1.1 (continued)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3-6, [Zai01]; Fig. 7, [Zai98]	References
RA0085a2	125.2	1010	9.901	C-H ₂ bend	H	DGB, NGD ; aliphatic sp ³ CH ₂ ; Table 9.3.2	3.18, 3.26 7.173	[Jan92, Fri91a] [Enc94, Dis87]
RA0115b	126.4	1020	9.808	LON ; lonsdaleite inclusions in polycrystalline diamond	7.27	[Bok86, Zai01]
RA0133a1	133.3	1075	9.302	C-H ₃ bend	H	DGB, NGD ; 3 lines a1-a3 (185.3 meV); sp ³ CH ₃ ; Table 9.3.2	3.17, 3.18 3.26, 7.5b	[Ghe92b, Jan92] [Fri91a, Dis87]

BAL ballias; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LON* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si-C interface; *PO* powder

Table 6.1.1.2 Diamond-related materials: absorption lines, far infrared, part 2 (0.135–0.18 eV)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3–6. [Zai01]; Fig. 7. [Zai98]	References
RA0109b	135.8	1095	9.130	NDC ; carbonate inclusions?	7.9	[Bok86, Zai01]
RA0115c	136.2	1100	9.103	LON ; lonsdaleite inclusions in polycrystalline diamond	7.27	[Bok86, Zai01]
RA0088a3	137.6	1110	9.009	C–H ₂ bend	H	DGB , olef. sp ² CH ₂ Table 9.3.2	3.17	[Ghe92b, Dis87]
RA0139a	138.5	1117	8.953	...	O?	PO ; (fine grained) surface C=O?; 2 lines a, b (0.1569 eV)	...	[Nov68, Zai01]
RA0144	143.8	1160	8.621	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0085a3	145.1	1170	8.547	C–H ₂ bend	H	NBD, NGD, DGB ; sp ² CH ₂ ; Table 9.3.2	3.8, 3.14 3.18, 7.173	[Rei98, Col82d] [Jan92, Enc94]
RA0115d	151.3	1220	8.194	LON ; lonsdaleite inclusions in polycrystalline diamond	7.27	[Bok86, Zai01]
RA0154	154.4	1245	8.030	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0139b	156.9	1266	7.901	...	O?	PO ; (fine grained) surface C=O vibration?	...	[Nov68, Zai01]
RA0108a2	159.9	1290	7.752	C–H ₁ bend	H	DGB ; olef. sp ² CH ₁ ; Table 9.3.2; DLC ; 159.9 meV	3.14	[Col82d]
RA0161	161.2	1300	7.692	...	O?	PO ; surface diffuse reflection Fourier transform spectra	...	[Mil95, Zai01]

(continued)

Table 6.1.1.2 (continued)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3–6. [Zai01]; Fig. 7. [Zai98]	References
RA0161	161.2	1300	7.692	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0133a2	164.9	1330	7.518	C–H ₃ bend	H	DGB, NGD ; sp ³ CH ₃ ; Table 9.3.2	3.17, 3.18	[Ghe92b, Jan92]
RA0115e	165.1	1332	7.509	LOn ; lonsdaleite inclusions in polycrystalline diamond	3.26, 7.5b 7.27	[Fri91a, Dis87] [Bok86, Zai01]
RA0171a	171.1	1380	7.246	C–H ₁ bend	H	DGB, PO [Che94b]; sp ³ CH ₁ ; Table 9.3.2	3.13, 3.18	[Che94b, Jan92]
RA0175	175.3	1414	7.072	...	NH ₂	PO ; amin terminated, surface diffuse reflection FT spectra	...	[Mil95, Zai01]
RA0095a2	177.3	1430	6.993	C–H ₁ bend	H	DGB , arom. sp ² CH ₁ ; Table 9.3.2	...	[Dis87]
RA0178	178.5	1440	6.944	...	O?	PO ; surface diffuse reflection Fourier transform spectra	...	[Mil95, Zai01]
RA0085a4	178.5	1440	6.944	C–H ₂ bend	H	DGB, NGD ; sp ³ CH ₂ ; Table 9.3.2	3.14, 3.18 7.173	[Col82d, Jan92] [Enc94, Dis87]
RA0109c	179.8	1450	6.900	NDC ; carbonate inclusions?	7.9	[Bok86, Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LOn* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder

Table 6.1.2 Diamond-related materials: absorption lines, mid-infrared (0.18–1.24 eV)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3–6, [Zai01]; Fig. 7, [Zai98]	References
RA0088a4	181.6	1465	6.827	C–H ₂ bend	H	DGB, NBD ; olef. sp ² CH ₂ Table 9.3.2	3.14	[Col82d, Dis87]
RA0133a3	185.3	1495	6.691	C–H ₃ bend	H	DGB, NGD ; sp ³ CH ₃ ; Table 9.3.2	3.17, 3.26 7.5b	[Ghe92b, Fri91a] [Dis87]
RA0188	187.8	1515	6.602	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0191	191.5	1545	6.474	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0196	195.9	1580	6.329	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0200	199.6	1610	6.211	...	O?	PO (KBr)	3.13	[Che94b]
RA0201	200.8	1620	6.173	C–C stretch	H	DLC, PAC ; Table 9.3.5	...	[Dis87]
RA0205a	204.6	1650	6.061	O–H bend?	H ₂ O?	NDC, PO (KBr); 2 lines a, b (419 meV)	3.13, 7.9	[Che94b, Bok86]
RA0216	215.6	1739	5.750	...	O?	DGB (flame grown CVD) or PO (fine grained)	3.10	[Jan91, Zai01]
RA0270	270.3	2180	4.587	C–C stretch	H	PAC ; acetylenic sp ¹ , Table 9.3.5	...	[Dis87]
RA0304	303.7	2450	4.082	...	CO ₂ ?	PO (KBr); var. 285–304 meV	3.13	[Che94b, Zai01]
RA0085b1	353.3	2850	3.509	C–H ₂ stretch	H	DGB, NGD ; 2 lines b1, 2 (361.6 meV); sp ³ CH ₂ ; Table 9.3.3	3.10 = 7.7 7.11, 7.12 7.18, 7.173	[Jan91] 2 × [Dis93] [Phi92, Enc94]

(continued)

Table 6.1.2 (continued)

Line-label	Energy (meV)	Frequ. (cm ⁻¹)	Wavel. (μm)	Name	Impur./defect	Material/comment	Figs. 3-6, [Zai01]; Fig. 7, [Zai98]	References
RA0133b1	356.4	2875	3.478	C-H ₃ stretch	H	DGB, PO ; 2 lines bl, 2 (0.3678 eV); sp ³ CH ₃ ; Table 9.3.3	3.13, 7.11	[Che94b, Dis93]
RA0171b	361.3	2914	3.432	C-H ₁ stretch	H	DGB ; sp ³ CH ₁ ; Table 9.3.3	7.11, 7.12	2 × [Dis93]
RA0085b2	361.6	2917	3.429	C-H ₂ stretch	H	DGB, NGD ; sp ³ CH ₂ ; Table 9.3.3	See line bl	
RA0133b2	367.8	2967	3.370	C-H ₃ stretch	H	DGB, PO ; sp ³ CH ₃ ; Table 9.3.3	3.13, 7.11	[Che94b, Dis93]
RA0088b1	368.5	2972	3.365	C-H ₂ stretch	H	DGB ; 2 lines bl, 2 (375.0 meV); olef. sp ² CH ₂ ; Table 9.3.3	7.11, 7.12	2 × [Dis93, Zai01]
RA0108b	371.9	3000	3.333	C-H ₁ stretch	H	DGB ; olef. sp ² CH ₁ ; Table 9.3.3	...	[Dis93, Zai01]
RA0088b2	375.0	3025	3.306	C-H ₂ stretch	H	DGB ; olef. sp ² CH ₂ ; Table 9.3.3	7.11, 7.12	2 × [Dis93, Zai01]
RA0095b	378.1	3050	3.279	C-H ₁ stretch	H	DGB ; arom. sp ² CH ₁ ; Table 9.3.3	...	[Dis93, Zai01]
RA0087b	412.0	3323	3.009	C-H ₁ stretch	H	DGB ; sp ¹ CH ₁ ; Table 9.3.3	...	[Dis93]
RA0205b	419.0	3380	2.958	O-H stretch?	H ₂ O?	NDC, PO(KBr)	3.13, 7.9	[Che94b, Bok86]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LOM* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si-C interface; *PO* powder

Table 6.1.3 Diamond-related materials: absorption lines, visible: green and blue (2.18–2.58 eV)

Line-label	Energy (eV)	Frequ. (10^3cm^{-1})	Wavel. (nm)	Name	Impur./defect	Comment	Figs. 3–6. [Zai01]; Fig. 7. [Zai98]	References
RA2308	2.308	18.62	537.2	NBD	...	[Bie67, Zai01]
RA2526	2.526	20.38	490.8	CAR ; coincides with ZPL of DAP76 ($V_1N_3^-$), see NL	...	[Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LN* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder

6.2 Luminescence Lines (RL)

Table 6.2.1 Diamond-related materials: luminescence lines, near infrared (1.24–1.77 eV)

Line-label	Energy (eV)	Frequ. (10^3cm^{-1})	Wavel. (nm)	Name	Impur./defect	Material/comment	Figs. 3–6, [Zai01]; Fig. 7, [Zai98]	References
RL1593	1.593	12.85	778.3	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]
RL1635	1.635	13.19	758.3	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]
RL1702	1.702	13.73	728.3	DGB ; coating of laser assisted CVD diam.	...	[Bad97a, Zai01]
RL1736	1.736	14.01	714.0	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LON* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder

Table 6.2.2 Diamond-related materials: luminescence lines, visible: purple to blue (1.77–2.58 eV)

Line-label	Energy (eV)	Frequ. (10^3 cm^{-1})	Wavel. (nm)	Name	Impur./defect	Material/comment	Figs. 3–6, [Zai01]; Fig. 7, [Zai98]	References
RL1773	1.773	14.30	699.3	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]
RL1855	1.855	14.96	668.3	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]
RL1884	1.884	15.20	658.1	LON ; lonsdaleite in natural polycryst. diam.	7.64	[Bok86, Zai01]
RL1949	1.949	15.72	636.1	BAL	...	[Bok86, Zai01]
RL1980	1.980	15.97	626.1	BAL	...	[Bok86, Zai01]
RL2010	2.010	16.21	616.8	BAL	...	[Bok86, Zai01]
RL2501	2.501	20.17	495.7	BAL	...	[Bok86, Zai01]
RL2523	2.523	20.35	491.4	...	N?	NBD ; coincides with ZPL of $^{*}(\text{V}_3\text{Si}_2)^{-}$ -DAP75	...	[Zai01]
RL2526	2.526	20.38	490.8	...	N?	CAR ; coincides with ZPL of $^{*}(\text{V}_1\text{N}_3)^{-}$ -DAP76	...	[Zai01]
RL2537	2.537	20.46	488.7	CAR ; main line of a group of narrow lines	...	[Bok86, Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LON* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder

6.3 Broad Bands (RB)

Table 6.3.1 Diamond-related materials: broad bands, near infrared (1.24–1.77 eV)

Line-label	Energy (eV)	Frequ. (10^3cm^{-1})	Wavel. (nm)	Name	Impur./defect	Material/observation/comment	Figs. 3–6. [Zai01]; Fig. 7. [Zai98]	References
RB1713	1.713	13.82	723.7	DGB; PL ; coating of laser assisted CVD diam.	...	[Bad97a, Zai01]
RB1734	1.734	13.99	715.0	BAL, LON; PL, XL	...	[Bok86, Zai01]
RB1746	1.746	14.08	710.0	LON; PL ; lonsdaleite in nat. polycryst. diam.	7.64	[Bok86, Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LON* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder
Observation: *A* absorption; *CL, EL, IL, PL, XL* luminescence; *PLE* photoluminescence excitation

Table 6.3.2 Diamond-related materials: broad bands, visible; purple to blue (1.77–2.58 eV)

Line-label	Energy (eV)	Frequ. (10^3 cm^{-1})	Wavel. (nm)	Name	Impur./defect	Comment	Figs. 3–6, [Zai01]; Fig. 7, [Zai98]	References
RB1771	1.771	14.29	700.0	NBD ; A; "chameleon" diamond	...	[Fri91a, Zai01]
RB1975	1.975	15.93	627.7	...	N, B?	BAL ; PL	...	[Bok86, Zai01]
RB2460	2.460	19.84	504.0	DLC ; PL ; nondiamond phases, W = 12%	...	[Ber93, Zai01]

BAL ballas; *CAR* carbonado; *DGB* diamond grain boundaries (in CVD diamond); *DLC* diamond-like carbon; *LON* lonsdaleite; *NBD* natural brown diamond; *NDC* natural diamond coat; *NGD* natural gray diamond; *PAC* polymer-like amorphous carbon; *SCI* Si–C interface; *PO* powder
Observation: A absorption; *CL*, *EL*, *IL*, *PL*, *XL* luminescence; *PLE* photoluminescence excitation