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Rotational Analysis of $A^2\Pi_u-X^2\Pi_g$ System of $^{16}\text{O}_2^+$ Cation

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The Doppler-limited absorption spectrum of $^{16}\text{O}_2^+$ cation was observed in the region of 11385–12100 cm^{-1} by optical heterodyne velocity modulation absorption spectroscopy (OH-VMS). The transitions were assigned to the (2, 19), (3, 20), and (5, 21) bands in the second negative system ($A^2\Pi_u-X^2\Pi_g$). All the available lines measured using OH-VMS were global fitted in a nonlinear least-squares fitting procedure, and precise molecular constants (B_v , A_v , D_v , p_v , q_v , γ_v) were obtained for the involved levels.

Key words: Oxygen molecule cation, Second negative system, Rotational resolution

I. INTRODUCTION

The oxygen molecule and its ions (O_2^+) have been extensively studied. The singly ionized molecular ion $^{16}\text{O}_2^+$ has four allowed electric dipole transitions in its low-lying electronic states: the first negative ($b^4\Sigma_g^- - a^4\Sigma_u$) system, the second negative ($A^2\Pi_u - X^2\Pi_g$) system, the Hopeld ($c^4\Pi_u - b^4\Pi_g$) system, and the ($B^2\Sigma_g^- - A^2\Pi_u$) system.

In this work, we mainly focused on the second negative system of $^{16}\text{O}_2^+$. The earlier experimental observation of this system was carried out by Stark in 1914 [1] and was identified until the work of Stevens in 1931 [2]. After that, Albritton *et al.* obtained a series of molecular constants of the states involved in the system through performing a least-squares fitting of 11 bands [3]. Later, a summarization was made by Huber *et al.* [4]. In 1984, Coxon and Haley [5] combined their data obtained from grating spectra with those of Colbourn and Douglas [6] performed a comprehensive least-squares analysis, merged constants were reported. Kong and Hepburn observed high vibrational levels ($v''=6-24$) in the $X^2\Pi_g$ state of $^{16}\text{O}_2^+$ using a coherent extreme ultraviolet (XUV) [7]. In 1997, Prasad *et al.* studied the second negative system using Fourier transform emission spectroscopy in the 15945–30210 cm^{-1} region and a set of equilibrium constants was obtained [8]. Using pulsed field ionization photoelectron technique, Song *et al.* studied the spectrum of $^{16}\text{O}_2^+$ in the 12.05–18.15 eV range and determined the Dunham-type expansion coefficients for vibrational, rotational, and spin-orbit splitting constants [9]. The $A^2\Pi_u - X^2\Pi_g$ transition has been the subject of several more recent spectroscopic studies. Zheng *et al.* observed high res-

olution spectrum of many bands in the $^{16}\text{O}_2^+$ second negative ($A^2\Pi_u - X^2\Pi_g$) system using optical heterodyne velocity modulation spectroscopy (OH-VMS) [10, 11]. Li *et al.* measured the spectrum of two bands ((8, 0) and (8, 1)) in the $A^2\Pi_u - X^2\Pi_g$ system using the laser-induced fluorescence technique [12]. Although the resolution is relatively lower ($\sim 0.2 \text{ cm}^{-1}$), the lines are the only available ones related to the $A^2\Pi_u$ ($v'=8$) and the $X^2\Pi_g$ ($v''=0, 1$) vibrational levels.

In this work, we study our new observation of the absorption spectrum of $^{16}\text{O}_2^+$ in the 11385–12100 cm^{-1} region. We performed a global fitting of all the available rotational resolution lines of second negative system of $^{16}\text{O}_2^+$ studied by optical heterodyne velocity modulation spectroscopy. A total of 1045 lines were included in our global fitting to determine 48 molecular constants.

II. EXPERIMENTS

The experimental setup has been detailedly described in our previous work [13]. A mixture of $^{16}\text{O}_2$ (3 Pa) and He (560 Pa) flowed continuously in the absorption cell. The gas was discharged at the current of 300 mA (peak to peak) at 23 kHz. The incident laser beam was frequency-modulated with an electro optical modulator (EOM) driven at 480 MHz. The acquired signal from a detector was first demodulated by a double-balance mixer at a frequency of 480 MHz and further demodulated by a lock-in amplifier at 23 kHz. The wavelength of the laser beam was determined by an attached wavemeter of the laser system and further calibrated by the iodine spectrum [14] using an additional iodine reference absorption cell.

III. SPECTRAL ANALYSIS AND RESULT

The involved two electronic states $X^2\Pi_g$ and $A^2\Pi_u$ in the second negative system of $^{16}\text{O}_2^+$ belong to Hund's case (a) and Hund's case (b), respectively. The same

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TABLE I Wavenumbers (in cm^{-1}) of rotational lines in the (4, 20) band of the second negative system for $^{16}\text{O}_2^+$. Numbers in the parentheses indicate $(\nu_{\text{cal.}} - \nu_{\text{obs.}}) \times 10^4 \text{ cm}^{-1}$.

J	P_{11}	R_{11}	P_{21}	R_{21}
1.5		12249.3638(21)		
2.5		12250.8473(28)		
3.5	12234.1797(6)	12251.5011(6)	12227.6191(18)	
4.5	12230.6406(13)	12251.9284(23)	12222.2575(31)	12239.8569(2)
5.5	12226.2125(19)	12251.3760(24)	12216.0623(17)	12237.4820(3)
6.5	12221.6177(16)	12250.7127(50)	12209.5486(19)	12234.8613(1)
7.5	12215.9872(50)	12248.9346(54)	12202.0892(17)	12231.2477(40)
8.5	12210.3016(18)	12247.1631(22)	12194.4540(8)	12227.5058(20)
9.5	12203.4485(42)	12244.1561(68)	12185.7589(1)	12222.6484(1)
10.5	12196.6675(34)	12241.2746(10)	12177.0061(9)	12217.7953(30)
11.5	12188.5842(28)	12237.0250(1)	12167.0809(3)	12211.7048(33)
12.5	12180.6987(7)	12233.0372(15)	12157.2160(22)	12205.7321(30)
13.5	12171.3839(28)	12227.5519(14)	12146.0616(15)	12198.4034(2)
14.5	12162.4027(17)	12222.4532(23)	12135.0974(59)	12191.3188(43)
15.5	12151.8573(5)	12215.7207(1)	12122.7096(3)	12182.7551(4)
16.5	12141.7670(11)	12209.5075(16)	12110.6296(1)	12174.5461(14)
17.5	12129.9922(31)	12201.5333(14)		12164.7560(26)
18.5	12118.7936(15)	12194.2041(46)		12155.4281(15)
19.5	12105.7829(9)	12184.9833(38)		12144.3988(7)
20.5		12176.5258(17)		12133.9516(16)
21.5		12166.0602(4)		12121.6906(36)
22.5		12156.4888(28)		12110.1176(20)
23.5		12144.7657(31)		
J	P_{12}	R_{12}	P_{22}	R_{22}
5.5			12038.8742(40)	12060.2957(38)
6.5			12032.0262(16)	12057.3370(21)
7.5	12038.3188(43)		12024.4257(26)	12053.5711(48)
8.5	12032.2030(28)		12016.3485(51)	12049.3915(127)
9.5	12025.1646(35)		12007.4790(35)	12044.3630(23)
10.5	12017.8479(24)		11998.1909(23)	12038.9776(9)
11.5	12009.5454(10)		11988.0437(19)	12032.6616(49)
12.5	12001.0346(24)	12053.3786(24)	11977.5531(26)	12026.0685(18)
13.5	11991.4663(1)	12047.6336(34)	11966.1402(26)	12018.4800(33)
14.5	11981.7577(7)	12041.8113(30)	11954.4471(17)	12010.6712(6)
15.5	11970.9202(0)	12034.7880(37)	11941.7676(58)	12001.8201(20)
16.5	11960.0193(47)	12027.7576(30)	11928.877(11)	11992.7989(28)
17.5	11947.9035(53)	12019.4548(33)		11982.6667(63)
18.5	11935.8085(15)	12011.2165(22)		11972.4412(3)
19.5	11922.4292(44)	12001.6330(18)		
20.5	11909.1355(20)	11992.1876(3)		
21.5		11981.3223(10)		
22.5		11970.6704(31)		

$^2\Pi$ case (a) matrix elements for the two states were employed in Refs.[5, 8, 10–12]. The A_D and γ_v cannot be determined simultaneously without isotopic parameters. Generally one of them was fixed to zero and the other was fitted. Prasad *et al.* fixed γ_v at zero to fit A_D

[8] while Coxon *et al.* fixed A_D to fit γ_v [5]. We fit γ_v in this work. For each vibrational level, the constants of T_v , A_v , B_v , D_v , p_v , q_v , and γ_v are fitted. Using OH-magnetic rotational (MR)-VMS, Zheng *et al.* recorded the (2, 18), (4, 20), (6, 20), (3, 18), (3, 19), and (4,

TABLE II Wavenumbers (in cm^{-1}) of rotational lines in the (2, 19) band of the second negative system for $^{16}\text{O}_2^+$.

J	P_{11}	R_{11}	P_{21}	R_{21}
0.5		11889.2437(22)		
1.5	11881.7112(30)	11891.1331(32)		11883.6890(35)
2.5	11878.9678(41)	11892.7587(1)		
3.5	11875.6880(23)	11893.6430(58)	11868.2418(5)	11882.6485(18)
4.5	11872.2090(35)	11894.3102(19)	11862.9876(1)	
5.5	11867.9114(2)	11894.0857(29)	11856.9203(43)	11879.3004(54)
6.5	11863.4825(27)	11893.7510(9)	11850.5569(41)	11876.9578(32)
7.5	11858.0871(58)	11892.3880(30)	11843.2940(5)	11873.6959(22)
8.5	11852.6470(17)	11891.0251(15)		11870.3154(42)
9.5	11846.1190(34)	11888.5159(8)	11827.4300(13)	11865.8833(17)
10.5	11839.6570(13)	11886.1259(32)	11818.9480(51)	11861.4482(27)
11.5	11831.9880(2)	11882.4607(12)		11855.8657(2)
12.5		11879.0335(53)	11789.0830(22)	11850.3875(14)
13.5		11874.2119(15)	11778.5210(99)	11843.6580(145)
14.5		11869.7319(48)	11766.6800(56)	11837.1150(43)
15.5	11797.1950(121)	11863.7591(31)		11829.2222(15)
16.5		11858.2462(31)	11755.0420(53)	11821.6553(43)
17.5		11851.1155(52)	11741.9870(165)	11812.6030(65)
18.5	11765.9500(55)	11844.5440(8)	11729.3450(184)	11803.9854(46)
19.5	11753.7060(70)		11715.1940(89)	11793.7620(90)
20.5	11742.0620(91)			11784.1123(45)
21.5				11772.7434(25)
22.5	11715.9850(143)			11762.0190(119)
23.5	11701.4380(96)			11749.4990(120)
24.5		11790.1970(281)		
J	P_{12}	R_{12}	P_{22}	R_{22}
2.5		11714.2400(70)	11694.5080(96)	
3.5	11697.1070(36)		11689.6450(140)	
4.5				11702.5680(19)
5.5	11688.9880(64)	11715.1530(2)		
6.5		11714.4670(125)		11697.6880(25)
7.5	11678.6500(96)			11694.2740(24)
8.5				11690.4360(104)
9.5				11685.8380(88)
10.5		11705.5260(30)		11680.8570(57)
11.5		11701.6310(16)	11628.5210(66)	11675.0320(33)
14.5	11624.6940(62)	11687.2440(118)		
15.5			11583.8450(58)	
16.5		11674.6190(28)		
17.5			11558.0440(86)	
23.5		11611.6390(2)		

19) bands in the $^{16}\text{O}_2^+$ second negative ($A^2\Pi_u-X^2\Pi_g$) system [10, 11]. In this work, the (2, 19), (3, 20), and (5, 21) bands are newly measured and the (4, 20) band was re-measured. The wavenumbers of rotational lines in these bands are shown in Tables I–IV. All the above bands except (5, 21) are included in a global fitting using the PGOPHER [15].

Figure 1 shows the interconnections of the vibrational levels. The new measured bands make the vibrational levels have good interconnection and make the global fit reasonable. The (5, 21) is individual fitted since $v'=5$ and $v''=21$ levels do not have good interconnection with the other levels.

TABLE III Wavenumbers (in cm^{-1}) of rotational lines in the (5, 21) band of the second negative system for $^{16}\text{O}_2^+$.

J	P_{11}	R_{11}	P_{21}	R_{21}
1.5		11798.1740(51)		11792.0990(12)
2.5	11786.4600(39)	11799.6420(22)	11782.0570(64)	11791.7210(16)
3.5	11783.2530(16)		11777.1790(13)	11790.5630(50)
4.5	11779.7860(50)		11771.8660(2)	11789.0490(24)
5.5	11775.4160(30)		11765.7090(9)	11786.6390(61)
6.5	11770.8800(60)			11784.0250(31)
7.5	11765.2930(14)	11797.5520(46)		
8.5	11759.6800(13)		11744.3290(36)	11776.6610(16)
9.5	11752.8590(0)	11792.7090(92)	11735.6960(21)	11771.7870(24)
10.5	11746.1510(34)	11789.8260(45)		11766.9570(13)
11.5	11738.1080(14)	11785.5160(5)	11717.1950(12)	11760.8500(56)
12.5	11730.3090(11)	11781.5340(9)	11707.4383(65)	11754.9110(50)
13.5	11721.0320(9)	11775.9870(32)	11696.3740(28)	11747.5790(63)
14.5	11712.1340(26)	11770.9090(42)		11740.5390(40)
15.5	11701.6310(4)	11764.1140(62)		
16.5	11691.6426(37)	11757.9270(4)		11723.8110(29)
17.5		11749.8980(38)		
18.5	11668.817 (37)	11742.6030(41)	11634.6990(8)	
20.5				11683.3420(31)
21.5			111589.8875(73)	
J	P_{12}	R_{12}	P_{22}	R_{22}
1.5				11617.3120(16)
3.5	11608.2697(34)		11602.2085(66)	
4.5			11596.6674(20)	11613.8465(41)
5.5		11624.7430(150)	11590.3901(135)	11611.3460(72)
6.5		11623.7450(106)	11583.6550(109)	11608.3978(46)
7.5		11621.7720(52)	11576.1003(20)	11604.6191(28)
8.5		11619.5930(90)	11568.1459(51)	11600.4678(102)
9.5		11616.3427(116)	11559.3294(0)	
10.5	11569.2910(120)		11550.1635(95)	
11.5	11561.0179(112)		11540.0899(64)	
12.5	11552.6265(142)	11603.8387(6)	11529.7435(56)	11577.2264(60)
13.5	11543.0760(64)		11518.4092(5)	11569.6241(3)
14.5	11533.4855(85)			11561.8852(71)
15.5			11494.2719(29)	11553.0325(58)
16.5			11481.5677(118)	11544.1033(26)
17.5	11499.8310(78)	11598.0257(30)	11467.6960(2)	11533.9736(75)
18.5	11487.9012(85)	11569.8376(9)	11453.7930(32)	11523.8624(148)
19.5	11474.5435(56)	11561.6911(42)	11438.6790(5)	11512.4390(49)
20.5		11542.6989(65)		
21.5	11446.8090(44)	11531.7596(74)		

What should be mentioned is that when $v' \leq 6$, the branches' names are different from those exported from PGOPHER and the subscript label i of P_{ij} and R_{ij} bands should be changed. For example, the P_{22} band in PGOPHER corresponds to the actual P_{12} band. All the lines are fitted with the same weight and the standard deviation of the global fitting is 0.0043 cm^{-1} , which is

less than the experimental uncertainty of 0.007 cm^{-1} . The estimated constants along with one standard deviation errors are listed in Table V for the $X^2\Pi_u$ state and in Table VI for the $A^2\Pi_u$ state, respectively. In Table V, the constants for $v''=18, 19, 20$ came from the global fitting with $T_{v''=18}$ fixed at the value in Ref.[8]. In the previous analysis [10, 11], the line positions are

TABLE IV Wavenumbers (in cm^{-1}) of rotational lines in the (3, 20) band of the second negative system for $^{16}\text{O}_2^+$.

J	P_{11}	R_{11}	P_{21}	R_{21}
0.5		11458.1667(16)		11452.6693(78)
1.5		11460.0362(6)		11453.0002(99)
2.5	11448.0680(30)	11461.6436(8)	11442.5510(147)	11452.8252(22)
3.5			11437.8170(105)	11451.9020(26)
4.5	11441.4350(34)			11450.6170(62)
5.5	11437.1930(44)	11462.8657(33)	11426.6310(162)	11448.5120(26)
6.5	11432.8240(6)	11462.5072(1)	11420.3130(2)	
7.5	11427.4940(198)	11461.1024(39)	11413.1252(20)	11442.8980(77)
8.5	11422.0950(43)	11459.7236(19)	11405.7671(30)	11439.5190(76)
9.5	11415.6141(34)	11457.1738(13)	11397.4184(24)	11435.0970(10)
10.5	11409.2268(0)	11454.7680(43)	11389.0269(29)	11430.6780(29)
11.5	11401.6023(36)	11451.0687(17)	11379.5253(47)	11425.0980(12)
12.5	11394.1919(19)	11447.6318(38)		11419.6464(11)
13.5	11385.4315(11)	11442.7802(12)		11412.9098(22)
14.5		11438.3095(25)		11406.4241(26)
15.5		11432.3034(34)		11398.5349(24)
16.5		11426.7964(84)		11391.0097(2)
17.5				11381.9720(28)
18.5		11413.0886(45)		
19.5		11404.7684(54)		
20.5		11397.1825(5)		
21.5		11387.7031(6)		
J	P_{12}	R_{12}	P_{22}	R_{22}
1.5		11278.4740		11271.4505
2.5	11269.1683 ^a	11279.9558	11260.8806	11271.1416
3.5	11266.3825	11280.7346	11256.0769	11270.1535
4.5	11263.1004	11281.1558	11250.6452	11268.6457
5.5	11259.4594	11280.7849	11244.5353	11266.4348
6.5	11255.1165	11280.1009	11237.9079	11263.7725
7.5	11250.4181	11278.5574	11230.5790	11260.3612
8.5	11244.9291	11276.7545	11222.8017	11256.5580
9.5	11239.1301	11274.0297	11214.2772	11251.9542
10.5	11232.4733	11271.1027	11205.3651	11247.0159
11.5	11225.5615	11267.1927	11195.6543	11241.2232
12.5	11217.7298	11263.1394	11185.6145	11235.1529
13.5	11209.7013	11258.0418	11174.7224	11228.1734
14.5	11200.6919	11252.8612	11163.5595	11220.9732
15.5	11191.5460	11246.5747	11151.4894	11212.8082
16.5	11181.3578	11240.2668	11139.2068	11204.4797
17.5	11171.0949	11232.7903	11125.9614	11195.1304
18.5	11159.7279	11225.3553	11112.5622	11185.6752
19.5	11148.3492	11216.6881	11098.1439	11175.1424
20.5	11135.8038	11208.1266	11083.6309	11164.5620
21.5	11123.3110	11198.2683	11068.0419	11152.8468

^a The calculated positions.

TABLE V Molecular constants (in cm^{-1}) for $X^2\Pi_g$ state of $^{16}\text{O}_2^+$.

Constants ^a	$v''=18$	$v''=19$	$v''=20$	$v''=21$
T_v	29659.556 ^b	30940.53921(72) ^c	32187.4863(12)	33399.4523(13)
B_v	1.3166795(100)	1.29491084(973)	1.2728851(127)	1.2506177(508)
A_v	182.54985(72)	180.89079(55)	179.11935(81)	177.2018(14)
$\gamma_v \times 10^2$	3.527(22)	4.036(16)	4.537(34)	5.176(67)
$p_v \times 10^2$	1.6250(90)	1.6118(74)	1.5826(86)	1.492(34)
$q_v \times 10^4$	0.857(95)	0.736(74)	0.30(17)	2.24(54)
$D_v \times 10^6$	6.3610(119)	6.4737(114)	6.594(21)	6.9781(853)

^a Constants for $v''=18, 19, 20$ based on the global fitting and constants for $v''=21$ based on the individual band fit.

^b Value was fixed.

^c Numbers in parentheses denote one standard deviation in unit of the last quoted digit.

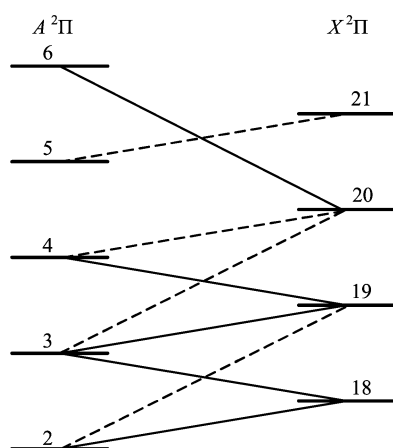


FIG. 1 Interconnections of the vibrational levels. Solid lines show the bands adopted from the Refs.[10, 11] and the dashed lines show the bands measured in this work. The (5, 21) band was not included in the global fitting.

weighted according to $(\nu_{\text{cal.}} - \nu_{\text{obs.}})$. Since the experimental uncertainties are the same for all the lines, the line positions were not weighted in this work. The precision is almost the same as the previous result and the constants are consistent with the previous ones (in 3σ). The (4, 20) band is corrected and the (3, 20) band was added and thus the constants for $v''=20$ should be more reliable. In Table VI, the constants for $v'=2, 3, 4, 6$ come from the global fitting. We fit γ_v and fixed A_D at zero as Coxon *et al.* did [5]. The precision of our constants is better than Coxon *et al.*'s. Prasad *et al.* [8] fitted the constants for $v'=2, 3, 4, 5$ using Coxon *et al.*'s line positions, they fitted A_D and fixed γ_v at zero for these levels. Though our line positions are obtained at higher resolution, our precision is close to Prasad *et al.*'s [8]. The reason is that Prasad *et al.*'s line positions have bigger rotational numbers (>30.5) than ours (≈ 22.5). The (5, 21) band including 106 lines is fitted and the reported standard deviation is 0.0058 cm^{-1} . The constants of $v''=21$ are newly reported and the constants of $v'=5$ are consistent with those in Refs.[5, 8].

IV. CONCLUSION

The rotational resolution lines positions of the $A^2\Pi_u$ - $X^2\Pi_g$ system of $^{16}\text{O}_2^+$ are reported and assigned in the 11385 – 12100 cm^{-1} region. The (4, 20) band is corrected and the (2, 19), (3, 20), and (5, 21) bands are first observed. A global fitting including 8 bands is performed and precise molecular constants are obtained for the involved levels. The line positions in 11385 – 14000 cm^{-1} of the system are now available. When line positions in other spectral region are available, these reported positions may be used to do a comprehensive and systematic analysis for the system, such as obtaining equilibrium molecular constants based on a global fitting.

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TABLE VI Molecular constants (in cm^{-1}) for $A^2\Pi_u$ state of $^{16}\text{O}_2^+$.

Constants		$v'=2$	$v'=3$	$v'=4$	$v'=5$	$v'=6$
T_v	Fitted	42734.83370(76) ^a	43551.85147(59)	44341.59584(91)	45103.6477 ^b	45839.3691(18)
	Ref.[8]	42734.4552(40)	43551.5277(40)	44341.2006(29)	45103.6477(53)	
	Ref.[5]	42733.92(13)	43550.92(13)	44340.57(13)	45103.03(13)	45838.27(12)
B_v	Fitted	1.0122870(103)	0.99206396(936)	0.9716480(104)	0.9510106(486)	0.9301201(203)
	Ref.[8]	1.012328(14)	0.992107(22)	0.971653(18)	0.951083(19)	
	Ref.[5]	1.01226(3)	0.99203(3)	0.97155(4)	0.95094(4)	0.93005(6)
A_v	Fitted	-2.7715(25)	-2.2912(19)	-1.7031(32)	-0.9933(50)	-0.175(13)
	Ref.[8]	-2.7782(53)	-2.3054(89)	-1.6913(77)	-0.9407(96)	
	Ref.[5]	-2.780(15)	-2.277(13)	-1.689(24)	-0.994(25)	-0.22(6)
$\gamma_v \times 10^2$	Fitted	-0.0222(48)	0.0935(30)	0.2662(47)	0.479(11)	0.837(10)
	Ref.[5]	0.018(22)	0.097(17)	0.285(28)	0.511(28)	0.91(4)
$p_v \times 10^2$	Fitted	-2.572(12)	-2.7993(91)	-3.075(11)	-3.620(49)	-4.105(17)
	Ref.[8]	-2.649(22)	-2.816(32)	-3.065(25)	-3.466(34)	
	Ref.[5]	-2.61(5)	-2.80(4)	-3.07(6)	-3.50(6)	-4.09(8)
$q_v \times 10^4$	Fitted	-0.048(21)	-0.205(12)	-0.425(19)	-0.827(55)	-1.227(42)
	Ref.[8]		-0.285(42)	-0.464(31)	-0.871(68)	
	Ref.[5]	-0.09(8)	-0.24(6)	-0.38(10)	-0.68(11)	-1.08(15)
$D_v \times 10^6$	Fitted	6.245(12)	6.3758(103)	6.543(13)	6.8311(786)	6.863(45)
	Ref.[8]	6.254(12)	6.463(21)	6.566(18)	6.741(25)	
	Ref.[5]	6.28(3)	6.43(2)	6.53(3)	6.68(3)	6.92(6)

^a Numbers in parentheses denote one standard deviation in unit of the last quoted digit.

^b Value was fixed at the one of Ref.[8].

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