

TABLE I. Comparison between calculated, *ab initio* and refined, and experimental spectroscopic parameters of OC⁷⁴Se, OC⁷⁶Se, OC⁷⁷Se, OC⁷⁸Se, OC⁸⁰Se, OC⁸²Se. (*p*) and (*v*) mean perturbative and variational calculations, respectively. Vibrational frequencies in cm⁻¹, rotational constants and *l*-doubling costants in MHz.

	16-12-74	16-12-76	16-12-77	16-12-78	16-12-80	16-12-82
B_{00^00}						
exp.	4095.82780(38) ^a	4068.44316(26) ^a	4055.24272(25) ^a	4042.41682(27) ^a	4017.65252(29) ^d	3994.06611(27) ^a
<i>ab in.</i>	4075.6	4048.4	4035.2	4022.4	3997.8	3974.3
ref. (<i>p</i>)	4095.56	4068.17	4054.97	4042.14	4017.38	3993.79
ref. (<i>v</i>)	-	-	-	-	4015.09	-
ν_{10^00}						
exp.	2023.68210(34) ^b	2023.62658(13) ^b	2023.60058(15) ^b	2023.57448(11) ^b	2023.529850(17) ^b	2023.47923(14) ^b
<i>ab in.</i>	2040.5	2040.4	2040.4	2040.4	2040.3	2040.3
ref. (<i>p</i>)	2023.610	2023.561	2023.538	2023.515	2023.471	2023.429
ref. (<i>v</i>)	-	-	-	-	2023.767	-
B_{10^00}						
exp.	4073.58(16) ^b	4046.385(39) ^b	4033.246(48) ^b	4020.478(33) ^b	3995.865(19) ^b	3972.471(45) ^b
<i>ab in.</i>	4053.9	4026.8	4013.7	4001.0	3976.5	3953.2
ref. (<i>p</i>)	4073.61	4046.38	4033.26	4020.51	3995.99	3972.43
ref. (<i>v</i>)	-	-	-	-	3993.24	-
ν_{01^10}						
exp.	-	463.23582(9) ^a	463.17873(12) ^a	463.12311(4) ^a	463.015666(25) ^a	462.91350(8) ^a
<i>ab in.</i>	481.3	481.2	481.1	481.1	480.9	480.8
ref. (<i>p</i>)	463.542	463.423	463.365	463.309	463.201	463.098
ref. (<i>v</i>)	-	-	-	-	462.958	-
B_{01^10}						
exp.	-	4075.4356(24) ^a	4062.2046(18) ^a	4049.36807(22) ^a	4024.56066(19) ^a	4000.9573(39) ^a
<i>ab in.</i>	4082.2	4054.9	4041.7	4028.9	4004.3	3980.7
ref. (<i>p</i>)	4102.67	4075.23	4062.01	4049.16	4024.35	4000.72
ref. (<i>v</i>)	-	-	-	-	4021.94	-
q_{01^10}						
exp.	-	3.240 ^{b,*}	3.208 ^{b,*}	3.20873(45) ^a	3.17228(37) ^a	3.1775(33) ^a
<i>ab in.</i>	3.19	3.15	3.14	3.12	3.08	3.05
ref. (<i>p</i>)	3.27	3.23	3.21	3.19	3.16	3.12
ref. (<i>v</i>)	-	-	-	-	3.15	-
ν_{00^01}						
exp.	-	647.810529(19) ^a	646.699141(19) ^a	645.617878(12) ^a	643.526287(7) ^a	641.528578(25) ^a
<i>ab in.</i>	656.8	654.5	653.4	652.3	650.2	648.2
ref. (<i>p</i>)	650.273	647.973	646.862	645.781	643.690	641.693
ref. (<i>v</i>)	-	-	-	-	643.566	-
B_{00^01}						
exp.	-	4054.94602(42) ^a	4041.80881(39) ^a	4029.04177(27) ^a	4004.39295(34) ^a	3980.91437(62) ^a
<i>ab in.</i>	4061.7	4034.6	4021.5	4008.8	3984.3	3960.9
ref. (<i>p</i>)	4082.42	4055.16	4042.02	4029.25	4004.60	3981.12
ref. (<i>v</i>)	-	-	-	-	4002.38	-
ν_{11^10}						
exp.	-	-	-	-	2480.652435(34) ^d	-
<i>ab in.</i>	2516.1	2515.9	2515.8	2515.7	2515.6	2515.4
ref. (<i>p</i>)	2481.188	2481.023	2480.943	2480.866	2480.717	2480.575
ref. (<i>v</i>)	-	-	-	-	2480.966	-
B_{11^10}						
exp.	-	-	-	-	4002.9970(13) ^d	-
<i>ab in.</i>	4060.5	4033.3	4020.2	4007.5	3983.0	3959.6
ref. (<i>p</i>)	4080.72	4053.44	4040.30	4027.52	4002.86	3979.36
ref. (<i>v</i>)	-	-	-	-	4001.48	-
ν_{10^01}						
exp.	-	2670.03829(18) ^b	2668.90192(25) ^b	2667.79553(14) ^b	2665.6604418(72) ^d	2663.61422(20) ^b
<i>ab in.</i>	2696.8	2694.4	2693.3	2692.2	2690.0	2687.9
ref. (<i>p</i>)	2672.579	2670.231	2669.097	2667.994	2665.859	2663.822
ref. (<i>v</i>)	-	-	-	-	2665.739	-
B_{10^01}						
exp.	-	4033.2827(21) ^b	4020.154(11) ^b	4007.4571(39) ^b	3982.92417(30) ^d	3959.5904(93)
<i>ab in.</i>	4040.0	4013.0	4000.0	3987.4	3963.0	3939.9
ref. (<i>p</i>)	4060.47	4032.37	4020.30	4007.61	3983.10	3959.76
ref. (<i>v</i>)	-	-	-	-	3981.24	-

	16-12-74	16-12-76	16-12-77	16-12-78	16-12-80	16-12-82
$\nu_{01^1 1}$						
exp.	-	-	-	-	1102.691994(22) ^{d,*}	-
<i>ab in.</i>	1134.3	1131.9	1130.7	1129.6	1127.4	1125.3
ref. (p)	1109.711	1107.323	1106.170	1105.048	1102.877	1100.804
ref. (v)	-	-	-	-	1102.762	-
$B_{01^1 1}$						
exp.	-	-	-	-	4011.6827(2) ^a	-
<i>ab in.</i>	4068.3	4041.1	4028.0	4015.3	3990.7	3967.3
ref. (p)	4089.53	4062.22	4049.05	4036.26	4011.57	3988.04
ref. (v)	-	-	-	-	4008.98	-
$\nu_{20^0 0}$						
exp.	-	-	-	4023.6267(16) ^c	4023.5376809(49) ^d	-
<i>ab in.</i>	4059.6	4059.4	4059.4	4059.3	4059.2	4059.2
ref. (p)	4023.652	4023.550	4023.500	4023.453	4023.361	4023.274
ref. (v)	-	-	-	-	4024.320	-
$B_{20^0 0}$						
exp.	-	-	-	3998.64(78) ^c	3973.92823(16) ^d	-
<i>ab in.</i>	4032.2	4005.2	3992.2	3979.6	3955.3	3932.0
ref. (p)	4051.66	4024.59	4011.55	3998.87	3974.39	3951.08
ref. (v)	-	-	-	-	3972.25	-
$\nu_{02^0 0}$						
exp.	-	928.48468(6) ^a	928.35765(8) ^a	928.23437(3) ^a	927.996659(28) ^a	927.77006(5) ^a
<i>ab in.</i>	962.1	961.9	961.7	961.6	961.4	961.1
ref. (p)	928.643	928.378	928.251	928.127	927.888	927.661
ref. (v)	-	-	-	-	927.700	-
$B_{02^0 0}$						
exp.	-	4081.62246(85) ^a	4068.3815(11) ^a	4055.5186(19) ^a	4030.67528(60) ^a	4007.0139(17) ^a
<i>ab in.</i>	4088.8	4061.4	4048.3	4035.4	4010.7	3987.2
ref. (p)	4109.78	4082.30	4069.05	4056.17	4031.32	4007.64
ref. (v)	-	-	-	-	4028.01	-
$\nu_{02^2 0}$						
exp.	-	-	-	-	926.6271(20) ^a	-
<i>ab in.</i>	962.5	962.2	962.2	962.0	961.8	961.6
ref. (p)	927.778	927.539	927.424	927.313	927.098	926.893
ref. (v)	-	-	-	-	926.500	-
$B_{02^2 0}$						
exp.	-	4082.36004(95) ^a	4069.1138(13) ^a	4056.2424(11) ^a	4031.39271(25) ^a	4007.72170(75) ^a
<i>ab in.</i>	4088.8 *	4061.4 *	4048.3 *	4035.4 *	4010.7 *	3987.2 *
ref. (p)	4109.78 *	4082.30 *	4069.05 *	4056.17 *	4031.32 *	4007.64 *
ref. (v)	-	-	-	-	4028.71	-
$\nu_{00^0 2}$						
exp.	-	-	-	-	1281.8676516(94) ^d	-
<i>ab in.</i>	1308.1	1303.5	1301.2	1299.1	1294.9	1290.9
ref. (p)	1294.782	1290.225	1288.024	1285.882	1281.738	1277.781
ref. (v)	-	-	-	-	1281.295	-
$B_{00^0 2}$						
exp.	-	-	-	4015.4461(16) ^a	3990.91871(33) ^a	-
<i>ab in.</i>	4047.8	4020.8	4007.8	3995.2	3970.8	3947.5
ref. (p)	4069.27	4042.14	4029.06	4016.35	3991.82	3968.44
ref. (v)	-	-	-	-	3988.74	-

^a Ref. [1]

^b Ref. [2]

^{b,*} Ref. [2]: values recalculated from the data given in Ref. [3].

^c Ref. [4]

^d Ref. [5]

^{d,*} Ref. [5]: effective state parameters evaluated from a global analysis.

* Identical to the corresponding values for the vibrational level 02⁰0 since the perturbation method used does not include *l*-doubling coupling.

TABLE II. Comparison between calculated, *ab initio* and refined, and experimental spectroscopic parameters of $\text{O}^{13}\text{C}^{74}\text{Se}$, $\text{O}^{13}\text{C}^{76}\text{Se}$, $\text{O}^{13}\text{C}^{77}\text{Se}$, $\text{O}^{13}\text{C}^{78}\text{Se}$, $\text{O}^{13}\text{C}^{80}\text{Se}$, $\text{O}^{13}\text{C}^{82}\text{Se}$. (*p*) and (*v*) mean perturbative and variational calculations, respectively. Vibrational frequencies in cm^{-1} , rotational constants and *l*-doubling costants in MHz.

	16-13-74	16-13-76	16-13-77	16-13-78	16-13-80	16-13-82
B_{00^00}						
exp.	4059.23718(55) ^a	4031.47843(29) ^a	4018.09727(38) ^a	4005.09632(38) ^a	3979.99214(32) ^a	3956.07864(47) ^a
<i>ab in.</i>	4039.1	4011.4	3998.1	3985.2	3960.2	3936.4
ref. (<i>p</i>)	4058.92	4031.16	4017.78	4004.78	3979.67	3955.76
ref. (<i>v</i>)	-	-	-	-	3977.45	-
ν_{10^00}						
exp.	-	1973.92147(47) ^b	1973.89596(52) ^b	1973.87138(12) ^b	1973.82425(8) ^b	1973.77905(36) ^b
<i>ab in.</i>	1990.5	1990.4	1990.4	1990.4	1990.4	1990.3
ref. (<i>p</i>)	1974.121	1974.075	1974.052	1974.030	1973.988	1973.948
ref. (<i>v</i>)	-	-	-	-	1974.261	-
B_{10^00}						
exp.	-	4010.61(26) ^b	3997.46(45) ^b	3984.480(54) ^b	3959.615(36) ^b	3936.21(24) ^b
<i>ab in.</i>	4018.7	3991.3	3978.0	3965.1	3940.3	3916.6
ref. (<i>p</i>)	4038.35	4010.75	3997.44	3984.51	3959.55	3935.76
ref. (<i>v</i>)	-	-	-	-	3957.26	-
ν_{01^10}						
exp.	-	-	-	-	-	-
<i>ab in.</i>	466.9	466.7	466.7	466.6	466.5	466.4
ref. (<i>p</i>)	449.604	449.481	449.421	449.363	449.262	449.146
ref. (<i>v</i>)	-	-	-	-	449.005	-
B_{01^10}						
exp.	-	-	-	-	3986.45073(28) ^a	-
<i>ab in.</i>	4045.2	4017.6	4004.2	3991.2	3966.2	3942.4
ref. (<i>p</i>)	4065.57	4037.76	4024.36	4011.33	3986.19	3962.23
ref. (<i>v</i>)	-	-	-	-	3983.79	-
q_{01^10}						
exp.	-	-	-	-	3.19907(56) ^a	-
<i>ab in.</i>	3.22	3.18	3.16	3.14	3.11	3.07
ref. (<i>p</i>)	3.31	3.26	3.24	3.22	3.19	3.15
ref. (<i>v</i>)	-	-	-	-	3.15	-
ν_{00^01}						
exp.	-	-	-	-	637.26827(8) ^a	-
<i>ab in.</i>	650.6	648.2	647.1	645.9	643.8	641.7
ref. (<i>p</i>)	644.070	641.733	640.603	639.505	637.379	635.349
ref. (<i>v</i>)	-	-	-	-	637.257	-
B_{00^01}						
exp.	-	-	-	-	3966.78697(41) ^a	-
<i>ab in.</i>	4025.2	3997.7	3984.5	3971.6	3946.7	3923.1
ref. (<i>p</i>)	4045.85	4018.22	4004.90	3991.95	3966.97	3943.16
ref. (<i>v</i>)	-	-	-	-	3965.36	-
ν_{10^01}						
exp.	-	-	-	-	2610.0047(10) ^c	-
<i>ab in.</i>	2640.8	2638.4	2637.2	2636.1	2633.9	2631.8
ref. (<i>p</i>)	2617.238	2614.852	2613.700	2612.579	2610.411	2608.340
ref. (<i>v</i>)	-	-	-	-	2610.284	-
B_{10^01}						
exp.	-	-	-	-	3946.675(35) ^c	-
<i>ab in.</i>	4004.9	3977.6	3964.4	3951.6	3926.8	3903.3
ref. (<i>p</i>)	4025.28	3997.80	3984.56	3971.69	3946.84	3923.17
ref. (<i>v</i>)	-	-	-	-	3945.27	-
ν_{02^00}						
exp.	-	-	-	-	-	-
<i>ab in.</i>	933.2	932.9	932.8	932.7	932.4	932.2
ref. (<i>p</i>)	900.575	900.301	900.170	900.042	899.796	899.561
ref. (<i>v</i>)	-	-	-	-	899.606	-
B_{02^00}						
exp.	-	-	-	-	3992.1704(16) ^a	-
<i>ab in.</i>	4051.4	4023.7	4010.3	3997.3	3972.2	3948.4
ref. (<i>p</i>)	4072.22	4044.36	4030.94	4017.89	3992.70	3968.70
ref. (<i>v</i>)	-	-	-	-	3989.94	-

^a Ref. [1]

^b Ref. [2]

^c Ref. [6]

TABLE III. Comparison between calculated, *ab initio* and refined, and experimental spectroscopic parameters of $^{18}\text{OC}^{74}\text{Se}$, $^{18}\text{OC}^{76}\text{Se}$, $^{18}\text{OC}^{77}\text{Se}$, $^{18}\text{OC}^{78}\text{Se}$, $^{18}\text{OC}^{80}\text{Se}$, $^{18}\text{OC}^{82}\text{Se}$. (*p*) and (*v*) mean perturbative and variational calculations, respectively. Vibrational frequencies in cm^{-1} , rotational constants and *l*-doubling costants in MHz.

	18-12-74	18-12-76	18-12-77	18-12-78	18-12-80	18-12-82
$B_{00^0 0}$						
exp.	3799.05008(37) ^a	3772.29886(21) ^a	3759.40347(49) ^a	3746.87476(37) ^a	3722.68279(28) ^a	3699.63943(42) ^a
<i>ab in.</i>	3780.5	3753.9	3741.0	3728.6	3704.5	3681.6
ref. (<i>p</i>)	3798.84	3772.08	3759.19	3746.66	3722.46	3699.42
ref. (<i>v</i>)	-	-	-	-	3720.30	-
$\nu_{10^0 0}$						
exp.	-	-	-	1983.606507(4) ^c	1983.551081(4) ^c	-
<i>ab in.</i>	1999.9	1999.8	1999.8	1999.7	1999.7	1999.6
ref. (<i>p</i>)	1983.316	1983.260	1983.233	1983.207	1983.158	1983.110
ref. (<i>v</i>)	-	-	-	-	1983.445	-
$B_{10^0 0}$						
exp.	-	-	-	-	3701.95(20) ^b	-
<i>ab in.</i>	3759.9	3733.4	3720.6	3708.2	3684.3	3661.5
ref. (<i>p</i>)	3777.98	3751.39	3738.57	3726.11	3702.06	3679.15
ref. (<i>v</i>)	-	-	-	-	3699.44	-
$\nu_{01^1 0}$						
exp.	-	-	-	-	-	-
<i>ab in.</i>	475.8	475.6	475.6	475.5	475.4	475.3
ref. (<i>p</i>)	458.215	458.095	458.036	457.980	457.871	457.767
ref. (<i>v</i>)	-	-	-	-	457.637	-
$B_{01^1 0}$						
exp.	-	-	-	-	3729.24523(27) ^a	-
<i>ab in.</i>	3786.8	3760.1	3747.3	3734.8	3710.6	3687.7
ref. (<i>p</i>)	3805.60	3778.80	3765.88	3753.32	3729.09	3705.98
ref. (<i>v</i>)	-	-	-	-	3726.80	-
$q_{01^1 0}$						
exp.	-	-	-	-	2.75808(54) ^a	-
<i>ab in.</i>	2.78	2.75	2.73	2.71	2.68	2.65
ref. (<i>p</i>)	2.85	2.81	2.80	2.78	2.75	2.72
ref. (<i>v</i>)	-	-	-	-	2.70	-
$\nu_{00^0 1}$						
exp.	-	-	-	-	-	-
<i>ab in.</i>	638.1	635.7	634.6	633.4	631.3	629.2
ref. (<i>p</i>)	631.705	629.358	628.224	627.120	624.985	622.946
ref. (<i>v</i>)	-	-	-	-	624.881	-
$B_{00^0 1}$						
exp.	-	-	-	-	3711.0412(11) ^a	-
<i>ab in.</i>	3768.3	3741.8	3729.0	3716.6	3692.6	3669.8
ref. (<i>p</i>)	3787.26	3760.62	3747.78	3735.31	3711.22	3688.28
ref. (<i>v</i>)	-	-	-	-	3708.73	-
$\nu_{02^0 0}$						
exp.	-	-	-	-	-	-
<i>ab in.</i>	951.3	951.0	950.9	950.8	950.5	950.3
ref. (<i>p</i>)	918.196	917.927	917.798	917.673	917.431	917.201
ref. (<i>v</i>)	-	-	-	-	917.215	-
$B_{02^0 0}$						
exp.	-	-	-	-	3735.0744(12) ^a	-
<i>ab in.</i>	3793.1	3766.3	3753.5	3740.9	3716.8	3693.8
ref. (<i>p</i>)	3812.37	3785.51	3772.57	3759.99	3735.71	3712.58
ref. (<i>v</i>)	-	-	-	-	3732.27	-

^a Ref. [1]

^b Ref. [2]

^c Ref. [7]

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