Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: Diagonal Born-Oppenheimer corrections to the ground electronic state potential energy surfaces of ozone: improvement of ab initio vibrational band centers for the $^{16}O_3$, $^{17}O_3$ and $^{18}O_3$ isotopologues

Attila Tajti,[*,†] Péter G. Szalay,[*,†] Roman Kochanov,[‡] and Vladimir G. Tyuterev[*,¶]

†*ELTE Eötvös Loránd University, Institute of Chemistry, Laboratory of Theoretical Chemistry, , P. O. Box 32, H-1518, Budapest 112, Hungary*

‡*Tomsk State Research University, Laboratory of Quantum Mechanics and Radiative Processes, Russia*

¶*Université de Reims, Groupe de Spectrométrie Moléculaire et Atmosphérique, France*

E-mail: tat@chem.elte.hu; szalay@chem.elte.hu; vladimir.tyuterev@univ-reims.fr

1 Comparison of observed and calculated band centers for various isotopologues of ozone

Table 1: Comparison of observed and calculated band centers (pure vibration energies) for the $^{16}O_3$ isotopologue of ozone. Each level is given by its symmetry ("SYMM"), vibrational quantum assignment ("v_1,v_2,v_3"), observed energy ("OBS"), and a set of calculated energies: Born-Oppenheimer PES without DBOC corrections ("BO"), and DBOC-corrected energy (BO+DBOC(n,n)). All band centers are given in wavenumbers. For each calculation, the zero point energies ("ZPE") are provided.

SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO +DBOC(4,4)	OBS -(BO+DBOC(4,4))	BO +DBOC(6,6)	OBS -(BO+DBOC(6,6))
		ZPE			1443.52		1443.87		1444.24	
A	0	1	0	700.93	700.68	0.25	700.93	0.00	700.95	−0.02
A	1	0	0	1103.14	1103.12	0.02	1103.34	−0.20	1103.38	−0.24
A	0	2	0	1399.27	1398.76	0.51	1399.25	0.02	1399.29	−0.02
A	1	1	0	1796.26	1796.05	0.21	1796.49	−0.23	1796.55	−0.29
A	0	0	2	2057.89	2056.88	1.01	2057.31	0.58	2057.62	0.27
A	0	3	0	2094.99	2094.23	0.76	2094.93	0.06	2095.00	−0.01
A	2	0	0	2201.16	2200.92	0.24	2201.31	−0.15	2201.38	−0.22
A	1	2	0	2486.58	2486.17	0.41	2486.82	−0.24	2486.91	−0.33
A	0	1	2	2726.11	2724.77	1.34	2725.37	0.74	2725.69	0.42
A	0	4	0	2787.9	2787.02	0.88	2787.92	−0.02	2788.00	−0.10
A	2	1	0	2886.18	2885.80	0.38	2886.39	−0.21	2886.49	−0.31
A	1	0	2	3083.70	3083.60	0.10	3084.24	−0.54	3084.45	−0.75
A	1	3	0	3173.93	3173.35	0.58	3174.18	−0.25	3174.29	−0.36
A	3	0	0	3289.93	3289.51	0.42	3290.05	−0.12	3290.11	−0.18
A	0	2	2	3390.92	3389.26	1.66	3390.01	0.91	3390.34	0.58
A	0	5	0	3478.	3477.09	0.91	3478.14	−0.14	3478.24	−0.24
A	2	2	0	3568.07	3567.56	0.51	3568.34	−0.27	3568.45	−0.38
A	1	1	2	3739.43	3739.15	0.28	3739.94	−0.51	3740.14	−0.71
A	1	4	0	3859.0	3857.36	1.64	3858.35	0.65	3858.47	0.53
A	3	1	0	3966.69	3966.16	0.53	3966.88	−0.19	3966.96	−0.27
A	0	0	4	4001.31	4000.53	0.78	4001.31	0.00	4001.49	−0.18
A					4050.29		4051.18		4051.49	
A	2	0	2	4141.42	4140.25	1.17	4141.04	0.38	4141.25	0.17
A					4164.36		4165.54		4165.65	
A	2	3	0	4246.70	4245.71	0.99	4246.64	0.06	4246.77	−0.07
A	4	0	0	4370.3	4369.24	1.06	4369.90	0.40	4369.94	0.36

SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO +DBOC(4,4)	OBS -(BO+DBOC(4,4))	BO +DBOC(6,6)	OBS -(BO+DBOC(6,6))
B	0	0	1	1042.08	1041.55	0.53	1041.74	0.34	1042.00	0.08
B	0	1	1	1726.52	1725.70	0.82	1726.11	0.41	1726.38	0.14
B	1	0	1	2110.78	2110.62	0.16	2111.05	−0.27	2111.27	−0.49
B	0	2	1	2407.93	2406.82	1.11	2407.42	0.51	2407.71	0.22
B	1	1	1	2785.24	2784.88	0.36	2785.50	−0.26	2785.73	−0.49
B	0	0	3	3046.09	3044.88	1.21	3045.51	0.58	3045.78	0.31
B	0	3	1	3086.22	3084.82	1.40	3085.59	0.63	3085.89	0.33
B	2	0	1	3186.41	3185.87	0.54	3186.48	−0.07	3186.70	−0.29
B	1	2	1	3455.82	3455.28	0.54	3456.06	−0.24	3456.31	−0.49
B	0	1	3	3698.29	3696.75	1.54	3697.52	0.77	3697.79	0.50
B					3759.55		3760.46		3760.76	
B	2	1	1	3849.91	3849.25	0.66	3850.01	−0.10	3850.24	−0.33
B	1	0	3	4021.85	4022.11	−0.26	4022.90	−1.05	4023.03	−1.18
B	1	3	1	4122.07	4121.36	0.71	4122.27	−0.20	4122.52	−0.45
B	3	0	1	4250.22	4249.67	0.55	4250.41	−0.19	4250.58	−0.36
B	0	2	3	4346.73	4344.87	1.86	4345.75	0.98	4346.02	0.71

Table 2: Comparison of observed and calculated band centers (pure vibration energies) for the $^{17}O_3$ isotopologue of ozone. Each level is given by its symmetry ("SYMM"), vibrational quantum assignment ("v_1,v_2,v_3"), observed energy ("OBS"), and a set of calculated energies: Born-Oppenheimer PES without DBOC corrections ("BO"), and DBOC-corrected energy (BO+DBOC(6,6)). All band centers are given in wavenumbers. For each calculation, the zero point energies ("ZPE") are provided.

SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO+DBOC(6,6)	OBS-(BO+DBOC(6,6))
		ZPE			1400.35		1401.00	
A					680.08		680.32	
A	1	0	0	1070.95	1070.93	0.02	1071.17	−0.22
A					1357.72		1358.21	
A					1743.75		1744.21	
A	0	0	2	1999.56	1998.73	0.83	1999.42	0.14
A					2032.90		2033.61	
A					2136.75		2137.18	
A					2413.95		2414.63	
A					2648.01		2648.87	
A					2705.59		2706.49	
A					2802.05		2802.68	
A					2998.15		2998.94	
A					3081.41		3082.29	
A					3193.96		3194.53	
A					3294.13		3295.13	
A					3375.72		3376.78	
A					3464.47		3465.29	
A					3636.05		3636.98	
A					3745.97		3747.00	
A					3851.62		3852.37	
A					3891.72		3892.63	
A					3937.03		3938.15	
A					4024.52		4025.45	
A					4043.24		4044.43	
A					4123.63		4124.61	
A					4242.83		4243.49	
A					4269.67		4270.70	
SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO+DBOC(6,6)	OBS-(BO+DBOC(6,6))
B	0	0	1	1012.16	1011.66	0.50	1012.07	0.09
B					1676.22		1676.84	
B	1	0	1	2050.82	2050.66	0.16	2051.26	−0.44
B					2337.95		2338.77	
B					2706.05		2706.84	
B					2960.24		2961.09	
B					2996.78		2997.77	
B					3095.09		3095.86	
B					3357.90		3358.85	
B					3594.48		3595.47	
B					3652.58		3653.70	
B					3740.42		3741.35	
B					3913.39		3914.26	
B					4005.82		4006.90	
B					4129.09		4129.95	
B					4225.24		4226.33	
B					4305.19		4306.41	

Table 3: Comparison of observed and calculated band centers (pure vibration energies) for the $^{18}O_3$ isotopologue of ozone. Each level is given by its symmetry ("SYMM"), vibrational quantum assignment ("v_1,v_2,v_3"), observed energy ("OBS"), and a set of calculated energies: Born-Oppenheimer PES without DBOC corrections ("BO"), and DBOC-corrected energy (BO+DBOC(6,6)). All band centers are given in wavenumbers. For each calculation, the zero point energies ("ZPE") are provided.

SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO+DBOC(6,6)	OBS-(BO+DBOC(6,6))
		ZPE			1360.98		1361.58	
A	0	1	0	661.49	661.28	0.21	661.51	−0.02
A	1	0	0	1041.56	1041.54	0.02	1041.76	−0.20
A	0	2	0	1320.69	1320.26	0.43	1320.71	−0.02
A	1	1	0	1696.17	1695.99	0.18	1696.42	−0.25
A	0	0	2	1946.45	1945.53	0.92	1946.18	0.27
A					1976.93		1977.58	
A	2	0	0	2078.37	2078.17	0.20	2078.57	−0.20
A	1	2	0	2348.33	2347.98	0.35	2348.61	−0.28
A	0	1	2	2578.99	2577.77	1.22	2578.58	0.41
A					2631.24		2632.08	
A	2	1	0	2725.88	2725.55	0.33	2726.15	−0.27
A	1	0	2	2919.96	2919.85	0.11	2920.60	−0.64
A					2997.43		2998.24	
A					3106.71		3107.23	
A					3207.06		3208.00	
A					3283.16		3284.15	
A					3370.27		3371.04	
A					3541.55		3542.43	
A					3644.18		3645.14	
A					3746.96		3747.66	
A					3791.90		3792.77	
A					3833.33		3834.39	
A					3918.59		3919.47	
A					3932.63		3933.74	
A					4012.01		4012.93	
A					4127.36		4127.98	
A					4159.30		4160.27	
A					4287.99		4289.07	

SYMM	v_1	v_2	v_3	OBS	BO	OBS-BO	BO+DBOC(6,6)	OBS-(BO+DBOC(6,6))
B	0	0	1	984.82	984.34	0.48	984.72	0.10
B	0	1	1	1631.72	1630.99	0.73	1631.57	0.15
B	1	0	1	1995.97	1995.83	0.14	1996.39	−0.42
B	0	2	1	2275.97	2275.00	0.97	2275.75	0.22
B	1	1	1	2634.24	2633.92	0.32	2634.65	−0.41
B	0	0	3	2883.86	2882.72	1.14	2883.52	0.34
B					2916.28		2917.20	
B	2	0	1	3012.54	3012.09	0.45	3012.81	−0.27
B	1	2	1	3269.22	3268.75	0.47	3269.64	−0.42
B	0	1	3	3502.23	3500.78	1.45	3501.71	0.52
					3554.74		3555.79	
					3640.85		3641.71	
B	1	0	3	3813.41	3813.60	−0.19	3814.43	−1.02
					3899.99		3901.00	
B	3	0	1	4019.28	4018.81	0.47	4019.62	−0.34
B	0	2	3	4117.32	4115.60	1.72	4116.62	0.70
					4190.25		4191.39	
					4265.40		4266.38	

2 Python routines of the analytical model fitted to ab initio DBOC points of ozone for various isotopologues and MRCI active spaces

```
"""
Analytical model was fitted to the ab initio DBOC points
separately for each isotopologue and active space.

Notations
================================================================
ISO    ACTIVE SPACE* PARAMETERS                  MODEL
================================================================
666    CAS(4,4)     DBOCModel_666_44_5_SY_PARS   MODEL_DBOC_666_44
666    CAS(6,6)     DBOCModel_666_66_5_SY_PARS   MODEL_DBOC_666_66
777    CAS(6,6)     DBOCModel_777_66_5_SY_PARS   MODEL_DBOC_777_66
888    CAS(6,6)     DBOCModel_888_66_5_SY_PARS   MODEL_DBOC_888_66
================================================================
*see manuscript text for a detailed description

In this module we provide four sets of parameters with
one generic class implementing the analytical form of the correction.

Usage example:
MODEL_DBOC_666_66(2.4,2.4,117)
// input: r1/a.u., r2/a.u., alpha/deg.;
   output: DBOC value (relative to the BO equilibrium geometry) for the r1;r2;alpha point (in cm-1),
           as provided by the invoked model (see above notaion table for description).

"""

import math

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    {"name":"poly_1_0_1", "value":-0.31592169593249175, "group":"polynom"},
    {"name":"poly_0_0_2", "value":-0.3560548287623085, "group":"polynom"},
    {"name":"poly_2_1_0", "value":-6.623448142676199, "group":"polynom"},
    {"name":"poly_3_0_0", "value":-4.938916996036866, "group":"polynom"},
    {"name":"poly_1_1_1", "value":0.8647095752369788, "group":"polynom"},
    {"name":"poly_2_0_1", "value":14.484557388604896, "group":"polynom"},
    {"name":"poly_1_0_2", "value":-9.148497399610251, "group":"polynom"},
    {"name":"poly_0_0_3", "value":18.206354547079748, "group":"polynom"},
    {"name":"poly_2_2_0", "value":-8.628404178336641, "group":"polynom"},
    {"name":"poly_3_1_0", "value":8.914913418963879, "group":"polynom"},
    {"name":"poly_4_0_0", "value":-11.897460403378824, "group":"polynom"},
    {"name":"poly_2_1_1", "value":-1.0454554135464362, "group":"polynom"},
    {"name":"poly_3_0_1", "value":-2.439317175109933, "group":"polynom"},
    {"name":"poly_1_1_2", "value":2.6297569094025466, "group":"polynom"},
    {"name":"poly_2_0_2", "value":-3.7426680640543744, "group":"polynom"},
    {"name":"poly_1_0_3", "value":-1.0236586163135444, "group":"polynom"},
    {"name":"poly_0_0_4", "value":-7.971404647082852, "group":"polynom"},
    {"name":"re_au", "value":2.448662452914793, "group":"gauss"},
    {"name":"alphae_deg", "value":120.52182645743281, "group":"gauss"},
    {"name":"slope_rgauss", "value":60.0, "group":"gauss"},
    {"name":"slope_agauss", "value":60.0, "group":"gauss"},
```

```
    {"name":"mul_gauss", "value":10.0, "group":"gauss"},
    {"name":"slope_rgauss_struct", "value":1.64942, "group":"struct"},
    {"name":"slope_agauss_struct", "value":5.32899, "group":"struct"},
    {"name":"mul_gauss_struct", "value":6.18143, "group":"struct"},
    {"name":"global_shift", "value":6.14733, "group":"globshift"},
]

class Parameters:
    """
    Container encapsulating model parameters.
    """
    def __init__(self,parlist):
        self.__objects__ = []
        self.__index__ = {}
        for dct in parlist:
            par = Par(name=dct['name'])
            par.load(dct)
            self.append(par)

    def __getitem__(self,name):
        return self.__objects__[self.__index__[name]]

    def append(self,pars):
        if type(pars) not in {list,tuple}:
            pars = [pars]
        for par in pars:
            if par.name not in self.__index__:
                self.__index__[par.name] = len(self.__objects__)
                self.__objects__.append(par)
            else:
                self.__objects__[self.__index__[par.name]] = par

    def get_values(self,group):
        return [par.value for par in self.__objects__ \
            if par.group==group]

class Par:
    """
    Basic class for parameters of the model.
    """
```

```
    def __init__(self,**kwargs):
        for arg in kwargs: setattr(self,arg,kwargs[arg])

    def load(self,dct):
        for name in dct:
            setattr(self,name,dct[name])

    def get_value(self):
        return self.value

def poly3d_rsymm(p,r1,r2,alpha,powers):
    """
    3D polynomial symmetrized by first 2 coordinates (r1,r2)
    """
    n = len(p)
    sum = 0.0
    for i in range(n):
        pow_r1 = powers[i][0]
        pow_r2 = powers[i][1]
        pow_alpha = powers[i][2]
        sum += p[i]*(r1**pow_r1*r2**pow_r2+r1**pow_r2*r2**pow_r1)*alpha**pow_alpha
    return sum


class DBOCModel:
    """
    Generic class for the DBOC functional representation.
    """
    def __init__(self,parlist):
        self.__powers__ = [
        #   r1 r2  alpha
            [0, 0,  0], # 0

            [1, 0,  0], # 1
            [0, 0,  1], # 1

            [1, 1,  0], # 2
            [2, 0,  0], # 2
            [1, 0,  1], # 2
            [0, 0,  2], # 2
```

```
            [2, 1,  0], # 3
            [3, 0,  0], # 3
            [1, 1,  1], # 3
            [2, 0,  1], # 3
            [1, 0,  2], # 3
            [0, 0,  3], # 3

            [2, 2,  0], # 4
            [3, 1,  0], # 4
            [4, 0,  0], # 4
            [2, 1,  1], # 4
            [3, 0,  1], # 4
            [1, 1,  2], # 4
            [2, 0,  2], # 4
            [1, 0,  3], # 4
            [0, 0,  4], # 4
        #])
        ]
        self.__params__ = Parameters(parlist)

    def __call__(self,r1_au,r2_au,alpha_deg):
        return self.__func__(r1_au,r2_au,alpha_deg)

    def __func__(self,r1_au,r2_au,alpha_deg):
        params = self.__params__

        # common variables
        re_au = params['re_au'].get_value()
        alphae_deg = params['alphae_deg'].get_value()

        alpha_rad = alpha_deg*math.pi/180.
        alphae_rad = alphae_deg*math.pi/180.
        r1_part = r1_au-re_au
        r2_part = r2_au-re_au
        alpha_part = math.cos(alpha_rad)-math.cos(alphae_rad)

        # get polynomial part
        p = params.get_values(group='polynom')
        poly = poly3d_rsymm(p,r1_part,r2_part,alpha_part,self.__powers__)
```

```
        # get correction damping Gaussian parameters
        center_rgauss = re_au
        center_agauss = alphae_deg
        slope_rgauss = params['slope_rgauss'].get_value()
        slope_agauss = params['slope_agauss'].get_value()
        mul_gauss = params['mul_gauss'].get_value()
        gauss_r1 = math.exp(-slope_rgauss*((r1_au-center_rgauss)/center_rgauss)**2)
        gauss_r2 = math.exp(-slope_rgauss*((r2_au-center_rgauss)/center_rgauss)**2)
        gauss_alpha = math.exp(-slope_agauss*((alpha_deg-center_agauss)/center_agauss)**2)
        gauss = mul_gauss*gauss_r1*gauss_r2*gauss_alpha

        # get structure Gaussian parameters
        center_rgauss_struct = re_au
        center_agauss_struct = alphae_deg
        slope_rgauss_struct = params['slope_rgauss_struct'].get_value()
        slope_agauss_struct = params['slope_agauss_struct'].get_value()
        mul_gauss_struct = params['mul_gauss_struct'].get_value()
        gauss_r1_struct = math.exp(-slope_rgauss_struct*((r1_au-center_rgauss_struct)/center_rgauss_struct)**2)
        gauss_r2_struct = math.exp(-slope_rgauss_struct*((r2_au-center_rgauss_struct)/center_rgauss_struct)**2)
        gauss_alpha_struct = math.exp(-slope_agauss_struct*((alpha_deg-center_agauss_struct)/center_agauss_struct)**2)
        gauss_struct = mul_gauss_struct*gauss_r1_struct*gauss_r2_struct*gauss_alpha_struct

        # get global shift
        global_shift = params['global_shift'].get_value()

        # get final result
        res = gauss*(global_shift-gauss_struct-poly)

        return res

MODEL_DBOC_666_66 = DBOCModel(DBOCModel_666_66_5_SY_PARS)
MODEL_DBOC_666_44 = DBOCModel(DBOCModel_666_44_5_SY_PARS)
MODEL_DBOC_777_66 = DBOCModel(DBOCModel_777_66_5_SY_PARS)
MODEL_DBOC_888_66 = DBOCModel(DBOCModel_888_66_5_SY_PARS)

MODELS = [MODEL_DBOC_666_66,MODEL_DBOC_666_44,MODEL_DBOC_777_66,MODEL_DBOC_888_66]
```

3 Details of the *ab initio* grid points used for the BO and DBOC surfaces

Table 4: Structural parameters and PES values (in wavenumbers, relative to the equilibrium configuration) for the BO and the (BO+DBOC) surfaces in the grid points used in the *ab initio* calculations, up to $V_{BO} < D_0/2$. The results correspond to the DBOC(6,6) model (see the main article for details).

r_1 / a.u.	r_2 / a.u.	α / deg.	V_{BO}	ΔV_{DBOC} $^{16}O_3$	ΔV_{DBOC} $^{18}O_3$	ΔV_{DBOC} $^{17}O_3$
2.4	2.4	117.0	−0.001	0.000	0.000	0.000
2.4	2.4	116.0	13.532	−0.117	−0.116	−0.110
2.5	2.4	117.0	53.998	0.379	0.326	0.357
2.4	2.5	116.0	56.743	0.455	0.401	0.428
2.4	2.4	115.0	61.158	−0.258	−0.234	−0.243
2.4	2.4	119.0	71.071	0.679	0.599	0.639
2.4	2.5	115.0	92.058	0.241	0.207	0.227
2.4	2.5	119.0	142.298	0.875	0.768	0.823
2.4	2.5	117.0	169.519	0.215	0.180	0.202
2.5	2.5	115.0	176.538	0.462	0.402	0.435
2.4	2.5	116.0	183.852	0.272	0.237	0.256
2.4	2.4	116.0	195.800	−0.258	−0.239	−0.243
2.4	2.4	119.0	221.155	0.507	0.448	0.477
2.4	2.5	115.0	232.253	0.025	0.014	0.024
2.4	2.5	119.0	238.925	0.694	0.604	0.653
2.4	2.4	115.0	257.237	−0.402	−0.362	−0.378
2.4	2.4	121.0	266.630	1.194	1.053	1.123
2.4	2.5	116.0	279.212	0.684	0.602	0.644
2.4	2.5	117.0	285.860	1.050	0.927	0.988
2.5	2.4	115.0	303.666	0.357	0.304	0.336
2.4	2.5	112.5	329.881	−0.418	−0.378	−0.393
2.4	2.4	112.5	336.807	−0.515	−0.462	−0.485
2.5	2.4	117.0	348.579	0.584	0.510	0.549
2.4	2.5	121.0	349.623	1.427	1.258	1.343
2.5	2.4	116.0	352.951	0.452	0.392	0.425
2.5	2.5	112.5	378.472	−0.124	−0.119	−0.117
2.4	2.5	119.0	388.755	1.197	1.056	1.126
2.5	2.4	115.0	389.846	0.234	0.197	0.220
2.4	2.4	117.0	396.711	−0.249	−0.231	−0.234
2.4	2.4	121.0	402.429	0.994	0.871	0.935
2.5	2.5	116.0	426.539	1.053	0.929	0.991
2.4	2.4	119.0	426.648	0.292	0.254	0.275
2.5	2.4	119.0	433.490	1.306	1.148	1.229
2.4	2.4	116.0	435.444	−0.422	−0.380	−0.397
2.5	2.5	115.0	439.868	0.723	0.640	0.680
2.5	2.5	121.0	483.503	1.642	1.448	1.545
2.5	2.4	112.5	507.546	0.008	−0.003	0.008
2.5	2.4	112.5	509.727	−0.479	−0.431	−0.451
2.4	2.4	115.0	511.511	−0.621	−0.556	−0.584
2.3	2.5	117.0	561.003	0.377	0.332	0.355
2.5	2.5	119.0	561.425	1.418	1.256	1.334
2.4	2.4	112.5	574.724	−0.734	−0.656	−0.691
2.4	2.4	123.0	579.699	1.818	1.603	1.711
2.5	2.3	116.0	588.298	0.170	0.146	0.160
2.4	2.4	121.0	592.705	0.869	0.768	0.818
2.4	2.5	121.0	605.409	1.743	1.540	1.640
2.5	2.5	112.5	609.588	0.142	0.120	0.134
2.4	2.3	117.0	618.645	−0.112	−0.106	−0.106
2.5	2.4	112.5	631.402	−0.158	−0.150	−0.149
2.4	2.5	121.0	637.258	1.550	1.364	1.458
2.4	2.5	116.0	641.683	1.002	0.884	0.943
2.3	2.4	119.0	647.024	0.388	0.338	0.365
2.3	2.5	115.0	651.213	−0.184	−0.174	−0.173
2.0	2.5	115.0	656.666	0.784	0.689	0.738
2.5	2.4	117.0	656.390	1.239	1.098	1.166
2.5	2.4	115.0	656.666	0.784	0.689	0.738

r_1 / a.u.	r_2 / a.u.	α / deg.	V_{BO}	ΔV_{DBOC} $^{16}O_3$	ΔV_{DBOC} $^{18}O_3$	ΔV_{DBOC} $^{17}O_3$
2.3	2.4	116.0	658.120	−0.386	−0.349	−0.363
2.4	2.5	116.0	663.506	0.845	0.742	0.795
2.4	2.5	117.0	667.695	1.091	0.964	1.027
2.5	2.4	123.0	669.373	2.048	1.806	1.927
2.5	2.4	115.0	690.349	0.696	0.611	0.655
2.3	2.5	116.0	701.366	0.434	0.382	0.408
2.4	2.4	123.0	706.491	1.727	1.527	1.625
2.3	2.4	115.0	734.904	−0.552	−0.499	−0.519
2.5	2.4	123.0	743.978	1.871	1.655	1.760
2.5	2.3	119.0	749.214	0.965	0.847	0.908
2.4	2.5	119.0	765.466	1.588	1.406	1.494
2.5	2.4	119.0	771.356	1.795	1.594	1.689
2.5	2.3	121.0	786.807	1.168	1.026	1.099
2.5	2.5	121.0	788.750	1.930	1.704	1.816
2.5	2.4	110.0	796.172	−0.750	−0.678	−0.706
2.5	2.5	123.0	809.577	2.309	2.044	2.173
2.5	2.4	112.5	830.326	0.322	0.275	0.303
2.5	2.5	116.0	838.751	1.221	1.073	1.149
2.4	2.4	110.0	851.799	−0.980	−0.879	−0.922
2.5	2.5	117.0	862.793	1.525	1.353	1.435
2.4	2.4	112.5	873.281	−0.953	−0.854	−0.897
2.4	2.4	123.0	887.111	1.489	1.316	1.401
2.5	2.5	112.5	892.069	0.522	0.460	0.491
2.4	2.5	112.5	899.880	0.249	0.212	0.234
2.4	2.3	117.0	904.585	−0.381	−0.350	−0.358
2.5	2.5	119.0	906.180	2.086	1.841	1.963
2.3	2.4	119.0	910.350	0.081	0.061	0.076
2.5	2.4	110.0	929.428	−0.405	−0.370	−0.381
2.5	2.4	123.0	929.589	2.412	2.137	2.269
2.5	2.3	121.0	937.860	1.863	1.653	1.753
2.3	2.5	117.0	949.933	0.887	0.777	0.835
2.4	2.5	123.0	953.300	2.210	1.953	2.079
2.4	2.3	116.0	957.870	−0.607	−0.551	−0.571
2.3	2.5	116.0	957.438	0.883	0.780	0.831
2.3	2.5	112.5	972.153	−0.596	−0.540	−0.561
2.4	2.5	1200.0	976.743	2.132	1.884	2.006
2.4	2.4	125.0	1003.970	2.565	2.270	2.414
2.5	2.3	112.5	1034.780	−0.201	−0.189	−0.189
2.3	2.4	112.5	1098.339	−0.791	−0.709	−0.744
2.4	2.6	117.0	1132.229	1.621	1.434	1.525
2.5	2.5	121.0	1142.006	2.242	1.983	2.110
2.4	2.6	112.5	1264.538	0.961	0.849	0.904
2.6	2.3	117.0	1322.925	1.497	1.326	1.409
2.4	2.5	125.0	1355.677	3.148	2.791	2.962
2.3	2.3	117.0	1474.332	−0.542	−0.490	−0.510
2.4	2.6	121.0	1485.297	2.664	2.364	2.507
2.3	2.4	125.0	1518.035	2.313	2.046	2.176
2.3	2.5	110.0	1556.168	−0.588	−0.533	−0.553
2.3	2.6	112.5	1571.589	0.596	0.520	0.561
2.3	2.3	121.0	1583.085	0.588	0.520	0.553
2.4	2.6	110.0	1609.738	0.364	0.311	0.342
2.3	2.6	121.0	1615.111	2.491	2.210	2.344
2.3	2.5	125.0	1660.461	2.952	2.622	2.778
2.3	2.4	110.0	1724.131	−1.230	−1.097	−1.157
2.5	2.6	117.0	1812.430	2.209	1.954	2.078
2.5	2.6	112.5	1849.329	1.146	1.006	1.078
2.3	2.6	110.0	2006.522	0.344	0.295	0.324
2.3	2.3	112.5	2114.987	−1.347	−1.203	−1.267
2.6	2.5	110.0	2117.990	0.909	0.805	0.855
2.4	2.6	125.0	2231.829	4.027	3.568	3.789
2.3	2.3	125.0	2253.445	1.947	1.723	1.832
2.7	2.3	117.0	2281.860	2.352	2.079	2.213
2.7	2.4	117.0	2290.271	2.548	2.261	2.397
2.6	2.3	125.0	2335.257	3.828	3.400	3.602
2.4	2.7	112.5	2356.192	1.645	1.458	1.548
2.2	2.5	117.0	2442.800	0.736	0.648	0.693
2.7	2.3	112.5	2453.575	1.533	1.350	1.442
2.4	2.5	105.0	2510.690	−0.937	−0.844	−0.882
2.4	2.4	130.0	2514.670	4.858	4.309	4.571
2.7	2.3	121.0	2594.498	3.522	3.119	3.314
2.2	2.5	121.0	2611.223	1.761	1.561	1.657
2.2	2.4	117.0	2621.450	0.010	−0.003	0.009
2.7	2.4	110.0	2639.364	1.252	1.106	1.178
2.4	2.7	121.0	2659.452	3.525	3.124	3.317
2.4	2.4	105.0	2692.411	−1.327	−1.190	−1.249
2.2	2.4	121.0	2718.827	0.958	0.841	0.901
2.7	2.3	110.0	2817.624	1.276	1.128	1.201
2.4	2.5	130.0	2834.404	5.422	4.815	5.102
2.6	2.2	117.0	2850.805	1.628	1.442	1.532
2.3	2.3	110.0	2865.138	−1.597	−1.425	−1.503
2.5	2.2	112.5	2945.484	−0.032	−0.031	−0.030
2.5	2.6	125.0	2969.751	4.402	3.904	4.142
2.4	2.6	105.0	2970.075	−0.150	−0.143	−0.141
2.6	2.6	112.5	2992.930	2.132	1.885	2.006
2.6	2.6	117.0	3030.595	3.138	2.781	2.953
2.4	2.3	130.0	3042.275	4.602	4.082	4.330
2.2	2.6	121.0	3066.737	2.586	2.292	2.433
2.7	2.5	112.5	3132.641	2.118	1.873	1.993
2.3	2.5	130.0	3151.359	5.236	4.649	4.927

r_1 / a.u.	r_2 / a.u.	α / deg.	V_{BO}	ΔV_{DBOC} $^{16}O_3$	ΔV_{DBOC} $^{18}O_3$	ΔV_{DBOC} $^{17}O_3$
2.5	2.7	117.0	3154.966	2.925	2.589	2.752
2.2	2.4	112.5	3272.764	−0.819	−0.732	−0.771
2.2	2.5	125.0	3290.522	3.130	2.773	2.945
2.7	2.3	125.0	3295.903	4.641	4.114	4.367
2.7	2.5	110.0	3345.887	1.749	1.547	1.646
2.5	2.5	130.0	3354.619	5.932	5.269	5.581
2.4	2.2	125.0	3376.435	2.340	2.073	2.202
2.4	2.7	125.0	3387.006	4.868	4.318	4.580
2.5	2.3	105.0	3407.226	−1.049	−0.942	−0.987
2.6	2.6	121.0	3457.966	4.334	3.848	4.078
2.8	2.3	112.5	3495.766	2.653	2.353	2.496
2.5	2.7	121.0	3567.241	4.124	3.652	3.880
2.8	2.4	117.0	3578.638	3.379	2.992	3.179
2.7	2.2	117.0	3593.398	2.431	2.148	2.287
2.4	2.8	112.5	3597.850	2.994	2.651	2.817
2.6	2.3	105.0	3609.320	−0.040	−0.039	−0.038
2.6	2.4	130.0	3660.687	5.973	5.301	5.620
2.8	2.3	121.0	3698.106	4.222	3.749	3.973
2.2	2.3	121.0	3739.192	0.461	0.401	0.434
2.3	2.2	117.0	3739.570	−0.628	−0.569	−0.591
2.6	2.2	125.0	3747.187	3.865	3.422	3.637
2.6	2.2	110.0	3772.801	0.472	0.407	0.444
2.3	2.6	130.0	3772.876	6.081	5.397	5.722
2.3	2.3	130.0	3789.922	4.310	3.825	4.055
2.8	2.3	110.0	3801.887	2.335	2.067	2.197
2.7	2.4	105.0	3812.870	0.884	0.774	0.832
2.4	2.8	110.0	3831.457	2.221	1.961	2.090
2.7	2.2	121.0	3836.935	3.559	3.155	3.349
2.3	2.4	105.0	3865.336	−1.661	−1.477	−1.563
2.7	2.2	112.5	3886.818	1.829	1.622	1.721
2.2	2.4	110.0	4027.583	−1.215	−1.091	−1.143