MCSCF Response Calculations of the Excited States Properties of the O_2 Molecule and a Part of its Spectrum

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TABLE I. Magnetizability properties (isotropic magnetizability, daimagnetic and paramagnetic contributions) and molecular g-factor of the $c^1\Sigma_u^-$ states of $^{16}O_2$ molecule calculated by MCSCF method with the "aug-cc-pVTZ" basis sets and complete active space 10e × 12 MOs (CAS-II). Components of molecular g-factor are: an isotropic g-factor, daimagnetic and electronic parts of g-factor. Nuclear part of g-factor is constant (0.5038).

		Magnetizabilities (a.u.)			Molecular g-factor		
r (Å)	E (a.u.)	Izotrop. ξ_i	Diamagn.	Paramag.	Izotrop.	Diamagn .	Electronic
1.0372	-149.42670	-1.814	-6.430	4.615	-0.4041	-0.0529	-0.8550
1.0583	-149.46561	-1.908	-6.535	4.627	-0.3703	-0.0545	-0.8197
1.2171	-149.64284	-2.470	-7.406	4.936	-0.2013	-0.0478	-0.6573
1.3200	-149.68750	-2.544	-8.026	5.482	-0.1619	-0.0553	-0.6104
1.4288	-149.70539	-2.449	-8.731	6.282	-0.1474	-0.0641	-0.5871
1.4817	-149.70854	-2.387	-9.093	6.706	-0.1426	-0.0645	-0.5819
1.5800	-149.70794	-2.162	-9.797	7.636	-0.1435	-0.0649	-0.5823
1.6934	-149.70192	-1.662	-10.661	8.999	-0.1603	-0.0652	-0.5989

TABLE II. Magnetizability properties (isotropic magnetizability, daimagnetic and paramagnetic contributions) and molecular g-factor of the $b^1\Sigma_g^+$ states of $^{16}O_2$ molecule calculated by MCSCF method with the "aug-cc-pVTZ" basis sets and complete active space 10e $\times$ 12 MOs (CAS-II). Components of molecular g-factor are: an isotropic g-factor, daimagnetic and electronic parts of g-factor. Nuclear part of g-factor is constant (0.5038).

		Magnetizabilities (a.u.)			Molecular g-factor		
r (Å)	E (a.u.)	Izotrop. ξ_i	Diamagn.	Paramag.	Izotrop.	Diamagn .	Electronic
1.0583	-149.73615	-2.072	-6.478	4.406	-0.3286	-0.0538	-0.7786
1.1000	-149.76322	-2.084	-6.695	4.611	-0.3026	-0.0567	-0.7497
1.1880	-149.79119	-2.024	-7.186	5.162	-0.2702	-0.0568	-0.7172
1.2408	-149.79364	-1.875	-7.496	5.621	-0.2688	-0.0618	-0.7107
1.2700	-149.79281	-1.796	-7.674	5.878	-0.2674	-0.0625	-0.7088
1.3700	-149.78093	-1.468	-8.309	6.841	-0.2675	-0.0639	-0.7074
1.4817	-149.75958	-1.078	-9.068	7.990	-0.2663	-0.0648	-0.7054
1.5875	-149.73805	-0.773	-9.835	9.062	-0.2571	-0.0652	-0.6957

TABLE III. Nuclear-spin-rotation constants, M_O total in kHz (including nuclear part, daimagnetic and paramagnetic contributions) and molecular g-factor of the $b^1\Sigma_g^+$ state of few isotope modifications of O_2 molecule calculated by MCSCF method with the "aug-cc-pVDZ" basis sets and small complete active space 10e × 6 MOs (2p-CAS). Large CAS-II and large basis sets are presented by ^{a,b} footnotes. Components of molecular g-factor are: an isotropic g-factor, daimagnetic and electronic parts.

		Spin-rotation constant (kHz)				Molecular g-factor		
r (Å)	Isotope	M_O,tot	Nuclear	Diamagn.	Paramag.	Izotrop.	Diamagn.	Electronic
1.1000	^{17}O-^{17}O	21.7551	-4.2852	1.5416	24.4986	-0.2615	-0.1 142	-0.6366
1.1000^a	^{16}O-^{16}O	-	-	-	-	-0.3026	-0.0567	-0.7497
1.1500	^{17}O-^{17}O	22.6607	-3.7502	1.2579	25.1539	-0.2509	-0.1 157	-0.6246
1.2000	^{17}O-^{17}O	23.6089	-3.3007	1.0403	25.8693	-0.2469	-0.1 167	-0.6195
1.2070	^{16}O-^{16}O	-	-	-	-	-0.2542	-0.1203	-0.6377
1.2270	^{17}O-^{17}O	24.1122	-3.0876	0.9443	26.2555	-0.2465	-0.1 172	-0.6187
1.2270^b	^{17}O-^{17}O	23.0055	-3.0876	1.0404	25.0526	-0.2205	- 0.1178	-0.5921
1.2270^a	^{17}O-^{17}O	23.6811	-3.0876	1.2484	25.5202	-0.2221	- 0.0622	-0.6493
1.2408	^{16}O-^{16}O	-	-	-	-	-0.2541	-0.1208	-0.6371
1.2408	^{17}O-^{17}O	24.3630	-2.9857	0.9001	26.4486	-0.2466	-0.1 174	-0.6187
1.2408^b	^{17}O-^{17}O	23.1520	-2.9857	0.9983	25.1394	-0.2204	- 0.1179	-0.5919
1.2408	^{18}O-^{18}O	-	-	-	-	-0.2400	-0.1145	-0.6029
1.2500	^{17}O-^{17}O	24.5262	-2.9202	0.8723	26.5642	-0.2468	-0.1 175	-0.6187
1.3000	^{17}O-^{17}O	25.3505	-2.5961	0.7410	27.2056	-0.2489	-0. 1180	-0.6202
1.4000	^{17}O-^{17}O	26.5489	-2.0786	0.5520	28.0755	-0.2537	-0. 1187	-0.6244
1.4500	^{17}O-^{17}O	26.8899	-1.8709	0.4816	28.2792	-0.2549	-0. 1190	-0.6253

[a] Large CAS-II-T (aug-cc-pVTZ-basis set). 85590 CSF's in the C_s point group.

[b] Large CAS-II-D (aug-cc-pVDZ-basis set). 85590 CSF's in the C_s point group.

Nuclear part of g-factor is presented by the following constants: ^{16}O-^{16}O (0.5038), ^{17}O-^{17}O (0.4894), ^{18}O-^{18}O (0.4774).

Nuclear g-value of the ^{17}O-isotope is -0.76.

Moment of inertia at r_e distance (1.2408 Å) is 43.9697 for the ^{16}O-^{16}O isotope, 45.3079 for the ^{17}O-^{17}O isotope and 46.5621 for the ^{18}O-^{18}O isotope. The nuclear contribution to $M_{^{17}O}$ is -2.9857 kHz.

TABLE IV. Perpendicular component of the quadrupole tensor Q_{xx} (ea_0^2), nuclear-spin-rotation constants, M_O total in kHz, for the ^{17}O-^{17}O isotope (including nuclear part, daimagnetic and paramagnetic contributions) and molecular g-factor of the $a^1\Delta_g$ state calculated by MCSCF method with the "aug-cc-pVDZ" basis sets and small complete active space 10e × 6 MOs (2p-CAS) at different internuclear distances r (Å). Components of molecular g-factor are: isotropic g-factor, daimagnetic and electronic parts.

		Spin-rotation constant (kHz)				Molecular g-factor		
r (Å)	Q_{xx}	M_O,tot	Nuclear	Diamagn.	Paramag.	Izotrop.	Diamagn.	Electronic
1.160	0.2258	21.4974	-3.6541	1.1905	23.9609	-0.2293	-0.1163	-0.6023
1.216	0.1640	22.6304	-3.1721	0.9668	24.8356	-0.2265	-0.1173	-0.5986
1.227	0.1524	22.8573	-3.0876	0.9300	25.0149	-0.2266	-0.1174	-0.5986
1.227[a]	0.1204	22.1037	-3.0876	1.2205	23.9708	-0.2156	-0.0619	-0.6431
1.270	0.1078	23.7555	-2.7844	0.8038	25.7361	-0.2286	-0.1179	-0.6000
1.300	0.0803	24.3278	-2.5961	0.7302	26.1936	-0.2306	-0.1182	-0.6017
1.400	-0.0050	26.0256	-2.0786	0.5449	27.5592	-0.2397	-0.1189	-0.6102
1.500	-0.0772	27.0574	-1.6900	0.4180	28.3294	-0.2458	-0.1193	-0.6159

[a] Large CAS-II-T (aug-cc-pVTZ-basis set). 85590 CSF's in the C_s point group.

Nuclear part of g-factor is 0.4894.

Nuclear g-value of the ^{17}O-isotope is -0.76.

Moment of inertia at r_e distance (1.227 Å) is 44.3057 for the ^{17}O-^{17}O isotope. The nuclear contribution to $M_{^{17}O}$ is -3.0876 kHz.

TABLE V. The $f' - X$ transition dipole moments (a.u.)[1] calculated by MCSCF QR method with CAS-II and the aug-cc-pVTZ basis set at different internuclear distances r (in Å) .

r_{OO} (Å)	$D_z(f' - X_0)$	$D_x(f' - X_1)$=$D_y(f' - X_1)$	$\tau_{f'}$, s	$\Delta E_{f'-X}$, eV	$E_{f'}$, hartree	E_X, hartree
1.2478	0.004534	0.004411	0.000007	12.85	-149.375405	-149.847820
1.3229	0.002751	0.003750	0.000017	11.56	-149.414568	-149.839438
1.3970	0.013907	0.002376	0.000000	10.47	-149.435686	-149.820456
1.4817	0.008531	0.002328	0.000012	9.62	-149.450079	-149.803900
1.5081	0.000902	0.002001	0.000133	9.27	-149.452524	-149.793394
1.5611	0.002915	0.000129	0.000160	8.76	-149.455247	-149.777313
1.5875	0.001334	0.000049	0.000845	8.54	-149.455723	-149.769646
1.6011	0.000827	0.000035	0.002283	8.44	-149.455780	-149.765772
1.6011[a]	0.001890	0.000022	0.000438	8.44	-149.465144	-149.775174
1.6298	0.000892	0.000009	0.002125	8.22	-149.455548	-149.757692
1.6404	0.001603	0.000296	0.000633	8.15	-149.455763	-149.755165
1.8521	0.001238	0.002754	0.000155	7.14	-149.445196	-149.707597
2.0109	0.000000	0.000000	-	6.77	-149.435182	-149.684153

[1] 1 a.u. = $e\times$bohr = 2.54 Debye

[a] Calculation with the aug-cc-pVQZ basis set