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Transition dipole moments of the lithium dimer

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a b s t r a c t

In addition to knowledge of interatomic adiabatic potential energy curves of diatomic systems, it is essential to know electronic transition dipole moments. They are needed in understanding processes like photodissociation, photoassociation, cooling, and trapping. Here, we present electronic transition dipole moments calculated for 74 allowed transitions between 26 states of Li_2 [P. Jasik, J.E. Sienkiewicz, Chem. Phys. 323 (2006) 563]. In the asymptotic internuclear region our results reasonably agree with previously calculated and measured results.

Contents

1. Introduction

Radiative transitions between different electronic states of diatomic lithium are of great interest to experimentalists as well as theoreticians who use them for comparisons and as an input data for further calculations. In general these transitions of diatomic molecules have been calculated in only a very scarce manner, although their behavior with change of internuclear distance is important in understanding several physical phenomena. On the other hand, they are rather difficult to obtain experimentally. The transition moments, which depend on the detailed electronic structure of the initial and final molecular states, may be used in estimations of the relative intensities of spectroscopic bands.

The recent development of computational techniques supported by availability of sophisticated computer program packages makes it possible, with great accuracy, to calculate, using *ab initio* methods, wavefunctions of the ground and excited electronic states of diatomic molecules. This in principle allows for accurate calculations of transition moments.

Quite recently we calculated electronic wavefunctions and adiabatic potential curves of the lithium dimer [1]. We presented and discussed the results for the twenty six lowest lying states. In the present paper we use the previously obtained electronic wavefunctions to calculate the allowed transition moments between these states. By covering the widest internuclear distance so far we gain insight into the behavior of the transition moments for small, intermediate, and large distances between the lithium atoms.

2. Theoretical outline

The interaction of an electromagnetic wave with a molecule may be written in the following form (see, e.g., Herzberg [2,3] or Wilson et al. [4])

$$E_\mu = \vec{E} \cdot \vec{\mu}^{mol}(\vec{r}, \vec{R}), \tag{1}$$

where $\vec{E}$ is the electric field vector and $\vec{\mu}^{mol}$ is the electronic transition dipole moment. The transition dipole moment operator can be split into electronic and nuclear parts

$$\vec{u}^{mol}(\vec{r}, \vec{R}) = \vec{\mu}^{el}(\vec{r}) + \vec{\mu}^{nuc}(\vec{R}), \tag{2}$$

where

$$\vec{u}^{el}(\vec{r}) = e \sum_i \vec{r}_i, \tag{3}$$

and

$$\vec{u}^{nuc}(\vec{R}) = \sum_j q_j \vec{R}_j. \tag{4}$$

Here, e and q_j are the electronic and nuclear charges, respectively, and $\vec{r}_i$ and $\vec{R}_j$ are the electronic and nuclear coordinate vectors, respectively. The probability of the transition between two molecular states is proportional to the square of the appropriate matrix element of the electronic dipole moment $\vec{\mu}^{mol}(\vec{r}, \vec{R})$, which is given by

$$\vec{\mu}_{fi}^{mol} = \iint \Psi_f^{mol*}(\vec{r}, \vec{R})\ \vec{\mu}^{mol}(\vec{r}, \vec{R})\ \Psi_i^{mol}(\vec{r}, \vec{R})\ d\vec{r}\ d\vec{R}, \tag{5}$$

where the subscripts i and f indicate, respectively, the initial and final state belonging to different electronic terms. In this description, we treat as negligible the existence of magnetic dipole and electric quadruple moments. The probability that arises from them is 10^5–10^8 times smaller than the one coming from the electric dipole moment [2]. Taking the molecular wavefunction in the adiabatic representation in the following form

$$\Psi_{f(i)}^{mol}(\vec{r}, \vec{R}) = \Psi_{f(i)}^{el}(\vec{r}; \vec{R})\Psi_{f(i)}^{nuc}(\vec{R}) \tag{6}$$

and noticing that the nuclear component of $\vec{\mu}_{fi}^{mol}$ vanishes due to the orthogonality of electronic wavefunctions $\int \Psi_f^{el*}(\vec{r}; \vec{R})\Psi_i^{el}(\vec{r}; \vec{R})d\vec{r}$, the molecular dipole moments becomes

$$\vec{\mu}_{fi}^{mol} = \int \Psi_f^{nuc*}(\vec{R})\vec{\mu}_{fi}^{el}(\vec{R})\Psi_i^{nuc}(\vec{R})d\vec{R}. \tag{7}$$

Here,

$$\vec{\mu}_{fi}^{el}(\vec{R}) = \int \Psi_f^{el*}(\vec{r}; \vec{R})\vec{\mu}^{el}(\vec{r})\Psi_i^{el}(\vec{r}; \vec{R})d\vec{r}, \tag{8}$$

is the matrix element of the electric dipole moment. Within the Born–Oppenheimer approximation we can assume that the electronic transition dipole changes very slowly along the internuclear separation, which leads to the following formula

$$\vec{\mu}_{fi}^{mol} = \overline{\vec{\mu}_{fi}^{el}} \int \Psi_f^{nuc*}(\vec{R})\Psi_i^{nuc}(\vec{R})d\vec{R}, \tag{9}$$

where $\overline{\vec{\mu}_{fi}^{el}}$ is an average value of the electronic dipole transition moment. The equation above is one way to constitute the Franck–Condon principle. Finally, we can write the probability for the transition between two molecular states as

$$P_{fi} \propto \left(\overline{\vec{\mu}_{fi}^{el}}\right)^2 \left[\int \Psi_f^{nuc*}(\vec{R})\Psi_i^{nuc}(\vec{R})d\vec{R}\right]^2, \tag{10}$$

where the square of the integrals from the nuclear wavefunction overlaps define the Franck–Condon coefficients and plays a decisive role in interpretation of diatomic spectral bands.

3. Computational method

The theoretical method is described in our previous papers [1,5]. Here we give the details of the computational approach, which is based on the restricted Hartree–Fock method, multiconfigurational self-consistent field/complete active space self-consistent field method, and multi-reference configuration interaction method. All calculations reported in this paper were

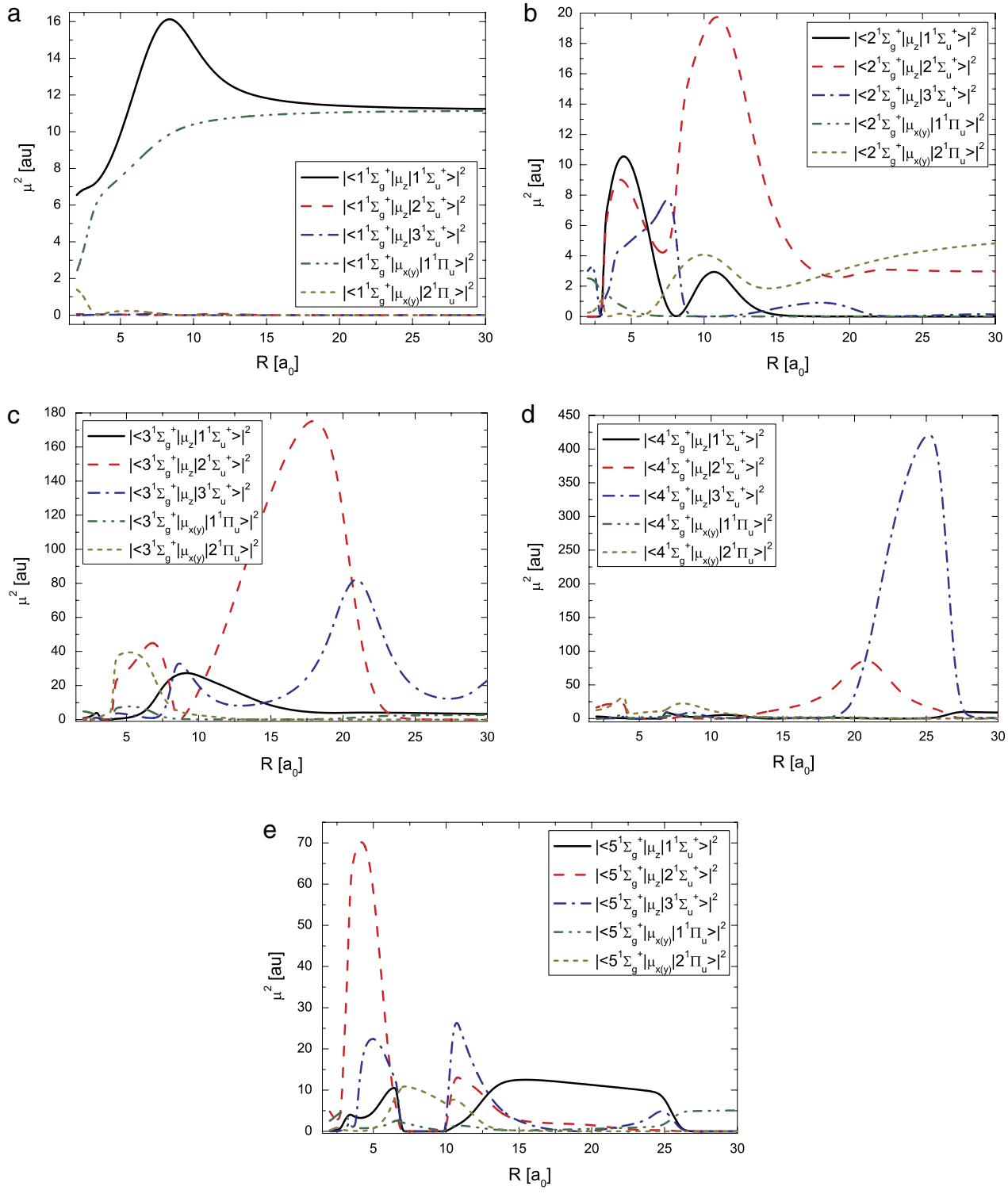

Fig. 1. The transition dipole moments for the $1^1\Sigma_g^+$ (a), $2^1\Sigma_g^+$ (b), $3^1\Sigma_g^+$ (c), $4^1\Sigma_g^+$ (d), and $5^1\Sigma_g^+$ (e) states of the lithium dimer.

performed by means of the MOLPRO program package [6]. The core electrons of the Li atoms are represented by the pseudopotential ECP2SDF [7], which was formed from the uncontracted (10s10p)/[8s8p] basis set. The basis for the s and p orbitals, which comes with this pseudopotential, is enlarged by functions for d, f, and g orbitals given by Feller [8] and assigned by CC-PV5Z. Additionally, our basis set was augmented by four short range correlation s functions (1979.970927, 392.169555, 77.676373, 15.385230), four p functions (470.456384, 96.625417, 19.845562, 4.076012), four d functions (7.115763, 3.751948, 1.978298, 1.043103), and four f functions (2.242072, 1.409302, 0.885847, 0.556818). Also, we added the following to the basis set of the diffused functions: two s functions (0.010159, 0.003894), two p functions (0.007058, 0.002598), two d functions (0.026579, 0.011581), and two f functions (0.055000, 0.027500). We checked the quality of our basis set by performing configuration interaction calculations for the ground and several excited states of the isolated lithium atom.

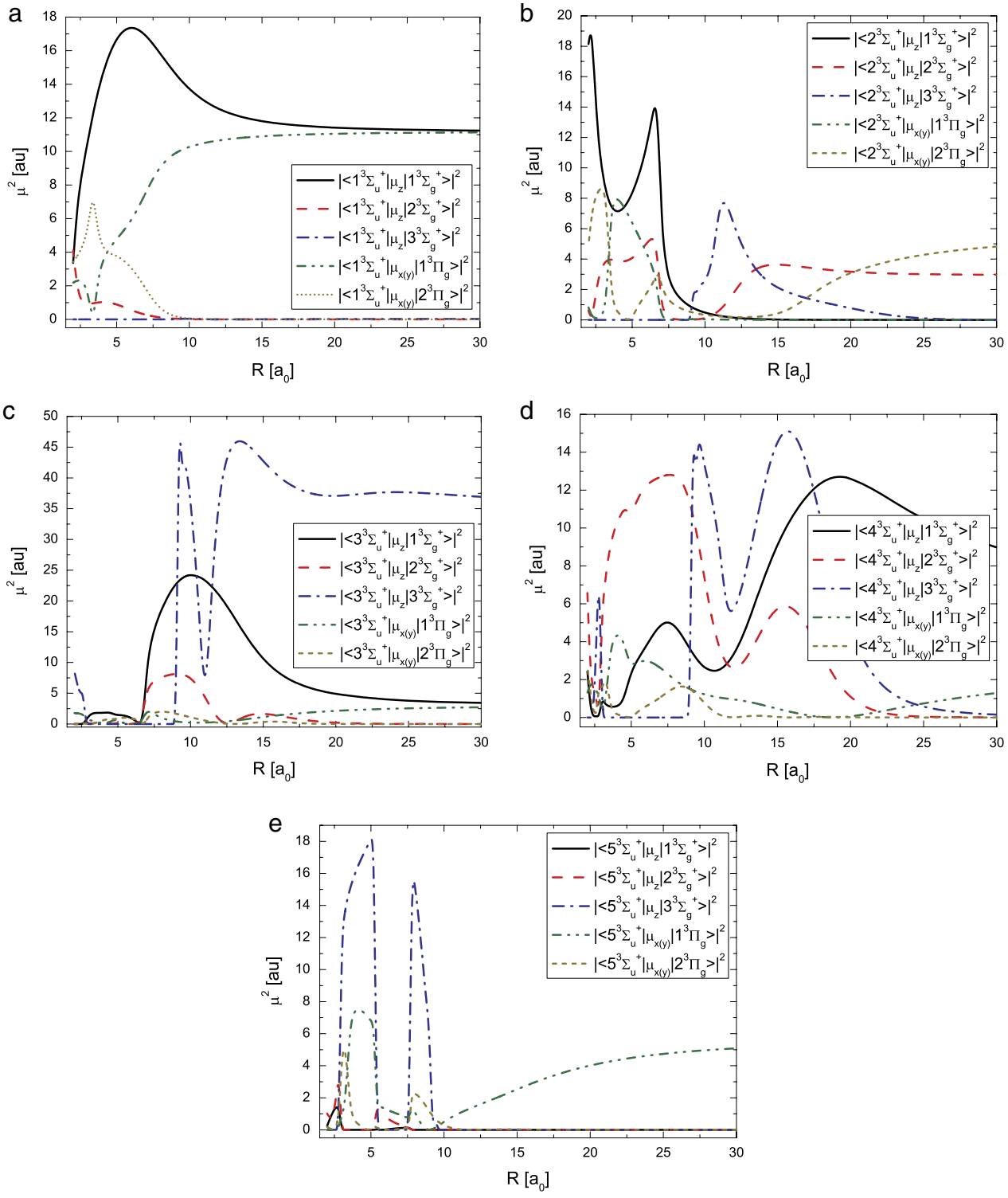

Fig. 2. The transition dipole moments for the $1^3\Sigma_u^+$ (a), $2^3\Sigma_u^+$ (b), $3^3\Sigma_u^+$ (c), $4^3\Sigma_u^+$ (d), and $5^3\Sigma_u^+$ (e) states of the lithium dimer.

4. Results and discussion

Electronic transition dipole moments are calculated for all 74 allowed transitions among the 26 adiabatic potential energy curves obtained previously [1]. We provide tables (Tables 1–16) with numerical values of calculated electronic transition dipole moments in a very wide range of the internuclear distance between the lithium atoms (2–90 a_0).

In Table A we show a comparison between our electronic transition moments calculated for very large internuclear distance ($R = 90\ a_0$) with the available atomic data. We refer to the atomic values given by Magnier [9], Marinescu and Dalgarno [10], Pipin and Bishop [11], Ratcliff et al. [12], Ponomarenko and Shestakov [13], Schmidt-Mink et al. [14], Ellis and Gościński [15], Moore et al. [16], Weiss [17], and Gaupp et al. [18]. For instance, the values of Marinescu and Dalgarno [10], Pipin and Bishop [11], and Ratcliff et al. [12] obtained for the transition between atomic asymptotes Li(2s) + Li(2s) and Li(2s) + Li(2p) are 3.3175, 3.3167, and 3.3400 ea_0, respectively. The agreement with the present asymptotic value (3.3419 ea_0) is very reasonable. The respective

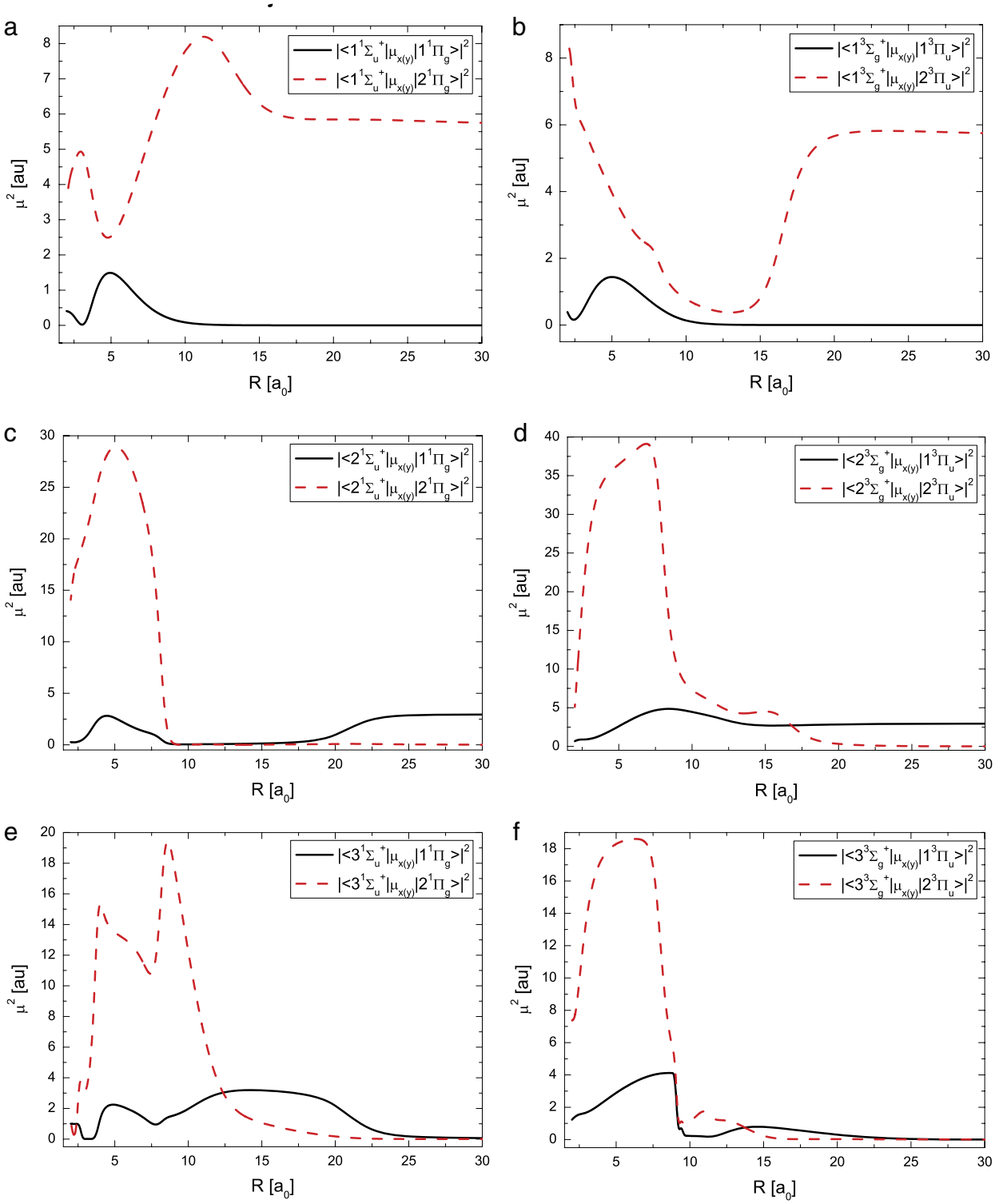

Fig. 3. The transition dipole moments for the $1^1\Sigma_u^+$ (a), $1^3\Sigma_g^+$ (b), $2^1\Sigma_u^+$ (c), $2^3\Sigma_g^+$ (d), $3^1\Sigma_u^+$ (e), and $3^3\Sigma_g^+$ (f) states of the lithium dimer.

differences between their values and the present one are 0.0244, 0.0252, and 0.0019 ea_0. The best agreement is obtained with Ratcliff et al. [12] for the transition between atomic asymptotes Li($2s$) + Li($2p$) and Li($2p$) + Li($2p$). The difference is only 0.0011 ea_0. We note that the biggest difference occurs for data of Schmidt-Mink et al. [14] for the transition Li($2s$) + Li($3s$) → Li($2s$) + Li($3p$) and it equals to 0.0574 ea_0.

In Table B, we give examples of the Franck–Condon coefficients (see Eq. (10)) for three chosen band systems (specific Franck–Condon coefficients may be calculated by the authors upon request). We calculated these coefficients using Le Roy's program LEVEL 8.0 [19].

In Figs. 1–4 we plot the squares of all presently calculated transitions along the internuclear axis. As one may easily notice they are by no means constants or slowly varying functions of R as it is quite often assumed. To the contrary, they often display quite rapid growth or decrease with the change of R. It has to be taken into account in any calculations that use transition probabilities,

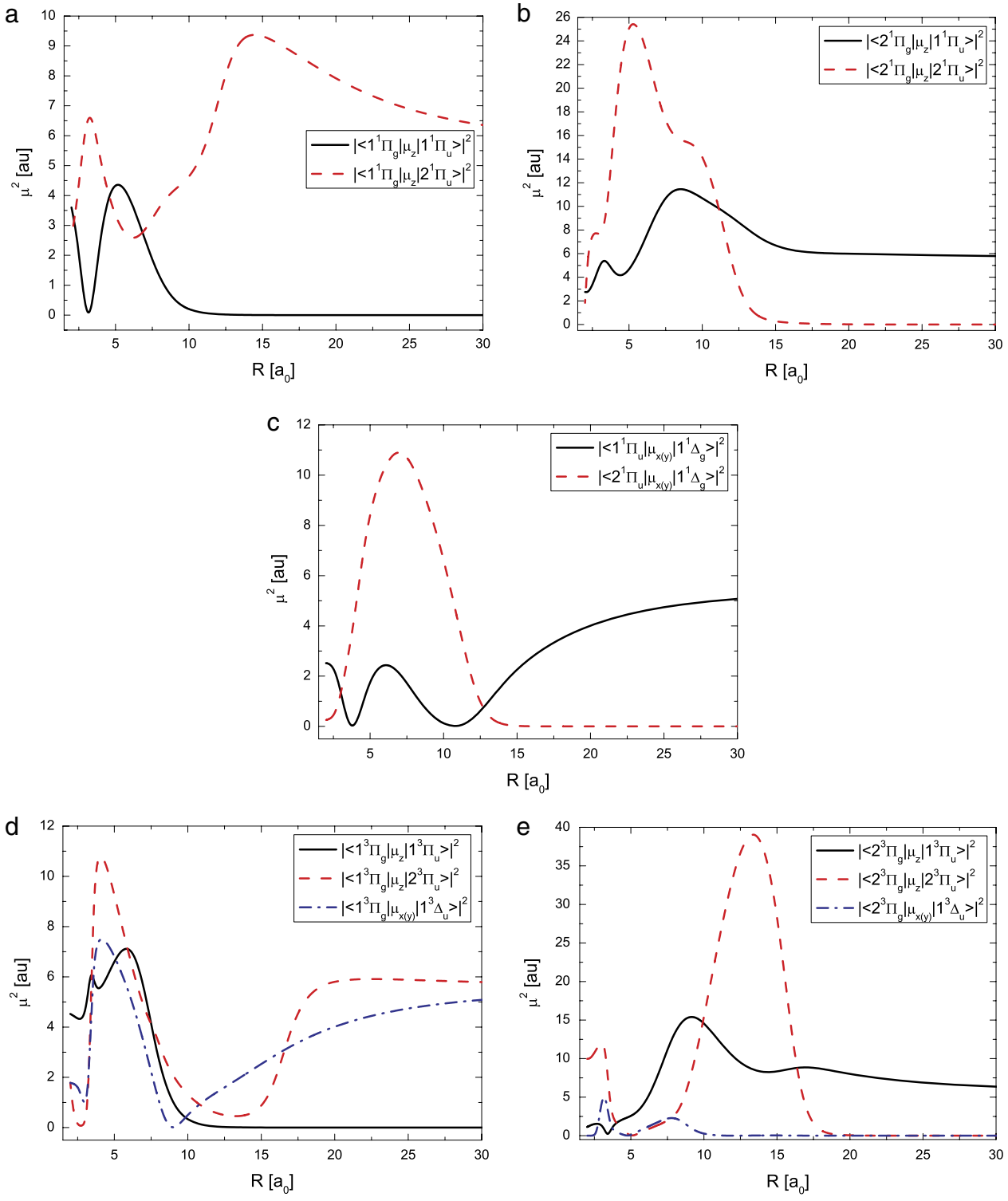

Fig. 4. The transition dipole moments for the $1^1\Pi_g$ (a), $2^1\Pi_g$ (b), $^1\Pi_u$ (c), $1^3\Pi_g$ (d), and $2^3\Pi_g$ (e) states of the lithium dimer.

for example, to describe photodissociation or photoassociation phenomena. As expected, the transition moments associated with allowed atomic transitions go to finite values with the increase of the interatomic separation. These moments display rather smooth monotonic changes for the full range of R. On the other hand, the transition moments associated with forbidden atomic transitions decrease to zero as one approaches the asymptotic region. When R decreases, several different atomic states start to contribute to the molecular states. These contributions become important at smaller interatomic distances and are responsible for the mixing of the basis states with different atomic orbital angular moments [20,21]. Some of molecular transition moments become quite large and may display rapid oscillations and discontinuities due to the oscillatory character of the expansion coefficients of the molecular wavefunction.

In Fig. 5 we present our transition dipole moment for the $1^1\Sigma_u^+$–$1^1\Sigma_g^+$ transition. We give a comparison with the results obtained from the fit of experimental transition dipole moment

Table A
Asymptotic values of electronic transition dipole moments and differences between our results and those obtained by other authors. Our results are given for the internuclear distance equal to 90 a_0. The symbol $*$ over the arrow stands for the atomic transition. All values are given in atomic units.

Electronic transition	Authors	μ_{fi}^{el}	$\lvert\triangle\mu_{fi}^{el}\rvert$
$Li(2s) + Li(2s) \rightarrow Li(2s) + Li(2p)$	Jasik and Sienkiewicz	3.341936	
	Marinescu and Dalgarno [10]	3.317500	0.0244
	Pipin and Bishop [11]	3.316700	0.0252
	Ratcliff et al. [12]	3.340000	0.0019
$Li(2s) + Li(2s) \rightarrow Li(2s) + Li(3s)$	Jasik and Sienkiewicz	0.000015	
$Li(2s) + Li(2s) \rightarrow Li(2p) + Li(2p)$	Jasik and Sienkiewicz	0.000005	
$Li(2s) + Li(2s) \overset{*}{\rightarrow} Li(2s) + Li(3p)$	Jasik and Sienkiewicz	0.169224	
	Marinescu and Dalgarno [10]	0.183400	0.0142
	Ponomarenko and Shestakov [13]	0.176700	0.0075
	Schmidt-Mink et al. [14]	0.133000	0.0362
	Ellis and Gościński [15]	0.140200	0.0290
$Li(2s) + Li(2p) \rightarrow Li(2s) + Li(2p)$	Jasik and Sienkiewicz	0.000027	
$Li(2s) + Li(2p) \overset{*}{\rightarrow} Li(2s) + Li(3s)$	Jasik and Sienkiewicz	1.718163	
	Ratcliff et al. [12]	1.704000	0.0142
	Schmidt-Mink et al. [14]	1.726000	0.0078
	Ellis and Gościński [15]	1.759000	0.0408
	Moore et al. [16]	1.724000	0.0058
	Weiss [17]	1.756000	0.0378
$Li(2s) + Li(2p) \overset{*}{\rightarrow} Li(2p) + Li(2p)$	Jasik and Sienkiewicz	2.363093	
	Salihoglu et al. [9]	2.352713	0.0104
	Pipin and Bishop [11]	2.345200	0.0179
	Ratcliff et al. [12]	2.362000	0.0011
	Schmidt-Mink et al. [14]	2.347000	0.0161
	Ellis and Gościński [15]	2.352000	0.0111
	Moore et al. [16]	2.348000	0.0151
	Weiss [17]	2.356000	0.0071
	Gaupp et al. [18]	2.337000	0.0261
$Li(2s) + Li(2p) \rightarrow Li(2s) + Li(3p)$	Jasik and Sienkiewicz	0.000174	
$Li(2s) + Li(3s) \rightarrow Li(2s) + Li(3s)$	Jasik and Sienkiewicz	0.000014	
$Li(2s) + Li(3s) \rightarrow Li(2p) + Li(2p)$	Jasik and Sienkiewicz	0.000611	
$Li(2s) + Li(3s) \overset{*}{\rightarrow} Li(2s) + Li(3p)$	Jasik and Sienkiewicz	5.992407	
	Schmidt-Mink et al. [14]	5.935000	0.0574
	Ellis and Gościński [15]	6.023000	0.0306
$Li(2p) + Li(2p) \rightarrow Li(2p) + Li(2p)$	Jasik and Sienkiewicz	0.000044	
$Li(2p) + Li(2p) \rightarrow Li(2s) + Li(3p)$	Jasik and Sienkiewicz	0.004064	

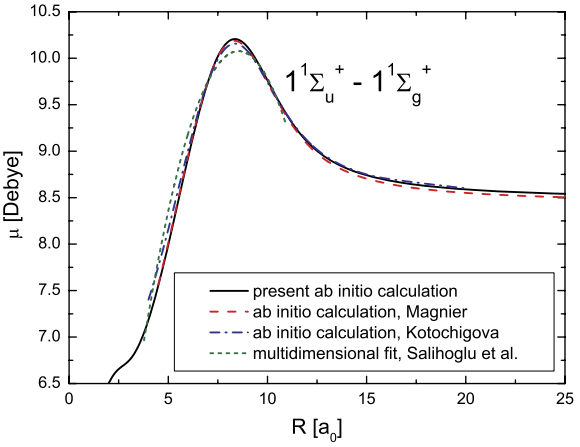

Fig. 5. The comparison between the experimental and theoretical transition dipole moments. Experimental data comes from Salihoglu et al. [9]. Theoretical results of Magnier and Kotochigova are cited in Ref. [9].

matrix elements with a quadratic polynomial expansion obtained by Salihoglu et al. [9] and other theoretical results obtained by *ab initio* calculations by Kotochigova and Magnier, as cited in Ref. [9]. We note that our results are in the excellent agreement with other theoretical results. However, at small internuclear distance our results agree with those of Magnier but we observe a small disagreement with ones of Kotochigova. At large distances, it is quite the opposite: our results agree better with those of Kotochigova but disagree with ones given by Magnier. The cause for these small deviations lies in different interaction models and different basis sets used in these calculations. We made quite an effort to control these two regions by careful choice of our basis set functions, which include short range as well as diffused functions.

5. Conclusions

For the first time the electronic transition dipole moments are calculated between all states correlated up to the $Li(2p) + Li(2p)$ configuration in atomic limits. Only $1^1\Sigma_u^-$ and $1^3\Sigma_g^-$ states are not taken into account. Additionally the transition moments are calculated for two Σ states ($3^1\Sigma_u^+$ and $3^3\Sigma_g^+$) correlated in the atomic asymptote to the $Li(2s) + Li(3p)$ level. Our transition dipole moments are calculated from very small internuclear distance ($2\ a_0$) up to $90\ a_0$. Overall, we note some very good agreement with electronic transition dipole moments calculated by other authors, but some significant discrepancies are still present.

Acknowledgments

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Appendix. Supplementary data

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.adt.2011.06.003.

Table B
The Franck–Condon coefficients from the three vibrational levels ($v'' = 0, 1, 2$) of the $1^1\Sigma_g^+$ ground state to all 17 vibrational levels of the $1^1\Pi_u$ state correlating to the atomic asymptote Li(2s) + Li(2p) and first 30 vibrational levels of the $1^1\Sigma_u^+$ and $2^1\Pi_u$ states correlating, respectively, to the atomic asymptotes Li(2s) + Li(2p) and Li(2p) + Li(2p).

	$1^1\Pi_u$–$1^1\Sigma_g^+$			$1^1\Sigma_u^+$–$1^1\Sigma_g^+$			$2^1\Pi_u$–$1^1\Sigma_g^+$		
v'	$v''=0$	$v''=1$	$v''=2$	$v''=0$	$v''=1$	$v''=2$	$v''=0$	$v''=1$	$v''=2$
0	0.2855370000	0.3769910000	0.2287400000	0.0525946000	0.1760000000	0.2704470000	0.0670734000	0.1956000000	0.2703590000
1	0.3260820000	0.0199861000	0.1151720000	0.1340110000	0.1960680000	0.0576827000	0.1548710000	0.1866680000	0.0402228000
2	0.2128820000	0.0653613000	0.1519240000	0.1878030000	0.0784480000	0.0152299000	0.1992710000	0.0581643000	0.0258317000
3	0.1053320000	0.1706400000	0.0053138300	0.1910240000	0.0032718800	0.0977962000	0.1886890000	0.0001455310	0.1039060000
4	0.0442678000	0.1632470000	0.0450818000	0.1574520000	0.0185471000	0.0895003000	0.1472250000	0.0291967000	0.0814064000
5	0.0167815000	0.1052190000	0.1195270000	0.1125990000	0.0687198000	0.0268561000	0.1012480000	0.0793156000	0.0201006000
6	0.0059917800	0.0549680000	0.1273480000	0.0724690000	0.1022580000	0.0000170902	0.0633041000	0.1063820000	0.0005421260
7	0.0020684900	0.0253801000	0.0937054000	0.0429491000	0.1053050000	0.0213938000	0.0368535000	0.1042470000	0.0250494000
8	0.0006992460	0.0108285000	0.0560757000	0.0239012000	0.0878567000	0.0567669000	0.0202986000	0.0848507000	0.0596809000
9	0.0002350410	0.0044192200	0.0296549000	0.0126660000	0.0637978000	0.0783435000	0.0106972000	0.0609394000	0.0800263000
10	0.0000794615	0.0017655600	0.0145512000	0.0064561500	0.0419746000	0.0798101000	0.0054345700	0.0399490000	0.0811284000
11	0.0000273506	0.0007026720	0.0068496000	0.0031886500	0.0256589000	0.0676442000	0.0026771400	0.0244383000	0.0692275000
12	0.0000097186	0.0002824890	0.0031705900	0.0015370600	0.0148488000	0.0506624000	0.0012798200	0.0141125000	0.0522497000
13	0.0000036064	0.0001157620	0.0014669100	0.0007263710	0.0082315700	0.0346946000	0.0005954480	0.0077704300	0.0359473000
14	0.0000014099	0.0000486892	0.0006853140	0.0003376420	0.0044041400	0.0221851000	0.0002707420	0.0041159000	0.0230320000
15	0.0000005870	0.0000212900	0.0003276830	0.0001551630	0.0022900500	0.0134543000	0.0001206230	0.0021087100	0.0139389000
16	0.0000002548	0.0000095296	0.0001576810	0.0000709344	0.0011655100	0.0078386300	0.0000527921	0.0010485300	0.0080460700
17	0.0000000969	0.0000036915	0.0000642500	0.0000324095	0.0005839740	0.0044283700	0.0000227580	0.0005070880	0.0044597700
18				0.0000148379	0.0002895320	0.0024424800	0.0000096962	0.0002391180	0.0023864600
19				0.0000068087	0.0001426760	0.0013217800	0.0000040980	0.0001103940	0.0012394700
20				0.0000031264	0.0000701281	0.0007044340	0.0000017186	0.0000500880	0.0006270360
21				0.0000014356	0.0000345126	0.0003714280	0.0000007127	0.0000224253	0.0003097800
22				0.0000006601	0.0000170494	0.0001946840	0.0000002903	0.0000099483	0.0001498170
23				0.0000003051	0.0000084551	0.0001018160	0.0000001150	0.0000043842	0.0000710763
24				0.0000001429	0.0000042042	0.0000532906	0.0000000440	0.0000019197	0.0000331685
25				0.0000000685	0.0000020921	0.0000279585	0.0000000162	0.0000008321	0.0000152728
26				0.0000000339	0.0000010406	0.0000147011	0.0000000059	0.0000003541	0.0000069586
27				0.0000000174	0.0000005179	0.0000077400	0.0000000022	0.0000001460	0.0000031419
28				0.0000000091	0.0000002588	0.0000040733	0.0000000009	0.0000000575	0.0000014035
29				0.0000000048	0.0000001306	0.0000021397	0.0000000004	0.0000000212	0.0000006164
30				0.0000000025	0.0000000668	0.0000011214	0.0000000002	0.0000000072	0.0000002630

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Explanation of Tables

Table 1–16 We present the numerical values of electronic transition dipole moments as functions of the internuclear distance R, ranging from 2 to 90 a_0.

$\langle \Psi_f^{el} \lvert \mu_{x(y)}^{el} \rvert \Psi_i^{el} \rangle = (\vec{\mu}_{fi}^{el}(\vec{R}))_{x(y)} = \int \Psi_f^{el*}(\vec{r};\vec{R}) \vec{\mu}_{x(y)}^{el}(\vec{r}) \Psi_i^{el}(\vec{r};\vec{R}) d\vec{r}$	the x or y component of the electronic dipole moment between the initial state Ψ_i^{el} and the final state Ψ_f^{el} of the diatomic molecule
$\langle \Psi_f^{el} \lvert \mu_{z}^{el} \rvert \Psi_i^{el} \rangle = (\vec{\mu}_{fi}^{el}(\vec{R}))_{z} = \int \Psi_f^{el*}(\vec{r};\vec{R}) \vec{\mu}_{z}^{el}(\vec{r}) \Psi_i^{el}(\vec{r};\vec{R}) d\vec{r}$	the z component of the electronic dipole moment between the initial state Ψ_i^{el} and the final state Ψ_f^{el} of the diatomic molecule

All values are given in atomic units.

Table 1
Electronic transition dipole moments for the molecular ground state $1^1\Sigma_g^+$.

R	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 1^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
90.0	−3.34232054	−0.00001646	−0.16922946	3.34174549	−0.00000998
88.0	3.34234728	0.00001620	0.16922018	3.34173137	0.00001111
86.0	3.34237710	0.00001661	0.16921815	3.34171684	0.00001210
84.0	−3.34240983	−0.00001705	−0.16921587	−3.34170086	−0.00001319
82.0	−3.34244584	−0.00001752	−0.16921324	3.34168326	−0.00001440
80.0	−3.34248555	−0.00001802	−0.16921015	3.34166384	−0.00001574
78.0	−3.34252943	−0.00001855	−0.16920635	3.34164234	−0.00001724
76.0	−3.34257807	−0.00001911	−0.16921090	3.34161848	−0.00001890
74.0	−3.34263213	−0.00001969	−0.16920486	3.34159195	−0.00002075
72.0	−3.34269236	−0.00002035	−0.16919703	3.34156235	−0.00002281
70.0	−3.34275969	−0.00002118	−0.16918690	3.34152923	−0.00002511
68.0	−3.34283535	−0.00002197	−0.16917534	3.34149206	−0.00002766
66.0	−3.34291994	−0.00002795	−0.16916091	3.34145017	−0.00003050
64.0	−3.34301553	−0.00002997	−0.16914653	3.34140284	−0.00003364
62.0	−3.34312357	−0.00003170	−0.16913139	3.34134912	−0.00003712
60.0	−3.34324603	−0.00003320	−0.16911506	3.34128790	−0.00004099
58.0	−3.34338538	−0.00003444	−0.16912875	3.34121783	−0.00004532
56.0	−3.34354486	−0.00003517	−0.16910771	3.34113728	−0.00005028
54.0	−3.34372872	−0.00003507	−0.16908368	3.34104423	−0.00005596
52.0	−3.34394237	−0.00003380	−0.16905605	3.34093623	−0.00006267
50.0	−3.34419251	−0.00003119	−0.16902415	3.34081020	−0.00004429
48.0	−3.34448680	−0.00002815	−0.16898487	−3.34066226	−0.00004942
46.0	−3.34483524	−0.00002542	−0.16898319	−3.34048763	−0.00005651
44.0	−3.34525169	−0.00002241	−0.16891710	−3.34028001	−0.00006614
42.0	−3.34581088	−0.00001898	−0.16882477	−3.34003123	−0.00007822
40.0	−3.34642459	−0.00001342	−0.16868380	−3.33973045	−0.00009088
38.0	−3.34717789	−0.00000094	−0.16845231	−3.33936323	−0.00009632
36.0	−3.34811073	0.00001594	−0.16803103	−3.33890950	−0.00008167
34.0	−3.34927942	0.00003541	−0.16680671	−3.33834205	−0.00004490
32.0	3.35076254	−0.00005810	0.16061981	3.33762481	−0.00000878
30.0	3.35267189	−0.00009491	0.11655061	3.33670636	−0.00007206
29.0	3.35383524	−0.00012869	0.08207824	3.33614910	−0.00010601
28.0	3.35517332	−0.00018394	0.06030999	3.33549123	−0.00010633
27.0	3.35672134	−0.00024801	0.04774945	3.33475462	−0.00012727
26.0	3.35843568	−0.00045423	0.04000734	3.33390965	−0.00016522
25.0	3.36053824	−0.00078693	0.03467778	3.33291750	−0.00020631
24.0	3.36302441	−0.00131480	0.03068916	−3.33175650	−0.00027873
23.0	3.36598415	0.00221979	0.02727482	−3.33038548	−0.00035724
22.0	3.36953672	0.00366580	0.02391557	−3.32876986	−0.00052956
21.0	3.37383691	0.00498547	0.02027082	−3.32682231	−0.00071045
20.0	3.37910547	0.00378233	0.01698006	−3.32450066	−0.00098283
19.5	3.38219589	0.00159455	0.01581810	3.32316395	−0.00113902
19.0	3.38554112	−0.00175275	0.01500082	3.32171822	−0.00135405
18.5	3.38942492	−0.00633850	0.01447375	3.32009429	−0.00149963
18.0	3.39381971	−0.01230395	0.01415767	3.31829712	−0.00165208
17.5	3.39882359	−0.01987369	0.01398391	3.31630429	−0.00176189
17.0	3.40456001	−0.02935442	0.01389443	−3.31409031	−0.00178890
16.5	3.41118583	−0.04113007	0.01384075	−3.31162589	−0.00167123
16.0	3.41890310	−0.05564706	0.01378362	−3.30887731	−0.00131391
15.5	3.42797307	−0.07337883	0.01371146	−3.30580563	−0.00055966
15.0	3.43873787	−0.09475145	0.01358361	−3.30236534	0.00077959
14.5	3.45165026	−0.12000775	0.01342994	−3.29849091	0.00303404
14.0	3.46729329	−0.14901172	0.01322739	−3.29416705	0.00652599
13.5	3.48655506	−0.18083883	0.01320261	−3.28927007	0.01191427
13.0	3.51060185	−0.21349132	0.01356546	−3.28371571	0.01932629
12.5	3.54103481	−0.24342652	0.01452528	−3.27737849	0.02808673
12.0	3.57978028	−0.26546911	0.01649142	−3.27012908	0.03609271
11.5	3.62888858	−0.27318407	0.01986287	−3.26166319	0.04047421
11.0	3.68970966	−0.25987191	0.02488818	−3.25164745	−0.03883022
10.5	3.76175777	−0.22012736	0.03148249	−3.23955998	−0.02921722
10.0	3.84107524	−0.15174541	0.03935664	−3.22465713	−0.00925941
9.8	3.87306697	0.11684063	0.04294603	−3.21766878	0.00230604
9.6	3.90401979	0.07830351	0.04713282	−3.20995541	0.01628241
9.4	3.93321146	−0.03684550	0.05202965	−3.20145459	0.03283106
9.2	3.95957729	0.00644790	0.05845621	−3.19205931	0.05215683
9.0	3.98209797	0.05000518	0.06767214	−3.18165461	0.07435798
8.8	3.99973111	0.09138423	0.08206814	−3.17012818	0.09944335
8.6	4.01155139	0.12631444	0.10555682	−3.15738802	0.12729631
8.4	4.01668975	0.14733049	0.14293945	−3.14333612	0.15763522
8.2	4.01445990	0.14730244	0.19193721	−3.12789982	0.19000981
8.0	4.00437867	0.13298585	0.23736166	−3.11103839	0.22381046
7.8	3.98618952	0.11922232	0.26794759	−3.09274431	0.25826196
7.6	3.95986999	0.11152558	0.28285823	−3.07304897	0.29248560
7.4	3.92562366	0.10920208	0.28430614	−3.05202021	0.32550760

(*continued on next page*)

Table 1 (*continued*)

R	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 1^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 1^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
7.2	3.88384699	0.11063387	0.27589373	−3.02975744	0.35655372
7.0	3.83511072	0.11458022	−0.26208732	−3.00641066	0.38496692
6.8	3.78012717	0.12019902	−0.24689349	−2.98203367	0.41015059
6.6	3.71970433	0.12692170	−0.23270184	−2.95689607	0.43173656
6.4	3.65470223	0.13436672	−0.22033944	−2.93111194	0.44959269
6.2	3.58600371	0.14216363	−0.20978613	−2.90481895	0.46368802
6.0	3.51448640	0.15011192	−0.20072775	−2.87816747	0.47416088
5.8	3.44100531	0.15803560	−0.19272428	−2.85129806	0.48114930
5.6	3.36638926	0.16580437	−0.18546082	−2.82433647	0.48475521
5.4	3.29145623	0.17324971	−0.17887823	−2.79739830	0.48498258
5.2	3.21700571	0.18042731	−0.17313406	−2.77054873	0.48178916
5.0	3.14384663	0.18719604	−0.16836795	−2.74385656	0.47482583
4.8	3.07277132	0.19350191	−0.16457238	−2.71734553	0.46344484
4.6	3.00457063	0.19931643	−0.16186244	−2.69096958	0.44644384
4.4	2.94003904	0.20464140	−0.16050978	−2.66454515	0.42169887
4.2	2.87996621	0.20949776	−0.16123093	−2.63762601	0.38554001
4.0	2.82512277	0.21390144	−0.16492727	−2.60926602	0.33183727
3.8	2.77625951	0.21788704	−0.16323985	−2.57756788	0.25115633
3.6	2.73412158	0.22161114	−0.14447269	−2.53885141	0.13149722
3.4	2.69934963	0.22528048	−0.13203593	−2.48640682	−0.03691349
3.2	2.67221064	0.22894796	−0.12744569	−2.40991888	−0.25285884
3.0	2.65229377	0.23248297	−0.12819956	−2.29932023	−0.49564693
2.8	2.63797886	0.23573791	−0.14163925	−2.15494404	−0.72742677
2.6	2.62604229	0.23892171	0.00000154	−1.99228828	−0.91438555
2.4	2.61174478	0.24245668	−0.00004348	−1.83009067	−1.04708308
2.2	2.59059964	0.24696914	−0.00007925	−1.67823755	−1.13316650
2.0	2.55921090	0.24919639	−0.00007037	−1.53705100	−1.18291423

Table 2
Electronic transition dipole moments for the molecular excited state $1^3\Sigma_u^+$.

R	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 1^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
90.0	3.34232711	−0.00001453	−0.16921895	3.34174074	0.00000978
88.0	3.34235411	−0.00001487	−0.16921336	3.34172730	0.00001089
86.0	3.34238375	−0.00001531	−0.16921138	3.34171285	0.00001186
84.0	3.34241630	−0.00001580	−0.16920919	3.34169696	0.00001293
82.0	3.34245212	−0.00001633	−0.16920673	3.34167945	0.00001413
80.0	3.34249163	−0.00001691	−0.16920397	3.34166011	0.00001545
78.0	3.34253531	−0.00001755	−0.16920084	3.34163871	0.00001692
76.0	3.34258375	−0.00001826	−0.16919727	3.34161495	0.00001856
74.0	3.34263759	−0.00001904	−0.16919315	3.34158852	0.00002039
72.0	3.34269763	−0.00001989	−0.16918837	3.34155903	0.00002242
70.0	3.34276479	−0.00002082	−0.16918278	3.34152602	0.00002469
68.0	3.34284013	−0.00002183	−0.16917618	3.34148896	0.00002720
66.0	3.34292501	−0.00002283	−0.16916855	3.34144722	0.00002997
64.0	3.34302091	−0.00002381	−0.16917469	3.34140001	0.00003300
62.0	3.34312969	−0.00002464	−0.16916298	3.34134642	0.00003629
60.0	3.34325350	−0.00002515	−0.16914896	3.34128533	0.00003982
58.0	3.34339496	−0.00002511	−0.16913228	3.34121539	0.00004357
56.0	3.34355719	−0.00002424	−0.16911269	3.34113494	0.00004758
54.0	−3.34374410	−0.00002229	−0.16908985	3.34104198	0.00005200
52.0	−3.34396061	−0.00001920	−0.16911267	3.34093402	0.00005711
50.0	−3.34421304	−0.00001524	−0.16907825	3.34080801	0.00006338
48.0	−3.34450957	−0.00002021	−0.16903628	3.34066008	0.00007155
46.0	−3.34486066	−0.00001714	−0.16898469	3.34048539	0.00004211
44.0	−3.34527971	−0.00001417	−0.16891827	3.34027764	0.00004967
42.0	−3.34578416	−0.00001124	−0.16882712	3.34002863	0.00005990
40.0	−3.34639696	−0.00000722	−0.16869607	3.33972754	0.00007179
38.0	−3.34714801	−0.00000015	−0.16850952	3.33935982	0.00007960
36.0	−3.34807774	0.00001230	−0.16829515	3.33890527	0.00007022
34.0	−3.34929107	0.00003032	−0.16797810	3.33833667	0.00003818
32.0	−3.35077633	0.00005361	−0.16754970	3.33761776	−0.00001021
30.0	−3.35268826	0.00008431	−0.16687063	3.33669706	−0.00006874
29.0	−3.35385247	0.00010109	−0.16634524	3.33613870	−0.00009939
28.0	−3.35519068	0.00012718	−0.16560748	3.33548052	−0.00013071
27.0	−3.35673763	0.00017223	−0.16455396	3.33474254	−0.00016469
26.0	−3.35853792	0.00025822	−0.16302054	3.33388762	−0.00016576
25.0	−3.36052893	0.00037400	−0.16104091	3.33291462	−0.00025720
24.0	−3.36300018	0.00050618	−0.15798264	3.33175382	−0.00039602
23.0	−3.36596002	0.00065798	−0.15365792	3.33038292	−0.00066947
22.0	−3.36950020	0.00082087	−0.14798213	3.32876530	−0.00108366
21.0	−3.37378408	−0.00106201	−0.14092996	3.32683355	−0.00190613
20.0	−3.37902432	−0.00134695	−0.13263952	3.32450892	−0.00341909
19.5	−3.38209118	−0.00150360	−0.12811999	3.32316738	−0.00460227
19.0	−3.38551475	−0.00166062	−0.12336858	3.32168576	−0.00616756
18.5	−3.38935136	−0.00183372	−0.11838584	3.32004811	−0.00830574
18.0	−3.39366633	−0.00196511	−0.11315564	3.31821088	−0.01110776
17.5	−3.39853914	−0.00206829	−0.10763615	3.31618337	−0.01465262
17.0	−3.40399447	−0.00213188	−0.10165016	3.31394728	−0.01899013
16.5	−3.41028384	−0.00214606	−0.09528101	3.31140896	−0.02370864
16.0	−3.41748881	−0.00211561	−0.08833066	3.30855167	−0.02848205
15.5	−3.42578848	−0.00206739	−0.08064924	3.30532144	−0.03295090
15.0	−3.43540482	−0.00204363	−0.07208197	3.30165203	−0.03703458
14.5	−3.44660221	−0.00225343	−0.06241315	3.29746233	−0.04100148
14.0	−3.45974030	−0.00293287	−0.05153270	3.29265281	−0.04537559
13.5	−3.47521553	−0.00453940	−0.03943265	3.28710693	−0.05084185
13.0	−3.49359308	−0.00790389	−0.02616785	3.28061440	−0.05824735
12.5	−3.51547865	−0.01421486	−0.01195153	3.27303855	−0.06864195
12.0	−3.54158796	−0.02483785	0.00363263	3.26408674	−0.08338631
11.5	−3.57274908	−0.04078426	0.02757082	3.25340460	−0.10435486
11.0	−3.60988444	−0.06229057	−0.11212289	3.24049288	−0.13421017
10.5	−3.65378342	−0.08941504	−0.17270480	3.22460663	0.17680257
10.0	−3.70528107	−0.12259601	−0.18925203	3.20453176	0.23740023
9.8	−3.72807738	−0.13780610	−0.19291941	3.19489776	0.26827675
9.6	−3.75212124	−0.15426519	−0.19675631	3.18408568	0.30379189
9.4	−3.77737669	−0.17208101	−0.19028655	3.17186872	0.34461787
9.2	−3.80377529	−0.19136968	−0.21449328	3.15789451	0.39141848
9.0	−3.83121906	−0.21224334	0.00000587	3.14178331	0.44490293
8.8	−3.85961069	−0.23483224	0.00013103	3.12305053	0.50576951
8.6	−3.88869240	−0.25920101	0.00007438	3.10111689	0.57456048
8.4	−3.91827360	−0.28547424	0.00001062	3.07530999	0.65166780
8.2	−3.94807470	−0.31373584	0.00000336	3.04491276	0.73712071
8.0	−3.97777496	−0.34405832	0.00000075	3.00923286	0.83045058
7.8	−4.00699743	−0.37649048	0.00000023	2.96772597	0.93054423
7.6	−4.03532099	−0.41105233	0.00000105	2.92014871	1.03557238
7.4	−4.06228284	−0.44771840	0.00000337	2.86671394	1.14303906

(*continued on next page*)

Table 2 (*continued*)

R	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 1^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 1^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
7.2	−4.08739321	−0.48640605	0.00000753	2.80820755	1.25000151
7.0	−4.11008128	−0.52695621	0.00001021	2.74586823	1.35344776
6.8	−4.12973353	−0.56912043	0.00000943	2.68139961	1.45070990
6.6	−4.14579508	−0.61258803	0.00001096	2.61657060	1.53977199
6.4	−4.15769039	−0.65696330	0.00001297	2.55299003	1.61958062
6.2	−4.16485938	−0.70176689	0.00001455	2.49189490	1.68981947
6.0	−4.16677545	−0.74643640	0.00001584	2.43403717	1.75086596
5.8	−4.16295782	−0.79032617	0.00001693	2.37966795	1.80354335
5.6	−4.15297682	−0.83269594	0.00001713	2.32857188	1.84884011
5.4	−4.13650796	−0.87274727	0.00000023	2.28009583	1.88752363
5.2	−4.11307056	−0.90947938	0.00000004	2.23316282	1.91964347
5.0	−4.08238997	−0.94201913	0.00000019	2.18633646	1.94424570
4.8	−4.04411958	−0.96946974	−0.00000007	2.13751009	1.96123775
4.6	−3.99786883	−0.99100963	−0.00000065	2.08372304	1.97578490
4.4	−3.94315486	−1.00593877	−0.00000099	2.02037522	1.99855761
4.2	−3.87933808	−1.01375256	−0.00000158	1.93938717	2.04035247
4.0	−3.80553985	−1.01425780	−0.00000289	1.82412082	2.11210254
3.8	−3.72058715	−1.00781333	−0.00000695	1.63245971	2.23440476
3.6	−3.62312050	−0.99567100	−0.00001508	1.23122757	2.45045905
3.4	−3.51189080	−0.98028761	0.00000222	0.26724492	2.70144117
3.2	−3.38648011	−0.96585470	0.00002153	0.80184711	2.55983347
3.0	−3.24822419	0.95990271	0.00005538	1.25344620	2.32927614
2.8	−3.09987642	0.97683908	0.00010669	1.43274702	2.17188026
2.6	−2.93872063	1.04615343	0.00005734	1.50570074	2.06154196
2.4	−2.73472664	1.22683781	−0.00013088	1.52411166	1.97946594
2.2	−2.39158151	1.59257925	−0.00018017	1.51029959	1.91246484
2.0	−1.83247184	−2.02618341	−0.00022499	1.47764164	1.84298836

Table 3
Electronic transition dipole moments for the molecular excited state $2^1\Sigma_g^+$.

R	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 2^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
90.0	0.00006128	−1.71826559	0.00018473	0.00002636	2.35714535
88.0	0.00006880	−1.71827762	0.00017466	−0.00003561	2.35670100
86.0	0.00007724	−1.71828974	0.00018952	−0.00003938	2.35624372
84.0	0.00008675	−1.71830290	0.00020611	−0.00004364	2.35574183
82.0	0.00009749	−1.71831712	0.00022479	0.00004846	2.35518977
80.0	0.00010967	−1.71833237	0.00024597	0.00005394	2.35458109
78.0	0.00012349	−1.71834839	0.00027043	0.00006017	2.35390836
76.0	0.00013925	−1.71836467	0.00025717	0.00006729	2.35316291
74.0	0.00015727	−1.71838041	0.00028745	0.00007545	2.35233465
72.0	0.00017792	−1.71839515	0.00032078	0.00008481	2.35141174
70.0	0.00020167	−1.71841023	0.00035842	0.00009559	2.35038028
68.0	0.00022905	−1.71842918	0.00040238	0.00010801	2.34922380
66.0	0.00026074	−1.71849463	0.00045475	0.00012249	2.34792280
64.0	0.00029747	−1.71852836	0.00052064	0.00013926	2.34645391
62.0	0.00034014	−1.71856628	0.00060730	0.00015879	2.34478912
60.0	0.00038980	−1.71860901	0.00072676	0.00018164	2.34289449
58.0	0.00044776	−1.71865732	0.00081709	0.00020849	2.34072865
56.0	0.00051575	−1.71871206	0.00105355	0.00024034	2.33824088
54.0	0.00059607	−1.71877403	0.00139235	0.00027856	2.33536765
52.0	0.00069186	−1.71884430	0.00186242	0.00032504	2.33202986
50.0	0.00080743	−1.71892457	0.00248618	0.00038221	2.32801657
48.0	0.00094876	−1.71901825	0.00328630	−0.00045331	2.32340259
46.0	0.00112412	−1.71912954	0.00415502	−0.00054226	2.31793641
44.0	0.00134465	−1.71926338	0.00557422	−0.00065422	2.31140987
42.0	0.00170955	−1.71941891	0.00778044	−0.00082514	2.30355224
40.0	0.00209253	−1.71964079	0.01121749	−0.00100929	2.29398918
38.0	0.00259027	−1.71994512	0.01682481	−0.00124773	2.28222977
36.0	0.00324657	−1.72038438	0.02688187	−0.00156033	2.26763007
34.0	0.00411448	−1.72102067	0.05200944	−0.00196882	2.24933084
32.0	0.00527498	−1.72196436	0.13982034	−0.00250947	2.22608257
30.0	0.00686588	−1.72348695	0.36861267	−0.00324301	2.19606808
29.0	0.00789217	−1.72466393	0.39645800	−0.00370891	2.17773590
28.0	0.00912937	−1.72633913	0.36647900	−0.00424701	2.15665685
27.0	0.01064021	−1.72882290	0.32676721	−0.00489584	2.13225581
26.0	0.01251211	−1.73266967	0.28534608	−0.00566921	2.10391359
25.0	0.01487258	−1.73843357	0.23635299	−0.00659567	2.07086662
24.0	0.01787467	−1.74696412	0.16605463	−0.00770253	2.03221609
23.0	0.02178842	1.75706921	0.04812551	−0.00902913	1.98698906
22.0	0.02700782	1.75701352	−0.16037150	−0.01063505	1.93388493
21.0	0.03423483	1.71328827	−0.47279772	−0.01260839	1.87187929
20.0	0.04467481	1.63199703	−0.76296094	−0.01501842	1.80013959
19.5	0.05175045	1.60602487	−0.85681970	0.01640908	1.76049312
19.0	0.06067958	1.60199242	−0.91604849	0.01793457	1.71840977
18.5	0.07189167	1.62254438	−0.94731490	0.01960205	1.67411001
18.0	0.08626637	1.66808213	−0.95692770	0.02141068	1.62791307
17.5	0.10490863	1.73872410	−0.94959829	0.02335954	1.58042002
17.0	0.12933699	1.83514344	−0.92855018	−0.02544051	1.53250566
16.5	0.16162995	1.95879693	−0.89591191	−0.02763785	1.48544679
16.0	0.20449147	2.11175255	−0.85315629	−0.02990420	1.44096609
15.5	0.26182543	2.29676038	−0.80107477	−0.03224699	1.40188407
15.0	0.33827921	2.51606442	−0.74019279	−0.03460548	1.37197821
14.5	0.43946071	2.77060644	−0.67109803	−0.03694587	1.35673048
14.0	0.57114975	3.05809757	−0.59444975	−0.03925112	1.36372285
13.5	0.73755382	3.36984621	−0.51149602	−0.04158151	1.40209116
13.0	0.93806092	3.68842339	−0.42464133	−0.04415236	1.47918682
12.5	1.16281973	3.98649687	−0.33743860	−0.04740213	1.59273093
12.0	1.38942015	4.23080814	−0.25474798	−0.05201415	1.72425898
11.5	1.58423767	4.39228182	−0.18123728	−0.05865769	1.84713716
11.0	1.70853369	4.45641699	−0.11864379	−0.06791090	−1.94183352
10.5	1.72789502	4.42751828	−0.06296343	−0.07975418	−2.00031241
10.0	1.61903928	4.32392390	−0.00038993	−0.09332591	−2.02027317
9.8	1.53694453	−4.26686734	0.03298787	−0.09886266	−2.01715885
9.6	1.43258511	−4.20307414	0.07650373	−0.10426058	−2.00747884
9.4	1.30626465	4.13363210	0.13656476	−0.10939657	−1.99097919
9.2	1.15855324	4.05875355	0.22372693	−0.11411670	−1.96720058
9.0	0.99038322	3.97660691	0.35594519	−0.11836410	−1.93564807
8.8	0.80298218	3.87922854	0.56443262	−0.12207703	−1.89571335
8.6	0.59780438	3.74309455	0.89794021	−0.12545685	−1.84665070
8.4	0.37663737	3.51201873	1.40118189	−0.12865601	−1.78770935
8.2	0.14152932	3.13351027	1.99804137	−0.13201693	−1.71814511
8.0	−0.10517554	2.70256140	2.45970039	−0.13602204	−1.63736650
7.8	−0.36087920	2.37465965	2.69682667	−0.14127380	−1.54501622
7.6	−0.62269500	2.17865787	2.77975908	−0.14847589	−1.44117623
7.4	−0.88745585	2.08036894	2.77608730	−0.15838625	−1.32625395

(*continued on next page*)

Table 3 (*continued*)

R	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 2^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 2^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
7.2	−1.15174260	2.04715274	2.72728682	−0.17176461	−1.20199449
7.0	−1.41204797	2.05747024	−2.65928767	−0.18928171	−1.07022689
6.8	−1.66475395	2.09769646	−2.59088276	−0.21153968	−0.93304625
6.6	−1.90636154	2.15889599	−2.53102796	−0.23905912	−0.79247776
6.4	−2.13368734	2.23496658	−2.48143742	−0.27201329	−0.65088809
6.2	−2.34407666	2.32021098	−2.44120045	−0.31042746	−0.51040062
6.0	−2.53516325	2.41155263	−2.40681741	−0.35427006	−0.37246471
5.8	−2.70546211	2.50548782	−2.37565788	−0.40309134	−0.23854143
5.6	−2.85393211	2.59912353	−2.34474822	−0.45628507	−0.10988885
5.4	−2.97982049	2.68945738	−2.31187860	−0.51305548	0.01202715
5.2	−3.08271473	2.77441552	−2.27659577	−0.57256652	0.12543544
5.0	−3.16204255	2.85099999	−2.23945902	−0.63389698	0.22778463
4.8	−3.21720278	2.91630525	−2.20090171	−0.69615200	0.31563375
4.6	−3.24730354	2.96691543	−2.16260600	−0.75856140	0.38415178
4.4	−3.25084532	2.99859107	−2.12690602	−0.82069220	0.42655688
4.2	−3.22535999	3.00573918	−2.09709836	−0.88281521	0.43365362
4.0	−3.16685510	2.98082764	−2.06450271	−0.94651199	0.39424998
3.8	−3.06938371	2.91403850	−1.88810859	−1.01565712	0.29860113
3.6	−2.92520495	2.79392463	1.50725180	−1.09802384	0.14788946
3.4	−2.72612964	2.61094225	1.25927534	−1.20405527	−0.02835804
3.2	−2.56460366	−2.45757626	−1.16229719	1.29877144	0.14494267
3.0	−0.00049144	0.00000452	−0.00013530	1.16788330	1.14406986
2.8	−0.00008917	0.00004217	0.01262042	1.35854999	0.91739959
2.6	0.00000099	0.00000875	−1.56227046	−1.48191106	−0.72629012
2.4	−0.00000830	−0.00002032	1.80637616	−1.54923309	−0.59784886
2.2	−0.00002124	−0.00006942	1.80524181	−1.57935396	−0.53137537
2.0	−0.00003161	−0.00052289	1.72835180	−1.58799238	−0.50396045

Table 4
Electronic transition dipole moments for the molecular excited state $2^3\Sigma_u^+$.

R	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 2^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
90.0	0.00005710	1.71826169	−0.00020711	−0.00003110	2.35714473
88.0	0.00006485	1.71827258	−0.00019632	−0.00003915	2.35670064
86.0	0.00007332	1.71828514	−0.00021189	−0.00004293	2.35624329
84.0	0.00008287	1.71829884	−0.00022922	−0.00004720	2.35574134
82.0	0.00009365	1.71831382	−0.00024859	−0.00005203	2.35518919
80.0	0.00010586	1.71833024	−0.00027027	−0.00005752	2.35458043
78.0	0.00011973	1.71834827	−0.00029473	−0.00006376	2.35390760
76.0	0.00013553	1.71836811	−0.00032238	−0.00007089	2.35316204
74.0	0.00015359	1.71838998	−0.00035381	−0.00007906	2.35233366
72.0	0.00017430	1.71841413	−0.00038973	−0.00008844	2.35141062
70.0	0.00019812	1.71844079	−0.00043121	−0.00009926	2.35037900
68.0	0.00022564	1.71847023	−0.00047987	−0.00011178	2.34922235
66.0	0.00025746	1.71850271	−0.00053845	−0.00012632	2.34792110
64.0	0.00029449	1.71853868	−0.00052060	−0.00014330	2.34645189
62.0	0.00033767	1.71857885	−0.00060919	−0.00016320	2.34478656
60.0	0.00038821	1.71862431	−0.00072901	−0.00018667	2.34289098
58.0	0.00044756	1.71867621	−0.00089840	−0.00021453	2.34072344
56.0	0.00051754	1.71873530	−0.00114245	−0.00024784	2.33823258
54.0	−0.00060052	1.71880205	−0.00149030	−0.00028794	2.33535481
52.0	−0.00069968	1.71887725	−0.00177484	−0.00033656	2.33201088
50.0	−0.00081941	1.71896253	−0.00239736	−0.00039593	2.32810122
48.0	−0.00096572	1.71901165	−0.00319144	−0.00046897	2.32350007
46.0	−0.00114701	1.71912002	−0.00420931	−0.00055947	2.31787940
44.0	−0.00137491	1.71925016	−0.00560286	−0.00067274	2.31134904
42.0	−0.00166560	1.71941112	−0.00767613	−0.00081591	2.30348813
40.0	−0.00204145	1.71962121	−0.01083518	−0.00099890	2.29393303
38.0	−0.00253280	1.71991605	−0.01540406	−0.00123650	2.28219084
36.0	−0.00317802	1.72034410	−0.02145747	−0.00154781	2.26761094
34.0	−0.00413207	1.72095776	−0.03017800	−0.00197212	2.24931924
32.0	−0.00529854	1.72187318	−0.04518111	−0.00251283	2.22607487
30.0	−0.00689515	1.72335398	−0.07499127	−0.00324568	2.19604664
29.0	−0.00792324	1.72433356	−0.09961365	−0.00371070	2.17769084
28.0	−0.00915975	1.72562812	−0.13358328	−0.00424617	2.15653363
27.0	−0.01066453	1.72738367	−0.17935609	−0.00489415	2.13201209
26.0	−0.01251754	1.72980645	−0.23947296	−0.00566733	2.10345551
25.0	−0.01482818	1.73309641	−0.31576463	−0.00659483	2.06987187
24.0	−0.01761586	1.73758989	−0.40901946	−0.00771018	2.03008204
23.0	−0.02140512	1.74381870	−0.51739837	−0.00905415	1.98244775
22.0	−0.02610630	1.75239326	−0.63588385	−0.01070201	1.92429266
21.0	−0.03219297	−1.76386220	−0.75712569	−0.01277058	1.85186901
20.0	−0.04020434	−1.77945025	−0.87427083	−0.01538019	1.75846911
19.5	−0.04516550	−1.78905610	−0.92999802	−0.01694300	1.70055364
19.0	−0.05089780	−1.80003695	−0.98343562	−0.01870091	1.63241755
18.5	−0.05759357	−1.81229569	−1.03546620	−0.02072118	1.55155388
18.0	−0.06541369	−1.82594953	−1.08646746	−0.02302478	1.45492043
17.5	−0.07457148	−1.84079655	−1.13739745	−0.02568359	1.34002605
17.0	−0.08532034	−1.85649960	−1.18954668	−0.02876415	1.20659720
16.5	−0.09796230	−1.87242964	−1.24459277	−0.03235566	1.05904925
16.0	−0.11285565	−1.88750821	−1.30469644	−0.03656900	0.90773764
15.5	−0.13042297	−1.89996029	−1.37265645	−0.04154031	0.76638431
15.0	−0.15115687	−1.90699146	−1.45215091	−0.04743411	0.64653803
14.5	−0.17567073	−1.90384312	−1.54798692	−0.05444480	0.55377814
14.0	−0.20448044	−1.88331130	−1.66639532	−0.06279396	0.48806089
13.5	−0.23829263	−1.83404400	−1.81506396	−0.07270966	0.44624378
13.0	−0.27787003	−1.73943301	−2.00139881	−0.08440372	0.42436710
12.5	−0.32402230	−1.58066124	−2.22790861	−0.09819546	0.41879800
12.0	−0.37764842	−1.34946564	−2.48684695	−0.11416988	0.42692839
11.5	−0.43967850	−1.06859642	−2.77147660	−0.13225993	0.44684571
11.0	−0.51120627	−0.78692737	2.81396036	−0.15206542	0.47763680
10.5	−0.59389535	−0.54293272	1.90298147	−0.17257937	−0.51927761
10.0	−0.68990078	−0.34634636	1.60461584	−0.19172946	−0.57268159
9.8	−0.73275026	−0.27941238	1.53539381	−0.19820540	−0.59772658
9.6	−0.77856413	−0.21792451	1.51127599	−0.20350395	−0.62510324
9.4	−0.82771594	−0.16098950	1.30144626	−0.20724686	−0.65506773
9.2	−0.88063262	−0.10770889	1.41482332	−0.20871512	−0.68788264
9.0	−0.93789663	−0.05715488	−0.00028107	−0.20722963	−0.72381816
8.8	−1.00029866	−0.00855449	−0.00062200	−0.20190776	−0.76317654
8.6	−1.06873082	0.03960462	−0.00035013	−0.19150009	−0.80640927
8.4	−1.14431165	0.08853133	−0.00005644	−0.17472003	−0.85387389
8.2	−1.22949781	0.13998336	−0.00002058	−0.14965204	−0.90620743
8.0	−1.32734089	0.19690878	−0.00000902	−0.11371293	−0.96434717
7.8	−1.44376421	0.26402079	−0.00000412	−0.06317595	−1.02993278
7.6	−1.59003866	0.35017094	−0.00000197	0.00835226	−1.10628963
7.4	−1.79028734	0.47400362	0.00000001	0.11386079	−1.20079780

(*continued on next page*)

Table 4 (*continued*)

R	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 2^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 2^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
7.2	−2.10285803	0.68096170	0.00000435	0.28545258	−1.33099959
7.0	−2.66998539	1.09369227	0.00000236	0.61235256	−1.53293143
6.8	−3.51798798	1.82982012	−0.00001446	1.20784937	−1.74700599
6.6	3.78564032	−2.25520735	−0.00002073	−1.65264382	1.68339729
6.4	3.67415977	−2.31634702	−0.00007658	−1.85092274	1.54776790
6.2	3.52881857	−2.29124766	−0.00012410	−1.98195408	1.43500470
6.0	3.39384730	−2.24520647	−0.00014292	−2.09127702	1.33248797
5.8	3.27156393	−2.19371752	−0.00014693	−2.18980698	1.22594495
5.6	3.16067690	−2.14231817	−0.00013001	−2.28131672	1.10122877
5.4	3.05978643	−2.09438885	−0.00006652	−2.36753395	0.94107407
5.2	2.96904985	−2.05147351	−0.00008026	−2.44942741	0.72704091
5.0	2.88816400	−2.01561301	−0.00008928	−2.52716163	0.44898856
4.8	2.81763796	−1.98819207	−0.00009804	−2.60074044	0.12962606
4.6	2.75850251	−1.97015315	−0.00010676	−2.66947535	−0.17294289
4.4	2.71241283	−1.96181707	−0.00012269	−2.73174718	−0.40795709
4.2	2.68177073	−1.96259035	−0.00014194	−2.78416734	−0.57529631
4.0	2.66989312	−1.97056963	−0.00016528	−2.81895436	−0.71974087
3.8	2.68116403	−1.98204750	−0.00019083	−2.81482821	−0.91960196
3.6	2.72090656	−1.99102249	−0.00021897	−2.68766697	−1.33007041
3.4	2.79499134	−1.98845825	−0.00006406	−2.09616848	−2.17499301
3.2	2.90900451	−1.96423959	−0.00006320	1.13737229	−2.80200921
3.0	3.06936030	1.89964837	−0.00005707	0.63538265	−2.93844815
2.8	3.28889562	1.76634973	−0.00008536	0.41059011	−2.93845216
2.6	3.59658155	1.50383399	−0.00010812	0.32153125	−2.88784334
2.4	4.01352418	1.00067166	−0.00024688	0.35225567	−2.79238477
2.2	4.39442295	0.12340025	−0.00018079	0.54876404	−2.59690728
2.0	4.25943325	0.79176555	−0.00005050	0.90778824	−2.20133861

Table 5
Electronic transition dipole moments for the molecular excited state $3^1\Sigma_g^+$.

R	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 3^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
90.0	−1.72287950	0.00001384	−5.99240557	1.71580126	0.00000693
88.0	−1.72321233	0.00001913	−5.99260433	−1.71563768	0.00000620
86.0	−1.72357672	0.00002218	−5.99281699	−1.71545480	0.00000642
84.0	−1.72397651	0.00002551	−5.99305094	−1.71525404	0.00000663
82.0	−1.72441604	0.00002912	−5.99330902	1.71503309	0.00000682
80.0	−1.72490021	0.00003287	−5.99359460	1.71478916	0.00000698
78.0	−1.72543454	0.00003642	−5.99391177	1.71451885	0.00000707
76.0	−1.72602520	0.00003914	−5.99426075	1.71421783	0.00000708
74.0	−1.72667918	0.00004006	−5.99465753	1.71388070	0.00000699
72.0	−1.72740519	0.00003852	−5.99510246	1.71350125	0.00000676
70.0	−1.72821527	0.00003574	−5.99559937	1.71307388	0.00000635
68.0	−1.72912556	0.00003478	−5.99614926	1.71259489	0.00000567
66.0	−1.73019207	0.00009921	−5.99672138	1.71212999	0.00000395
64.0	−1.73135737	0.00011609	−5.99741188	1.71154113	0.00000206
62.0	−1.73267773	0.00013559	−5.99818449	1.71087288	−0.00000064
60.0	−1.73417977	0.00015831	−5.99904780	1.71011128	−0.00000444
58.0	−1.73589583	0.00018548	−5.99999105	1.70923965	−0.00000970
56.0	−1.73786526	0.00021934	−6.00107024	1.70823772	−0.00001688
54.0	−1.74013622	0.00026392	−6.00228347	1.70708046	−0.00002679
52.0	−1.74276840	0.00032577	−6.00366241	1.70573647	−0.00004045
50.0	−1.74583688	0.00041463	−6.00525484	1.70416617	−0.00008061
48.0	−1.74943742	0.00054532	−6.00712872	−1.70231915	−0.00011118
46.0	−1.75369222	0.00073706	−6.00931966	−1.70012966	−0.00015286
44.0	−1.75875607	0.00102177	−6.01201000	−1.69751664	−0.00021081
42.0	−1.76481090	0.00146612	−6.01525590	−1.69436895	−0.00029287
40.0	−1.77218380	0.00220359	−6.01921058	−1.69053965	−0.00041164
38.0	−1.78122245	0.00346342	−6.02410310	−1.68583358	−0.00059008
36.0	−1.79244632	0.00565835	−6.02955539	−1.67997644	−0.00086161
34.0	−1.80655918	0.00963313	−6.02864152	−1.67256478	−0.00127367
32.0	−1.82456419	0.01761171	−5.93662670	−1.66298374	−0.00188542
30.0	−1.84800120	0.03619317	−4.84135900	−1.65019996	−0.00272963
29.0	−1.86250423	0.05486983	−3.94534346	−1.64204123	−0.00320847
28.0	−1.87947732	0.08670842	−3.50917498	−1.63217598	−0.00361460
27.0	−1.89961717	0.14324828	−3.46789561	−1.61981268	−0.00382513
26.0	−1.92396522	0.24807633	−3.72338909	−1.60364501	−0.00343348
25.0	−1.95370269	0.45230705	−4.27013545	−1.58090370	−0.00145741
24.0	−1.99029953	0.87574237	−5.17872902	−1.54561425	0.00402629
23.0	2.03282708	1.80592291	6.55485652	1.48351747	−0.01755368
22.0	2.06777761	3.85317323	8.29860677	1.36242268	−0.04748580
21.0	2.05620563	7.46836258	9.36305593	1.14339723	−0.10096015
20.0	1.99813134	11.04608634	8.53488566	0.87268613	−0.16495572
19.5	1.98020602	12.16862540	7.71188542	−0.75432561	−0.19372989
19.0	1.98315604	12.84086345	6.88055002	−0.65631414	−0.21864989
18.5	2.01048958	13.17248576	6.13005797	−0.57757488	−0.23935028
18.0	2.06291859	13.26524006	5.48486419	−0.51488758	−0.25548419
17.5	2.14021746	13.19305006	4.94067739	−0.46488906	−0.26621636
17.0	2.24215904	13.00477504	4.48426548	0.42476180	−0.27018738
16.5	2.36876455	12.73120720	4.10174794	0.39234005	−0.26536536
16.0	2.52020425	12.39082799	3.78141290	0.36602825	−0.24888515
15.5	2.69647624	11.99363826	3.51452472	0.34468951	−0.21684700
15.0	2.89688950	11.54354983	3.29451659	0.32755414	−0.16385251
14.5	3.11934552	11.03997369	3.11797464	0.31419722	−0.08283850
14.0	3.35961648	10.47915334	2.98363793	0.30430252	0.03505139
13.5	3.61017850	9.85660134	2.89344318	0.29806270	0.19850692
13.0	3.86097427	9.16960819	2.85211495	0.29579110	0.41057502
12.5	4.10111460	8.42158359	2.86931693	0.29809611	0.65824287
12.0	4.32286102	7.62415216	2.96059765	0.30599227	0.90800892
11.5	4.52577980	6.79382010	3.14793987	0.32065577	1.12621936
11.0	−4.71728227	−5.94018053	−3.45535708	−0.34348836	1.30573171
10.5	−4.90455684	−5.05060249	−3.89530001	−0.37544129	1.46156598
10.0	−5.07819536	−4.08106322	−4.44530259	−0.41661242	1.61154057
9.8	−5.13608579	3.65516289	−4.68135253	−0.43572659	1.67326466
9.6	−5.18241677	3.19796694	−4.91757766	−0.45685085	1.73803779
9.4	−5.21385526	−2.69933813	−5.14771542	−0.48085592	1.80826177
9.2	−5.22767968	−2.14187010	−5.36536614	−0.50910783	1.88748417
9.0	−5.22195261	−1.49559676	−5.56155315	−0.54364201	1.98039156
8.8	−5.19530296	−0.70404044	−5.71569011	−0.58717303	2.09291157
8.6	−5.14671525	0.31991034	−5.76984758	−0.64270109	2.23097963
8.4	−5.07444520	1.66146993	−5.57889703	−0.71395024	2.40179209
8.2	−4.97565433	3.18216068	−4.95703881	−0.80494388	2.61257265
8.0	−4.84583652	4.45312429	−4.00921607	−0.91986301	2.87028566
7.8	−4.67868172	5.30442384	−3.06997607	−1.06243663	3.18035246
7.6	4.46677334	−5.86612556	2.29070394	1.23461261	−3.54379859
7.4	4.20398135	−6.25571515	1.69276845	1.43435842	−3.95329031

(*continued on next page*)

Table 5 (*continued*)

R	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 3^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 3^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
7.2	3.89006409	−6.52071885	1.27899179	1.65332553	−4.38786803
7.0	3.53557454	−6.67283335	−1.04205436	1.87670085	−4.81525355
6.8	3.16221966	−6.71854308	−0.95375991	2.08715822	−5.20180686
6.6	2.79559285	−6.67388245	−0.96978442	2.27115938	−5.52456297
6.4	2.45558981	−6.56304982	−1.04680621	2.42255648	−5.77687554
6.2	2.15171062	−6.41098692	−1.15456486	2.54157117	−5.96465667
6.0	1.88618002	−6.23546999	−1.27167568	2.63127067	−6.09828787
5.8	1.65548647	−6.04928958	−1.38857509	2.69575497	−6.18927832
5.6	1.45503188	−5.86010650	−1.49973525	2.73853369	−6.24692668
5.4	1.28055446	−5.67190855	−1.60228960	2.76221553	−6.27802984
5.2	1.12869873	−5.48980227	−1.69476335	2.76862683	−6.28716608
5.0	0.99738366	−5.31581434	−1.77678851	2.75907272	−6.27710100
4.8	0.88628104	−5.15264710	−1.84484603	2.73393824	−6.24840013
4.6	0.79592329	−5.00355914	−1.89779955	2.69367048	−6.20135178
4.4	0.73716924	4.89048964	1.92727792	2.65142945	−6.15832897
4.2	0.68778390	4.76381177	1.93693242	2.55652808	6.01513606
4.0	0.00018877	0.00030922	0.00010726	−0.32515976	−2.15452924
3.8	−0.00016545	−0.00030656	−0.00050400	−0.01446098	−1.95945035
3.6	−0.00044089	−0.00071237	−0.00064462	0.30729167	−1.76812697
3.4	−0.00006053	0.00001335	−0.00005150	0.62270914	−1.57587982
3.2	0.00131412	0.00090134	0.00003297	0.91509992	−1.36982011
3.0	−2.15776613	−2.07008433	−1.05101242	1.54035730	−0.26948320
2.8	−1.82529831	−1.76137818	−1.12363607	1.74779636	−0.26316901
2.6	−1.51328573	−1.47435092	−0.00011831	1.93236399	−0.20400540
2.4	1.22309176	1.19131888	0.00040421	−2.08160877	−0.14375973
2.2	−1.06387421	−1.00127363	0.00050109	2.15071387	−0.13331279
2.0	0.92879338	0.74358550	0.00005439	−2.19976607	0.15266381

Table 6
Electronic transition dipole moments for the molecular excited state $3^3\Sigma_u^+$.

R	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 3^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
90.0	−1.72287411	−0.00001399	5.99240803	−1.71580511	0.00000670
88.0	−1.72320731	−0.00001910	5.99260620	−1.71564057	0.00000602
86.0	−1.72357213	−0.00002230	5.99281776	−1.71545748	0.00000624
84.0	−1.72397246	−0.00002589	5.99305040	−1.71525655	0.00000645
82.0	−1.72441273	−0.00002996	5.99330681	−1.71503558	0.00000663
80.0	−1.72489805	−0.00003461	5.99359008	−1.71479196	0.00000678
78.0	−1.72543434	−0.00003996	5.99390377	−1.71452272	0.00000686
76.0	−1.72602847	−0.00004619	5.99425205	−1.71422438	0.00000685
74.0	−1.72668842	−0.00005347	5.99463968	−1.71389284	0.00000673
72.0	−1.72742357	−0.00006201	5.99507214	−1.71352331	0.00000644
70.0	−1.72824487	−0.00007201	5.99555564	−1.71311006	0.00000590
68.0	−1.72916524	−0.00008366	5.99609710	−1.71264626	0.00000503
66.0	−1.73019999	−0.00009694	5.99670373	−1.71212370	0.00000370
64.0	−1.73136752	−0.00011203	5.99737489	−1.71153253	0.00000173
62.0	−1.73269008	−0.00012916	5.99813668	−1.71086121	−0.00000111
60.0	−1.73419472	−0.00014916	5.99898731	−1.71009636	−0.00000519
58.0	−1.73591410	−0.00017361	5.99993655	−1.70922214	−0.00001093
56.0	−1.73788749	−0.00020503	6.00099840	−1.70821879	−0.00001894
54.0	1.74016273	−0.00024734	6.00219375	−1.70706090	−0.00002993
52.0	1.74279940	−0.00030706	6.00351251	−1.70571625	−0.00004489
50.0	1.74587250	−0.00039415	6.00508691	−1.70414448	−0.00006521
48.0	1.74942592	−0.00055694	6.00714464	−1.70235075	−0.00009497
46.0	1.75367670	−0.00074944	6.00940248	−1.70016674	−0.00016403
44.0	1.75873669	−0.00103512	6.01211894	−1.69755893	−0.00022402
42.0	1.76480917	−0.00147996	6.01541921	−1.69441955	−0.00030840
40.0	1.77217028	−0.00220960	6.01951038	−1.69060205	−0.00042921
38.0	1.78119809	−0.00343125	6.02482359	−1.68590710	−0.00060723
36.0	1.79241003	−0.00545476	6.03210595	−1.68005896	−0.00087844
34.0	1.80648743	−0.00878160	6.04247762	−1.67266976	−0.00129366
32.0	1.82446180	−0.01440310	6.05702585	−1.66317834	−0.00191289
30.0	−1.84787672	0.02431366	−6.07629528	1.65066043	0.00275510
29.0	−1.86217792	0.03213741	−6.08829811	1.64298443	0.00327876
28.0	−1.87876179	0.04282637	−6.10145193	1.63405842	0.00381894
27.0	−1.89815418	0.05746053	−6.11506195	1.62357599	0.00428137
26.0	−1.92105043	0.07748105	−6.12765110	1.61119616	0.00440553
25.0	−1.94828073	0.10473884	−6.13698901	1.59646872	0.00383162
24.0	−1.98098435	0.14170590	−6.14001627	1.57883684	0.00172088
23.0	−2.02078858	0.19160957	−6.13408138	1.55758160	−0.00347799
22.0	−2.06999080	0.25841339	−6.11868724	1.53179868	−0.01462933
21.0	−2.13158962	−0.34638738	−6.09981486	1.50041973	−0.03713906
20.0	−2.21087969	−0.46055456	−6.08775646	1.46187696	−0.08043689
19.5	−2.25924018	−0.52867348	−6.08843763	1.43936707	−0.11454743
19.0	−2.31491420	−0.60451738	−6.09585148	1.41432814	−0.16014930
18.5	−2.37932634	−0.68797023	−6.11151552	1.38643018	−0.21985402
18.0	−2.45419590	−0.77852164	−6.13673878	1.35528012	−0.29505045
17.5	−2.54154077	−0.87486306	−6.17296937	1.32041659	−0.38405206
17.0	−2.64384589	−0.97481540	−6.22058845	1.28119530	−0.47950113
16.5	−2.76372100	−1.07459272	−6.28052946	1.23692756	−0.56615474
16.0	−2.90405627	−1.16807918	−6.35409296	1.18680467	−0.62294317
15.5	−3.06725113	−1.24586473	−6.44025992	1.12981897	−0.63189241
15.0	−3.25470135	−1.29328179	−6.53683446	1.06504049	−0.58474085
14.5	−3.46530053	−1.28799790	−6.63812329	0.99187235	−0.48461614
14.0	−3.69428777	−1.19798295	−6.73055208	0.91064563	−0.34174873
13.5	3.93213353	0.98121475	6.78903530	−0.82335344	0.16920444
13.0	4.16580413	0.59273386	6.77098223	−0.73411314	−0.01963494
12.5	4.38183926	0.00894492	6.60310645	−0.64892694	−0.21277488
12.0	4.56969260	−0.72584802	6.14828664	−0.57423376	−0.40099528
11.5	4.72256017	−1.47595786	5.00342577	−0.51578309	−0.57900770
11.0	4.83587255	−2.08810661	−0.22827236	−0.47827544	−0.74509669
10.5	4.90474397	−2.49715799	4.73539230	−0.46594205	0.89971963
10.0	4.92264774	−2.72681604	−6.03179693	−0.48379078	1.04378796
9.8	4.91365341	−2.78032968	−6.33488005	−0.50078840	1.09840704
9.6	4.89450647	−2.81692055	−6.54260179	−0.52417602	1.15114514
9.4	4.86455806	−2.83945862	−6.38675985	−0.55443077	1.20163353
9.2	4.82318048	−2.85032089	−7.24459957	−0.59234197	1.24925379
9.0	4.76980470	−2.85156813	−0.00164359	−0.63847956	1.29341066
8.8	4.70368003	−2.84427084	−0.00581582	−0.69337564	1.33304989
8.6	4.62468571	−2.83025711	−0.00359010	−0.75757194	1.36689086
8.4	4.53216347	−2.80986079	−0.00069733	−0.83127709	1.39323161
8.2	4.42572923	−2.78341049	−0.00039328	−0.91453055	1.41005948
8.0	4.30435096	−2.75069559	−0.00025659	−1.00664669	1.41465100
7.8	4.16580649	−2.71091510	−0.00018654	−1.10620766	1.40339056
7.6	4.00444411	−2.66209015	−0.00014720	−1.21052012	1.37062527
7.4	3.80509276	−2.59866183	−0.00013472	−1.31417819	1.30500808

(*continued on next page*)

Table 6 (*continued*)

R	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 3^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 3^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
7.2	3.52014361	−2.50277778	−0.00012477	−1.40255844	1.17722820
7.0	2.97375192	−2.29514005	−0.00007393	−1.41922325	0.89002153
6.8	1.66899332	−1.68492394	−0.00000836	−1.13841090	0.21762743
6.6	0.25210991	−0.90425236	−0.00003638	−0.63947670	−0.44623922
6.4	−0.41601618	−0.50338333	−0.00005582	−0.33734095	−0.73993926
6.2	−0.73914592	−0.29735866	−0.00006229	−0.15115033	−0.87710323
6.0	−0.92527376	−0.16440329	−0.00006303	−0.00757887	−0.95176059
5.8	−1.04442469	−0.05730312	−0.00006256	0.12396929	−0.99339071
5.6	−1.12351036	0.04729160	−0.00005938	0.26032219	−1.01197690
5.4	−1.17379976	0.16331190	−0.00000422	0.41333873	−1.00986969
5.2	−1.19920352	0.29151620	−0.00001219	0.58636819	−0.98574541
5.0	−1.20953731	0.38999300	−0.00002706	0.75245408	−0.94155095
4.8	−1.23931503	0.33335133	−0.00005888	0.82356268	−0.89900853
4.6	−1.31013222	0.03085051	−0.00008743	0.71940889	−0.89213968
4.4	−1.35902456	−0.31051130	0.00010255	0.54656843	−0.89467179
4.2	−1.36232199	−0.49482047	0.00011043	0.44463022	−0.85617811
4.0	−1.35109289	−0.55392044	0.00011608	0.41722433	−0.77820137
3.8	−1.34433191	−0.54791283	0.00012099	0.44081782	−0.68064652
3.6	−1.34405727	−0.50143598	0.00012571	0.51929744	−0.55481908
3.4	−1.33782139	−0.40940566	0.00001496	0.66458128	−0.31315963
3.2	−1.29312700	−0.23309695	−0.00000643	−0.74173765	−0.01806975
3.0	−1.14218372	−0.11046667	−0.00002651	−0.79958549	0.14464295
2.8	−0.77947613	−0.64600578	−0.00043192	−0.96236683	0.16151617
2.6	0.00025863	0.00090894	−2.29691436	1.23741603	−0.41702273
2.4	0.00005724	0.00009551	−2.21138176	1.29846181	−0.01704903
2.2	−0.00006271	0.00025146	−2.54387431	1.32458539	0.06060886
2.0	0.00487576	0.00751290	−2.93946081	1.33520164	−0.08058350

Table 7
Electronic transition dipole moments for the molecular excited state $4^1\Sigma_g^+$.

R	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 4^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
90.0	−2.25962672	0.00033764	−0.01309353	1.70296346	0.00004362
88.0	−2.22594257	0.00033837	−0.01405670	−1.73347174	0.00004079
86.0	−2.26506854	0.00039796	−0.01509839	−1.72194370	0.00003650
84.0	−2.29520804	0.00045786	−0.01624145	−1.70689026	0.00003114
82.0	−2.31971438	0.00052113	−0.01749821	1.69321962	0.00002578
80.0	−2.34031167	0.00058982	−0.01888279	1.68105632	0.00002054
78.0	−2.35828291	0.00066618	−0.02041136	1.67000332	0.00001542
76.0	−2.37452845	0.00075255	−0.02209968	1.65967565	0.00001037
74.0	−2.38967873	0.00085152	−0.02397779	1.64976467	0.00000533
72.0	−2.40423438	0.00096619	−0.02606697	1.63999044	0.00000022
70.0	−2.41854948	0.00110019	−0.02839773	1.63012803	−0.00000501
68.0	−2.43290381	0.00125796	−0.03100622	1.61990840	−0.00001051
66.0	−2.44553128	0.00146148	−0.03440768	1.60672327	−0.00001862
64.0	−2.46253796	0.00166999	−0.03724011	1.59975736	−0.00002074
62.0	−2.47805124	0.00193798	−0.04098038	1.58802986	−0.00002697
60.0	−2.49413803	0.00226038	−0.04523509	1.57593810	−0.00003318
58.0	−2.51085371	0.00264988	−0.05008481	1.56325235	−0.00003951
56.0	−2.52827121	0.00312265	−0.05567441	1.54988105	−0.00004594
54.0	−2.54651662	0.00369984	−0.06213557	1.53571133	−0.00005226
52.0	−2.56883127	0.00447582	−0.06911258	1.51846674	−0.00007252
50.0	−2.58936444	0.00537808	−0.07778973	1.50210154	−0.00007306
48.0	−2.61155931	0.00651200	−0.08800734	−1.48420987	−0.00007799
46.0	−2.63585995	0.00795246	−0.10009119	−1.46437510	−0.00007933
44.0	−2.66270440	0.00980683	−0.11458968	−1.44216828	−0.00007350
42.0	−2.69204996	0.01234719	−0.13126618	−1.41772103	−0.00003682
40.0	−2.72565768	0.01560361	−0.15262827	−1.38906248	0.00001017
38.0	−2.76402002	0.02004197	−0.17930069	−1.35571529	0.00010021
36.0	−2.80866582	0.02628026	−0.21347281	−1.31596673	0.00026580
34.0	−2.86134128	0.03552798	−0.26007800	−1.26762558	0.00057724
32.0	−2.92352740	0.05087903	−0.33748193	−1.20833863	0.00122539
30.0	−2.99980620	0.08375172	−0.54210723	−1.13131778	0.00276075
29.0	−3.04695399	0.12229445	−0.79582363	−1.07976153	0.00461128
28.0	−3.10774857	0.21845585	−1.43493008	−1.00354708	0.00925814
27.0	−3.19518324	0.65174807	−4.15378707	−0.80706255	0.02961061
26.0	1.36230584	−3.50698835	20.44685944	−0.23365446	−0.15836384
25.0	0.60323313	−4.21656184	20.70782950	−0.37283038	−0.17682499
24.0	0.38112773	−5.13001947	19.58213905	−0.46620552	−0.19458591
23.0	0.18580642	6.51025515	17.77445298	−0.60436801	−0.21800653
22.0	−0.08836339	8.30935285	14.75995400	−0.81445089	−0.24496015
21.0	−0.46877552	9.55350762	10.11498069	−1.07642840	−0.26991175
20.0	−0.82256905	8.93328761	5.45533393	−1.28178670	−0.29241682
19.5	−0.94186676	8.17300212	3.77529135	1.34217670	−0.30735092
19.0	−1.01974573	7.37989942	2.53565001	1.37954736	−0.32747985
18.5	−1.06140324	6.65298229	1.62698867	1.40043497	−0.35416958
18.0	−1.07203610	6.02360700	0.94761668	1.40997053	−0.38849649
17.5	−1.05480016	5.49089787	0.42351057	1.41164677	−0.43164709
17.0	−1.01058901	5.04246668	0.00552836	−1.40773671	−0.48513283
16.5	−0.93805187	4.66336983	−0.33763632	−1.39971430	−0.55104414
16.0	−0.83343821	4.33902679	−0.62516385	−1.38852845	−0.63235290
15.5	−0.69006428	4.05532943	−0.86739723	−1.37471107	−0.73322237
15.0	−0.49725213	3.79715963	−1.06823879	−1.35827384	−0.85990326
14.5	0.23880521	−3.54531852	1.22285250	1.33819945	1.02062200
14.0	−0.10762268	−3.27127945	1.31532364	1.31142988	1.22498238
13.5	−0.56351839	−2.93207935	1.31431655	1.27085250	1.47848462
13.0	−1.11707236	−2.47969698	1.18438963	1.20641148	1.76932580
12.5	−1.67177358	−1.91637938	0.94135739	1.11933901	2.06099224
12.0	−2.08726240	−1.33331869	0.69561937	1.03828869	2.32195318
11.5	−2.30699644	−0.81692248	0.56861258	0.99840693	2.55533622
11.0	−2.35052134	−0.38609422	0.62737958	1.01640941	−2.79304156
10.5	−2.24632222	−0.04110920	0.91446413	1.09909447	−3.07950140
10.0	−2.02768206	0.18760500	1.44969483	1.24963487	−3.44705041
9.8	−1.92272539	−0.23216550	1.72126369	1.32778129	−3.61572869
9.6	−1.81807729	−0.24249080	2.00954689	1.41419617	−3.79149540
9.4	−1.72220900	0.21367057	2.29779709	1.50667105	−3.96803269
9.2	−1.64357820	0.14014508	2.56675142	1.60284571	−4.14003052
9.0	−1.58964755	0.01220373	2.79659523	1.69997684	−4.30073497
8.8	−1.56650765	−0.18869797	2.96544862	1.79529518	−4.44441787
8.6	−1.57862856	−0.49334981	3.04536411	1.88646910	−4.56694375
8.4	−1.62918147	−0.92644926	2.99100135	1.97046238	−4.66321847
8.2	−1.72063568	−1.40181205	2.77368742	2.04381751	−4.72735987
8.0	−1.85464347	−1.68852659	2.50263903	2.10206581	−4.75117176
7.8	−2.03116022	−1.67699618	2.34225258	2.13943028	−4.72348880
7.6	−2.24623228	−1.40959755	2.33676392	2.14893814	−4.63061344
7.4	−2.48859659	−0.93973625	2.45975480	2.12363238	−4.45984920

(*continued on next page*)

Table 7 (*continued*)

R	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 4^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 4^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
7.2	−2.73621274	−0.31223633	2.66796278	2.05924558	−4.20592748
7.0	−2.96063490	0.43375230	−2.91747348	1.95807881	−3.87828541
6.8	−3.13173575	1.24458158	−3.17467620	1.83500787	−3.51405872
6.6	−0.00723391	0.00396018	−0.00768378	−1.52776653	−3.29532499
6.4	−0.00157667	0.00053516	−0.00196674	−1.54836512	−3.27096411
6.2	0.00001917	−0.00007634	−0.00025788	−1.56059162	−3.24329203
6.0	0.00008422	−0.00001281	−0.00007661	−1.56185298	−3.20880696
5.8	0.00007001	−0.00000675	−0.00006066	−1.55004356	−3.16693263
5.6	0.00000436	0.00001165	−0.00005135	−1.52337112	−3.11655552
5.4	0.00000793	0.00010118	−0.00008265	−1.47922790	−3.05714226
5.2	−0.00021028	0.00125273	−0.00014775	−1.41412301	−2.98550493
5.0	−0.00028839	0.00173890	−0.00009904	−1.32407966	−2.89973176
4.8	−0.00009268	0.00063064	−0.00004151	−1.20436272	−2.79683257
4.6	0.00079054	0.00491868	−0.00126305	−1.05913907	−2.68371494
4.4	−0.00068781	−0.00443151	0.00270591	−0.84709454	−2.51300465
4.2	−0.00010621	−0.00027999	0.00049573	−0.60715629	−2.34475767
4.0	−0.67864702	−4.68297637	1.87524856	2.45500581	5.85630482
3.8	−0.70781193	−4.63361907	1.56134554	2.32452611	5.63544204
3.6	−0.78141931	−4.61830460	1.06323817	2.15512202	5.34133026
3.4	0.90188851	4.63148430	−0.77315251	−1.93620336	−4.99949488
3.2	1.06306478	4.65415392	−0.61845507	−1.65867024	−4.65827328
3.0	1.24865227	4.65951532	−0.53991375	−1.32775440	−4.36148368
2.8	1.43504874	4.62534972	−0.61176707	−0.97207830	−4.11099677
2.6	1.59043650	4.54112304	0.00019216	−0.65047194	−3.89332385
2.4	1.69351705	4.36869624	−0.00011295	−0.41774636	3.70850057
2.2	1.72686525	4.20582431	−0.00005482	−0.33373978	3.61634822
2.0	1.74256784	4.05584388	−0.00134835	−0.26044819	3.52730998

Table 8
Electronic transition dipole moments for the molecular excited state $4^3\Sigma_u^+$.

R	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 4^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
90.0	−2.29676846	−0.00036426	0.01307076	−1.69574475	0.00002998
88.0	−2.23268005	−0.00034562	0.01404911	−1.72536896	0.00003969
86.0	−2.27097003	−0.00040488	0.01509087	−1.71773956	0.00003581
84.0	−2.29999224	−0.00046402	0.01623420	−1.70366542	0.00003034
82.0	−2.32358208	−0.00052659	0.01749128	−1.69063480	0.00002484
80.0	−2.34343413	−0.00059468	0.01887626	−1.67896812	0.00001947
78.0	−2.36079785	−0.00067052	0.02040555	−1.66831666	0.00001425
76.0	−2.37654880	−0.00075645	0.02209815	−1.65831615	0.00000911
74.0	−2.39129949	−0.00085509	0.02397630	−1.64867012	0.00000399
72.0	−2.40553721	−0.00096958	0.02606589	−1.63910716	−0.00000118
70.0	−2.41960661	−0.00110362	0.02839750	−1.62940884	−0.00000649
68.0	−2.43376353	−0.00126168	0.03100711	−1.61932578	−0.00001209
66.0	−2.44820392	−0.00144909	0.03393764	−1.60626156	−0.00002023
64.0	−2.46325273	−0.00167339	0.03722855	−1.59923200	−0.00002256
62.0	−2.47879810	−0.00194207	0.04096737	−1.58748751	−0.00002902
60.0	−2.49498846	−0.00226582	0.04521689	−1.57532198	−0.00003560
58.0	−2.51187074	−0.00265771	0.05007036	−1.56251884	−0.00004246
56.0	−2.52948335	−0.00313429	0.05564272	−1.54899783	−0.00004962
54.0	2.54791556	−0.00371707	0.06207773	−1.53467875	−0.00005698
52.0	2.56734243	−0.00443458	0.06949733	−1.51940885	−0.00006431
50.0	2.58804020	−0.00532548	0.07823629	−1.50294807	−0.00007112
48.0	2.61157193	−0.00653672	0.08773095	−1.48430210	−0.00007904
46.0	2.63584897	−0.00798603	0.09980622	−1.46449383	−0.00007765
44.0	2.66268091	−0.00985276	0.11425370	−1.44230644	−0.00007097
42.0	2.69254852	−0.01229289	0.13171960	−1.41724396	−0.00005055
40.0	2.72610856	−0.01553847	0.15310605	−1.38862077	−0.00000493
38.0	2.76357427	−0.02008951	0.17869680	−1.35614024	0.00011727
36.0	2.80821359	−0.02623806	0.21202224	−1.31641668	0.00028388
34.0	2.86071554	−0.03500301	0.25470589	−1.26828402	0.00058493
32.0	2.92244392	−0.04790409	0.31010037	−1.20968029	0.00114610
30.0	2.99472750	−0.06765711	0.38384539	−1.13805147	0.00224031
29.0	3.03549936	−0.08178950	0.43061835	−1.09604708	0.00316067
28.0	3.07988302	−0.10022760	0.48664164	−1.04871237	0.00450439
27.0	3.12834501	−0.12481916	0.55499459	−0.99505943	0.00649738
26.0	3.18136288	−0.15837235	0.64007592	−0.93344035	0.00958873
25.0	3.23926434	−0.20526611	0.74820100	−0.86189279	0.01419767
24.0	3.30238459	−0.27250121	0.88954268	−0.77734299	0.02129366
23.0	3.36986030	−0.37092292	1.07791658	−0.67632910	0.03244988
22.0	3.43934285	−0.51652805	1.33247063	−0.55446597	0.04969511
21.0	3.50459345	0.73001598	1.67535459	−0.40734184	0.07622833
20.0	3.55286989	1.03096311	2.12395471	−0.23268985	0.11382362
19.5	3.56459360	1.21506386	2.38512655	−0.13631655	0.13579884
19.0	3.56441251	1.41683898	2.66259870	−0.03591477	0.15760033
18.5	3.55019728	1.62861134	2.94435260	0.06622820	0.17569255
18.0	3.52065595	1.83833984	3.21595804	0.16746915	0.18450109
17.5	3.47581591	2.03317654	3.46028839	0.26544479	0.17732589
17.0	3.41633386	2.20013114	3.66152641	0.35852213	0.14764615
16.5	3.34263016	2.32797578	3.80660809	0.44601089	0.09217847
16.0	3.25392789	2.40797155	3.88578412	0.52805660	0.01397131
15.5	3.14766654	2.43391815	3.89226386	0.60526426	−0.07707919
15.0	3.01962147	2.40187554	3.82211844	0.67818582	−0.16720904
14.5	2.86473755	2.31272740	3.67399767	0.74678798	−0.24246263
14.0	2.68066612	2.17206317	3.45306457	0.81005617	−0.29045620
13.5	2.46945590	1.99511221	3.17500398	0.86602043	−0.30075449
13.0	2.24138585	1.80943177	2.86791189	0.91273857	−0.26579248
12.5	2.01531920	1.65711246	2.57382960	0.94895754	−0.18068555
12.0	1.81431664	1.59283177	2.35485746	0.97655745	−0.04445397
11.5	1.66084612	1.67018038	2.35177731	1.00010052	0.14073887
11.0	1.57297147	1.91193956	−3.07223494	1.02598078	0.36875389
10.5	1.56134002	2.28776011	−3.40734884	1.06005451	−0.62475401
10.0	1.62530503	2.71766397	3.65389540	1.10494622	−0.87913411
9.8	1.66914735	2.88186986	3.76571885	1.12587775	−0.97132153
9.6	1.72124566	3.03281535	3.83536403	1.14844749	−1.05422868
9.4	1.77979694	3.16623515	3.55775814	1.17257405	−1.12513109
9.2	1.84284149	3.27958568	3.94817416	1.19865841	−1.18359781
9.0	1.90829821	3.37192016	0.00192184	1.22685389	−1.22834252
8.8	1.97378910	3.44281965	0.00385920	1.25752934	−1.25909807
8.6	2.03727324	3.49628954	0.00235109	1.29071266	−1.27612218
8.4	2.09617077	3.53373154	0.00053312	1.32660664	−1.27993640
8.2	2.14797677	3.55798208	0.00031700	1.36513961	−1.27135780
8.0	2.19022025	3.57189233	0.00020790	1.40599671	−1.25142801
7.8	2.22065819	3.57809117	0.00014313	1.44858444	−1.22140907
7.6	2.23753714	3.57879582	0.00009836	1.49201179	−1.18278916
7.4	2.23987817	3.57571025	0.00005550	1.53509841	−1.13728386

(*continued on next page*)

Table 8 (*continued*)

R	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 4^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 4^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
7.2	2.22745452	3.57001830	−0.00001099	1.57716801	−1.08690090
7.0	2.20169709	3.56248917	−0.00007929	1.61560669	−1.03341961
6.8	−2.16378558	−3.55342712	−0.00011753	−1.64996272	0.97888834
6.6	−2.11601396	−3.54280362	−0.00009710	−1.67911947	0.92440012
6.4	−2.06071099	−3.53012637	−0.00005078	−1.70217924	0.87178559
6.2	−2.00060345	−3.51451095	−0.00003120	−1.71847380	0.81928883
6.0	−1.93742978	−3.49435109	−0.00001697	−1.72701228	0.76451138
5.8	−1.87208040	−3.46738770	−0.00000554	−1.72670844	0.70232798
5.6	−1.80395315	−3.43104826	0.00000689	−1.71671915	0.62363845
5.4	−1.73019909	−3.38441691	0.00009463	−1.69821052	0.51468238
5.2	−1.64419531	−3.33134180	0.00007304	−1.67865053	0.35877947
5.0	−1.53038297	−3.29203367	0.00010071	−1.68562141	0.15612458
4.8	−1.36524564	−3.29296590	0.00010471	−1.75922305	−0.05357930
4.6	−1.14105439	−3.31564708	0.00009889	−1.90233103	−0.19921657
4.4	−0.93906760	−3.29755145	0.00004560	−2.02278508	−0.28198264
4.2	−0.82136066	−3.25188231	0.00014982	−2.07916325	−0.34839108
4.0	−0.76769804	−3.19673264	0.00016627	−2.08359634	−0.42306884
3.8	−0.74807515	−3.12593053	0.00020891	−2.03475033	−0.53575506
3.6	−0.75168580	−3.02654950	0.00018652	−1.88482817	−0.76899685
3.4	−0.78164734	−2.88010735	−0.00007115	−1.44555006	−1.23373256
3.2	−0.85353699	−2.66432093	−0.00034766	0.83968420	−1.44586132
3.0	−0.99722391	2.36208834	0.00861404	0.54669208	−1.22148791
2.8	0.00031799	0.00027102	2.92819219	−1.07504419	1.33111493
2.6	0.29926191	1.03020519	1.86857430	1.19115921	0.15378357
2.4	−0.13215462	1.20580923	−0.00138487	1.33245767	0.62581921
2.2	−0.72914796	1.56128357	0.00042795	1.33186336	1.12655168
2.0	1.55679232	2.56401808	0.00008685	−1.14505396	−1.65833421

Table 9
Electronic transition dipole moments for the molecular excited state $5^1\Sigma_g^+$.

R	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 5^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
90.0	0.00143663	0.00000420	0.00004207	2.35010653	0.00000683
88.0	0.00125221	0.00000560	0.00005892	2.36925098	−0.00002052
86.0	0.00141944	0.00000601	0.00006346	2.36893882	−0.00002305
84.0	0.00162596	0.00000648	0.00006894	2.36866483	−0.00002593
82.0	0.00188653	0.00000704	0.00007568	−2.36844538	−0.00002924
80.0	0.00222576	0.00000771	0.00008423	−2.36831476	−0.00003304
78.0	0.00268183	0.00000855	0.00009539	−2.36831950	−0.00003741
76.0	0.00332304	0.00000962	0.00011003	−2.36854862	−0.00004248
74.0	0.00428467	0.00001108	0.00013323	−2.36918638	−0.00004836
72.0	0.00587052	0.00001325	0.00017083	−2.37065012	−0.00005526
70.0	0.00894775	0.00001698	0.00024299	−2.37414795	−0.00006346
68.0	0.07810044	0.00006051	0.00162192	−2.45907107	−0.00011149
66.0	0.06397048	0.00005580	0.00142696	−2.44277371	−0.00011074
64.0	0.04983486	0.00005108	0.00123192	−2.42647097	0.00011258
62.0	0.04521491	0.00004698	0.00121726	−2.41016921	−0.00015383
60.0	0.01775262	0.00001887	0.00052087	−2.37245554	−0.00016625
58.0	0.00946737	0.00000979	0.00029996	−2.35996933	−0.00018685
56.0	0.00595576	0.00000554	0.00020407	−2.35364678	−0.00021263
54.0	0.00415916	0.00000312	0.00015412	−2.34939208	−0.00024431
52.0	0.00314711	0.00000147	0.00012598	−2.34587451	−0.00028288
50.0	0.00254883	0.00000014	0.00011019	−2.34252563	−0.00034613
48.0	0.00117257	0.00000806	0.00007740	−2.33473420	0.00042230
46.0	0.00078822	0.00000879	0.00007064	−2.33156019	0.00049644
44.0	0.00054364	0.00001023	0.00006603	−2.32751919	0.00058654
42.0	0.00042035	0.00001251	0.00006821	−2.32249128	0.00069678
40.0	0.00040598	0.00001619	0.00007895	−2.31626428	0.00083223
38.0	0.00041120	0.00002254	0.00009258	−2.30854720	0.00099904
36.0	0.00038024	0.00000882	0.00006719	−2.30003430	0.00119015
34.0	0.00022786	0.00000856	0.00005314	−2.28854024	0.00145261
32.0	0.00005862	0.00000842	0.00001372	−2.27401692	0.00179910
30.0	−0.00004749	0.00001425	−0.00009517	−2.25522428	0.00227044
29.0	−0.00006654	0.00002465	−0.00024608	−2.24375510	0.00257063
28.0	−0.00004787	0.00004992	−0.00048589	−2.23045292	0.00295173
27.0	0.00005168	0.00009365	−0.00091871	−2.21517983	0.00338457
26.0	0.02590530	0.01890576	−0.10130693	2.21952426	−0.00296371
25.0	3.02231557	0.56132919	−2.52921926	1.12143464	0.02662036
24.0	3.12432438	0.52445435	−1.72578618	1.02434736	0.02486617
23.0	3.19083741	−0.61927483	−1.36443709	0.95645758	0.02950522
22.0	3.24797392	−0.80937504	−1.08495476	0.89625171	0.03957092
21.0	3.30188119	−1.04950535	−0.74447187	0.83755091	0.05621606
20.0	−3.35462761	1.22737610	0.34205458	−0.77706191	−0.08180994
19.5	−3.38076026	1.27885970	0.14723659	0.74537287	−0.09880043
19.0	−3.40663306	1.31419031	−0.03763554	0.71239019	−0.11906151
18.5	−3.43208778	1.34077210	−0.21570565	0.67797367	−0.14291388
18.0	−3.45681212	1.36400515	−0.39125137	0.64212494	−0.17054329
17.5	−3.48016551	1.38749567	−0.56890613	0.60516702	−0.20219388
17.0	−3.50139565	1.41446363	−0.75169367	−0.56784911	−0.23777074
16.5	−3.51940756	1.44831229	−0.94212994	−0.53158589	−0.27707997
16.0	−3.53269375	1.49363549	−1.14243566	−0.49874144	−0.31991019
15.5	−3.53906702	1.55734487	−1.35511060	−0.47299819	−0.36657420
15.0	−3.53492061	1.65012900	−1.58510518	−0.45986499	−0.41881283
14.5	−3.51342311	1.78799775	−1.84022275	−0.46728077	−0.48279789
14.0	−3.45935976	1.99219273	−2.13596628	−0.50640326	−0.57501591
13.5	−3.34165420	2.28142772	−2.49071353	−0.58948077	−0.72956248
13.0	−3.11028567	2.64171370	−2.91389278	−0.71996515	−0.99649777
12.5	−2.73671681	2.99399116	−3.38540185	−0.87427019	−1.39723843
12.0	−2.27720167	3.25260518	−3.87770035	−1.01151474	−1.86855799
11.5	−1.82062138	3.42137733	−4.39575031	−1.11311752	−2.30862501
11.0	−1.40274967	3.56366717	−4.93709176	−1.18164633	2.64954294
10.5	−1.01100487	3.74367110	−5.44690636	−1.21751731	2.85277662
10.0	−0.00004334	0.00022676	−0.00017788	0.34529222	−2.57452466
9.8	−0.00000366	−0.00010027	0.00005205	0.42866309	−2.66102886
9.6	0.00001528	−0.00001100	0.00016715	0.51097075	−2.74106604
9.4	0.00001591	−0.00004055	0.00015207	0.59246331	−2.81498032
9.2	0.00000005	0.00000379	0.00001778	0.67335056	−2.88310983
9.0	0.00000338	−0.00001254	0.00002973	0.75385595	−2.94659217
8.8	0.00002476	−0.00001567	−0.00002805	0.83393993	−3.00539329
8.6	0.00003112	−0.00001346	−0.00003094	0.91331950	−3.05974400
8.4	0.00003813	−0.00002128	−0.00006051	0.99165092	−3.10970417
8.2	0.00005041	0.00001592	−0.00010516	1.06837461	−3.15515654
8.0	0.00008297	0.00010547	−0.00016623	1.14276502	−3.19572455
7.8	0.00018722	0.00030262	−0.00031833	1.21393923	−3.23074394
7.6	0.00040074	0.00076320	−0.00058850	1.28094077	−3.25945659
7.4	−0.00062766	−0.00002437	0.00064312	1.34413313	−3.28368033

(*continued on next page*)

Table 9 (*continued*)

R	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|1^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|2^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_z^{el}\|3^1\Sigma_u^+\rangle$	$\langle 5^1\Sigma_g^+\|\mu_{x(y)}^{el}\|1^1\Pi_u\rangle$	$\langle 5^1\Sigma_g^+\|\mu_{x(y)}^{el}\|2^1\Pi_u\rangle$
7.2	−0.00042825	−0.00027722	0.00050821	1.40039642	−3.29818262
7.0	0.00156100	0.00219846	0.00056944	−1.45975815	−3.30201938
6.8	1.94574756	0.84336172	2.06287331	1.54826927	−3.13924795
6.6	3.24759723	2.36588577	3.50642922	1.63717596	2.97574566
6.4	3.25395533	2.89618053	−3.65792528	1.54790445	−2.73630841
6.2	3.20679760	3.70084360	−3.88383258	1.42014636	−2.39257261
6.0	3.10036362	4.48853787	−4.09870508	1.30778701	−2.08000138
5.8	2.94716167	5.25378858	−4.29739317	1.21117702	−1.79257544
5.6	2.76187098	5.97667210	−4.47299560	1.12882064	−1.52290705
5.4	2.56046229	6.63285553	−4.60978701	1.05885419	−1.26665776
5.2	2.36065586	7.19579962	−4.70169384	0.99996275	−1.02430198
5.0	2.17929241	7.64439810	−4.74065518	0.95180007	−0.80442912
4.8	2.02737634	7.97937378	−4.72537178	0.91394639	−0.61326642
4.6	1.91187230	8.20696265	−4.64783596	0.88679972	−0.45882439
4.4	1.83552166	8.33969592	−4.47882451	0.87072571	−0.34613395
4.2	1.79940937	8.38822557	−4.12345981	0.86707369	−0.27901838
4.0	1.80414294	8.36003641	−3.24218815	0.87907334	−0.25930561
3.8	1.85033810	8.25919394	−1.04996756	0.91466580	−0.28587226
3.6	1.93723894	8.08478370	1.04233782	0.99677134	−0.35264004
3.4	2.05181204	7.77056617	1.66753917	1.21203923	−0.43341800
3.2	1.88884950	5.99743780	1.05612784	1.94795030	−0.45180114
3.0	1.58047638	4.70924969	−0.29603516	2.05953784	−0.56058408
2.8	−0.90795480	−1.98096700	−0.54121374	−2.17078447	0.66903030
2.6	0.69694546	1.67815043	−0.02268742	2.05229443	−0.89429954
2.4	−0.52652502	−1.68348658	0.04693232	−1.91417949	0.93090584
2.2	−0.37497960	−1.92537435	0.00014853	−1.73161215	0.72966246
2.0	−0.25905703	−2.20326136	−0.00075871	−1.59768382	0.50001515

Table 10
Electronic transition dipole moments for the molecular excited state $5^3\Sigma_u^+$.

R	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 5^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
90.0	0.00217686	−0.00000652	−0.00006747	−2.34490029	0.00001341
88.0	0.00125224	−0.00000564	−0.00005825	2.36924909	−0.00002265
86.0	0.00141948	−0.00000606	−0.00006277	2.36893692	−0.00002520
84.0	0.00162600	−0.00000654	−0.00006823	2.36866289	−0.00002812
82.0	0.00188657	−0.00000710	−0.00007499	2.36844339	−0.00003145
80.0	0.00222579	−0.00000777	−0.00008362	2.36831273	−0.00003528
78.0	0.00268187	−0.00000860	−0.00009499	2.36831742	−0.00003968
76.0	0.00332309	−0.00000965	−0.00011069	2.36854651	−0.00004478
74.0	0.00428472	−0.00001106	−0.00013384	2.36918419	−0.00005070
72.0	0.00587059	−0.00001313	−0.00017148	2.37064789	−0.00005763
70.0	0.00894798	−0.00001671	−0.00024378	2.37414586	−0.00006588
68.0	0.07773065	−0.00005979	−0.00161537	2.45858428	−0.00011372
66.0	0.06395971	−0.00005566	−0.00142854	2.37014483	−0.00011433
64.0	0.05018327	−0.00005152	−0.00124162	−2.28167383	0.00011493
62.0	0.04516064	−0.00004682	−0.00121498	2.41006540	−0.00015667
60.0	0.01776993	−0.00001879	−0.00052087	2.37244067	−0.00016958
58.0	0.00949905	−0.00000975	−0.00030306	2.35996999	−0.00019100
56.0	0.00597565	−0.00000555	−0.00020725	2.35365111	−0.00021829
54.0	−0.00417930	−0.00000313	−0.00015733	2.34939423	−0.00025176
52.0	−0.00316843	−0.00000147	−0.00012252	2.34587502	−0.00029253
50.0	−0.00258846	−0.00000004	−0.00010716	2.34252346	−0.00034196
48.0	−0.00126581	−0.00000801	−0.00008432	−2.33468708	0.00041702
46.0	−0.00092796	−0.00000872	−0.00007517	−2.33149289	0.00049488
44.0	−0.00072254	−0.00001029	−0.00007238	−2.32743295	0.00058490
42.0	−0.00059828	−0.00001292	−0.00007460	−2.32240672	0.00069530
40.0	−0.00051693	−0.00001667	−0.00008004	−2.31625158	0.00083148
38.0	−0.00039135	−0.00002180	−0.00008265	−2.30873968	0.00099944
36.0	−0.00010158	−0.00003093	−0.00010096	−2.29946016	0.00120858
34.0	−0.00029782	−0.00000893	−0.00004575	−2.28872390	0.00145366
32.0	−0.00018070	−0.00000784	−0.00003493	−2.27415178	0.00180089
30.0	−0.00006273	0.00002604	−0.00002154	−2.25539648	0.00227084
29.0	0.00001018	−0.00003257	0.00001572	2.24397402	−0.00256821
28.0	−0.00003466	−0.00003881	0.00001058	2.23074531	−0.00291720
27.0	−0.00007261	−0.00004082	0.00000743	2.21560191	−0.00332400
26.0	−0.00010480	−0.00003785	0.00000674	2.19804308	−0.00379881
25.0	−0.00012971	−0.00004120	0.00001381	2.17758483	−0.00429924
24.0	−0.00015099	−0.00004492	0.00003592	2.15363719	−0.00478736
23.0	0.00017496	0.00004342	0.00000628	−2.12551929	0.00513861
22.0	0.00002997	0.00001790	0.00001335	−2.09201385	0.00496215
21.0	0.00003686	−0.00001144	0.00001921	−2.05218043	0.00359860
20.0	0.00004342	−0.00000869	0.00002436	−2.00453247	−0.00072180
19.5	0.00004537	−0.00000525	0.00002547	−1.97725802	−0.00502728
19.0	0.00004572	0.00000038	0.00002749	−1.94737671	−0.01171498
18.5	0.00004255	0.00001038	0.00002796	−1.91469661	−0.02167503
18.0	0.00003503	0.00001463	0.00002878	−1.87885606	−0.03605577
17.5	0.00002565	0.00001869	0.00002968	−1.83976296	−0.05578307
17.0	0.00000269	−0.00000338	−0.00001788	−1.79716860	−0.08082699
16.5	0.00000162	−0.00000675	−0.00002141	−1.75098272	−0.10984812
16.0	0.00000153	−0.00001183	−0.00002624	−1.70112093	−0.13906067
15.5	0.00000353	−0.00001852	−0.00003273	−1.64763645	−0.16368297
15.0	0.00000832	−0.00002763	−0.00003922	−1.59070527	−0.17957687
14.5	0.00000262	−0.00003376	−0.00005665	−1.53062089	−0.18427234
14.0	0.00000178	0.00000257	−0.00002056	−1.46785009	−0.17677702
13.5	0.00000182	0.00000487	−0.00001848	−1.40262229	−0.15649412
13.0	0.00000485	0.00001184	0.00000005	−1.33503875	−0.12279516
12.5	0.00000562	0.00002836	0.00000202	−1.26476390	−0.07448442
12.0	0.00000562	0.00004651	0.00000247	−1.19021609	−0.00948277
11.5	0.00000878	0.00005990	0.00000244	−1.10786256	0.07557333
11.0	−0.00001493	0.00002374	0.00006650	1.01107380	−0.18555122
10.5	−0.00000414	−0.00003503	−0.02080034	0.88608822	0.32920259
10.0	−0.00000292	−0.00001365	0.05635098	0.70833684	0.51867000
9.8	0.00000118	0.00001301	−0.11561797	0.61362724	0.61053237
9.6	0.00000686	0.00003679	−0.00540377	0.50028942	0.71280114
9.4	0.00001385	−0.00000967	0.82740175	−0.36477173	−0.82494428
9.2	0.00002685	−0.00005381	0.00405794	−0.20400300	−0.94579569
9.0	0.00006570	−0.00007337	2.49182248	−0.01672596	−1.07180934
8.8	0.00004101	−0.00001418	2.82219053	0.19150820	−1.19437923
8.6	0.00004384	−0.00000926	3.14902668	0.41438705	−1.30609869
8.4	0.00003593	−0.00001176	3.44908211	0.64019148	−1.39798211
8.2	0.00001683	−0.00000930	3.70766965	0.85826516	−1.46426576
8.0	−0.00003102	0.00002176	3.91771302	1.06168419	−1.50313219
7.8	0.00037437	−0.00026723	4.03585018	−1.19454640	1.51493474
7.6	−0.37302467	0.32972374	0.01600480	0.85011907	−0.34843260
7.4	−0.36424446	0.39399284	−0.03993018	0.90068709	−0.34678477

(*continued on next page*)

Table 10 (*continued*)

R	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|1^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|2^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_z^{el}\|3^3\Sigma_g^+\rangle$	$\langle 5^3\Sigma_u^+\|\mu_{x(y)}^{el}\|1^3\Pi_g\rangle$	$\langle 5^3\Sigma_u^+\|\mu_{x(y)}^{el}\|2^3\Pi_g\rangle$
7.2	−0.34984618	0.47531185	−0.04344676	0.94451713	−0.30789576
7.0	−0.33208007	0.54751120	−0.00860597	0.96897098	−0.24762533
6.8	−0.30958230	0.61481210	−0.00108079	1.00157474	−0.18913121
6.6	−0.28071143	0.68030431	0.00033433	1.03527329	−0.12606521
6.4	−0.24335918	0.74719796	0.00066935	1.06891137	−0.05805951
6.2	−0.19518427	0.81895416	0.00039989	1.10350174	0.01495910
6.0	−0.13235274	0.89884129	0.00016197	1.13949980	0.09313573
5.8	−0.04954929	0.98973230	−0.00111403	1.17748074	0.17639764
5.6	0.05918977	1.09197992	−0.00645888	1.21657125	0.26474307
5.4	0.20254888	1.19918570	−0.02234352	1.25134418	0.35935897
5.2	−0.02258646	−0.07711427	4.28347944	−2.62906698	0.46712164
5.0	−0.00043481	−0.00132393	4.25522320	−2.61055112	0.26812641
4.8	0.00004602	0.00010857	4.21619825	−2.65347701	0.01076541
4.6	0.00006296	0.00015891	4.17405473	−2.69131069	−0.23235686
4.4	0.00005804	0.00014793	4.12847195	−2.72087503	−0.42165709
4.2	0.00005488	0.00014195	4.07881675	−2.73848340	−0.55733708
4.0	0.00005401	0.00014816	4.02399607	−2.73672617	−0.67473110
3.8	0.00005351	0.00016849	3.96218885	−2.69558414	−0.83757415
3.6	0.00005635	0.00030046	3.89024505	−2.54268014	−1.17758101
3.4	−0.00026952	−0.00035324	3.80191271	−1.99738959	−1.88311671
3.2	−0.00006109	0.00050523	3.68127943	1.20745699	−2.32327838
3.0	−0.00113691	0.00218943	3.46439829	0.94601781	−2.12803119
2.8	−1.18283196	1.90748645	0.00156756	0.37066386	−0.79913224
2.6	−1.20048914	1.33540851	−0.00046504	0.21629874	−0.41148954
2.4	−1.05402939	0.95879807	−0.00097497	0.13133106	−0.23793534
2.2	−0.84273256	0.85054038	−0.00146730	0.08811949	−0.22324685
2.0	−0.48573570	−1.01229556	0.00257236	−0.02888848	−0.44474917

Table 11
Electronic transition dipole moments for the molecular excited states $1^1\Sigma_u^+$ and $1^3\Sigma_g^+$.

R	$\langle 1^1\Sigma_u^+ \mid \mu_{x(y)}^{el} \mid 1^1\Pi_g\rangle$	$\langle 1^1\Sigma_u^+ \mid \mu_{x(y)}^{el} \mid 2^1\Pi_g\rangle$	$\langle 1^3\Sigma_g^+ \mid \mu_{x(y)}^{el} \mid 1^3\Pi_u\rangle$	$\langle 1^3\Sigma_g^+ \mid \mu_{x(y)}^{el} \mid 2^3\Pi_u\rangle$
90.0	0.00003186	2.36488917	0.00003517	2.36488962
88.0	0.00003954	2.36502112	0.00004306	2.36502152
86.0	0.00004373	2.36515414	0.00004725	2.36515455
84.0	−0.00004846	2.36529967	0.00005199	2.36530008
82.0	−0.00005380	2.36545917	−0.00005734	2.36545959
80.0	−0.00005986	2.36563436	−0.00006341	2.36563478
78.0	−0.00006676	2.36582718	−0.00007032	2.36582761
76.0	−0.00007462	2.36603987	−0.00007819	2.36604032
74.0	−0.00008361	2.36627503	−0.00008719	2.36627549
72.0	−0.00009392	2.36653564	−0.00009752	2.36653612
70.0	−0.00010578	2.36682518	−0.00010942	2.36682571
68.0	−0.00011942	2.36714768	−0.00012316	2.36714829
66.0	−0.00013529	2.36750785	−0.00013909	2.36750860
64.0	−0.00015364	2.36791119	−0.00015764	2.36791222
62.0	−0.00017497	2.36836415	−0.00017932	2.36836571
60.0	−0.00019983	2.36887436	−0.00020479	2.36887682
58.0	−0.00022897	2.36945086	−0.00023491	2.36945480
56.0	−0.00026339	2.37010456	−0.00027076	2.37011074
54.0	−0.00030456	2.37084904	0.00031377	−2.37085800
52.0	−0.00035446	2.37170078	0.00036575	−2.37171280
50.0	−0.00041569	2.37267996	0.00042910	−2.37269508
48.0	0.00049168	2.37381113	0.00050691	−2.37382873
46.0	0.00058668	2.37512398	0.00060320	−2.37514348
44.0	0.00070576	2.37669681	0.00072327	−2.37667544
42.0	0.00088108	2.37851172	−0.00087390	−2.37846836
40.0	0.00107130	2.38061801	−0.00106358	−2.38057523
38.0	0.00131071	2.38309917	−0.00130285	−2.38305820
36.0	0.00161514	2.38601362	−0.00160613	−2.38597528
34.0	0.00201024	2.38941386	−0.00201290	−2.38942287
32.0	0.00253897	2.39336202	−0.00254107	−2.39336898
30.0	0.00326502	2.39789656	−0.00326614	−2.39789609
29.0	0.00374557	2.40037637	−0.00373105	−2.40036294
28.0	0.00430306	2.40302532	−0.00430770	−2.40293103
27.0	−0.00496852	2.40572789	−0.00497393	−2.40559466
26.0	−0.00576635	2.40845947	−0.00577316	−2.40814776
25.0	−0.00672934	2.41112458	−0.00673786	−2.41042349
24.0	−0.00789351	2.41358139	−0.00787049	−2.41203127
23.0	−0.00931729	2.41566352	−0.00934258	−2.41230148
22.0	0.01109284	2.41716379	−0.01113463	−2.40978698
21.0	0.01329044	2.41791551	−0.01336898	−2.40165214
20.0	0.01605908	2.41798357	−0.01620007	−2.38150541
19.5	0.01770046	2.41794174	−0.01790149	−2.36265826
19.0	0.01960128	2.41805374	−0.01983703	−2.33362129
18.5	0.02169945	2.41863549	−0.02204776	−2.28817493
18.0	0.02407601	2.42014889	−0.02460596	−2.21597630
17.5	0.02677864	2.42327478	−0.02754060	−2.10063512
17.0	0.02986629	2.42896908	−0.03095428	−1.92112582
16.5	0.03341574	2.43853471	−0.03495894	−1.66756118
16.0	0.03752828	2.45353136	−0.03970330	−1.37026495
15.5	0.04234287	2.47579581	−0.04538776	−1.09425851
15.0	0.04805202	2.50716111	−0.05228443	−0.88431487
14.5	0.05492667	2.54900829	−0.06081515	−0.74493009
14.0	0.06335000	2.60152726	−0.07138887	−0.66236642
13.5	0.07385478	2.66274286	−0.08480981	−0.62127283
13.0	0.08718914	2.72771411	−0.10189428	−0.61017409
12.5	0.10421827	2.78864922	−0.12393020	−0.62127085
12.0	0.12610220	2.83631313	−0.15247470	−0.64941802
11.5	0.15413979	2.86286493	−0.18937558	−0.69119145
11.0	0.18976237	2.86404545	−0.23668760	−0.74431315
10.5	0.23433499	2.83966091	−0.29605057	−0.80749111
10.0	0.28911063	2.79196603	−0.36846701	−0.88094943
9.8	0.31412301	2.76700947	−0.40104670	−0.91379246
9.6	0.34098939	2.73893492	−0.43555685	−0.94916713
9.4	0.36975420	2.70778924	−0.47184513	−0.98772027
9.2	0.40045046	2.67390142	−0.50974850	−1.03034819
9.0	0.43310176	2.63720945	−0.54905741	−1.07836584
8.8	0.46770978	2.59785315	−0.58958629	−1.13344170
8.6	0.50426484	2.55581247	−0.63109898	−1.19752980
8.4	0.54273372	2.51116217	−0.67320076	−1.27183645
8.2	0.58306270	2.46392932	−0.71571488	1.35422644
8.0	0.62517185	2.41411935	−0.75837964	1.43492825
7.8	0.66894459	2.36175613	−0.80093284	1.49795181
7.6	0.71421894	2.30684904	−0.84311026	1.53582729
7.4	0.76077623	2.24948096	−0.88464700	1.55716859

(*continued on next page*)

Table 11 (*continued*)

R	$\langle 1^1\Sigma_u^+\|\mu_{x(y)}^{el}\|1^1\Pi_g\rangle$	$\langle 1^1\Sigma_u^+\|\mu_{x(y)}^{el}\|2^1\Pi_g\rangle$	$\langle 1^3\Sigma_g^+\|\mu_{x(y)}^{el}\|1^3\Pi_u\rangle$	$\langle 1^3\Sigma_g^+\|\mu_{x(y)}^{el}\|2^3\Pi_u\rangle$
7.2	0.80834126	2.18982704	−0.92524578	1.57429645
7.0	0.85653391	2.12828847	−0.96454423	1.59418601
6.8	0.90489441	2.06533499	−1.00223125	1.61905583
6.6	0.95291911	2.00148698	−1.03798635	1.64920141
6.4	0.99997758	1.93744332	−1.07141365	1.68368457
6.2	1.04534375	1.87406207	−1.10209822	1.72182092
6.0	1.08818095	1.81239469	−1.12959982	1.76287923
5.8	1.12752023	1.75372249	−1.15345099	1.80618902
5.6	1.16221583	1.69961209	−1.17313484	1.85114175
5.4	1.19085829	1.65198161	−1.18801581	1.89713347
5.2	1.21169084	1.61324972	−1.19746779	1.94372057
5.0	1.22251440	1.58634844	−1.20063974	1.99048499
4.8	1.22057030	1.57483347	−1.19662262	2.03717127
4.6	1.20233833	1.58283964	−1.18439186	2.08366708
4.4	1.16325093	1.61479481	−1.16277991	2.12996633
4.2	1.09743358	1.67455033	−1.13045836	2.17615608
4.0	0.99764068	1.76344469	−1.08594859	2.22236237
3.8	0.85618909	1.87686079	−1.02769311	2.26868522
3.6	0.66818742	2.00092980	−0.95424611	2.31513549
3.4	−0.43745941	2.11380040	−0.86493511	2.36115549
3.2	−0.18188954	2.19314915	−0.75983809	2.40570305
3.0	0.06902278	2.22659135	−0.64279385	2.44667686
2.8	0.28595457	2.21620653	−0.52341873	2.48416247
2.6	0.45109743	2.17346800	−0.42210086	2.53319267
2.4	0.55991046	2.11211884	−0.37759587	2.64863480
2.2	0.61813722	2.04205323	−0.44757898	2.87385543
2.0	0.63826273	1.88659945	−0.62474911	2.90828809

Table 12
Electronic transition dipole moments for the molecular excited states $2^1\Sigma_u^+$ and $2^3\Sigma_g^+$.

R	$\langle 2^1\Sigma_u^+\|\mu_{x(y)}^{el}\|1^1\Pi_g\rangle$	$\langle 2^1\Sigma_u^+\|\mu_{x(y)}^{el}\|2^1\Pi_g\rangle$	$\langle 2^3\Sigma_g^+\|\mu_{x(y)}^{el}\|1^3\Pi_u\rangle$	$\langle 2^3\Sigma_g^+\|\mu_{x(y)}^{el}\|2^3\Pi_u\rangle$
90.0	1.71811122	0.00121757	−1.71811637	−0.00121745
88.0	1.71811041	0.00133248	−1.71811326	−0.00133231
86.0	1.71810422	0.00146081	−1.71810685	−0.00146064
84.0	−1.71809744	0.00160499	−1.71809990	−0.00160481
82.0	−1.71808990	0.00176741	1.71809233	−0.00176724
80.0	−1.71808132	0.00195092	1.71808406	−0.00195075
78.0	−1.71807119	0.00215887	1.71807501	−0.00215873
76.0	−1.71805855	0.00239527	1.71806506	−0.00239521
74.0	−1.71804192	0.00266488	1.71805406	−0.00266501
72.0	−1.71801970	0.00297344	1.71804182	−0.00297390
70.0	−1.71799177	0.00332793	1.71802806	−0.00332892
68.0	−1.71796086	0.00373691	1.71801235	−0.00373857
66.0	−1.71800061	0.00421244	1.71799414	−0.00421325
64.0	−1.71798150	0.00476485	1.71797271	−0.00476581
62.0	−1.71795937	0.00541100	1.71794749	−0.00541210
60.0	−1.71793354	0.00617067	1.71791839	−0.00617196
58.0	−1.71790346	0.00706870	1.71788572	−0.00707027
56.0	−1.71786867	0.00813644	1.71784952	−0.00813844
54.0	−1.71782857	0.00941379	1.71780880	−0.00941641
52.0	−1.71778216	0.01095203	1.71776170	−0.01095543
50.0	−1.71772795	0.01281769	1.71770599	−0.01282188
48.0	1.71766376	0.01509803	1.71769544	−0.01509676
46.0	1.71758690	0.01790877	1.71762277	−0.01790745
44.0	1.71749349	0.02140218	1.71753506	−0.02140401
42.0	1.71737531	0.02579317	−1.71742741	−0.02579763
40.0	1.71722683	0.03137009	−1.71729148	−0.03137907
38.0	1.71703554	0.03853867	−1.71711077	−0.03855505
36.0	1.71677839	0.04787740	−1.71686238	−0.04790211
34.0	1.71639863	0.06021478	−1.71650421	−0.06022896
32.0	1.71576955	0.07676784	−1.71596624	−0.07680005
30.0	1.71455613	0.09935545	−1.71503266	−0.09942813
29.0	1.71345192	0.11371708	−1.71444107	−0.11390109
28.0	1.71168900	0.13063141	−1.71365181	−0.13112415
27.0	−1.70867282	0.15071098	−1.71261570	−0.15170799
26.0	−1.70327587	0.17455490	−1.71122452	−0.17670065
25.0	−1.69288435	0.20256538	−1.70934911	−0.20729450
24.0	−1.67136005	0.23471540	−1.70681734	−0.24534013
23.0	1.62313206	−0.26891788	−1.70338694	−0.29359896
22.0	−1.51003935	−0.29669885	−1.69879475	−0.35660431
21.0	−1.27783056	−0.29954954	1.69282894	0.44189888
20.0	−0.97365725	−0.27415399	1.68501866	0.56348641
19.5	−0.84009560	−0.25953022	1.68037427	0.64561088
19.0	−0.73029034	−0.24709579	1.67523703	0.74866468
18.5	−0.64276970	−0.23711173	1.66971661	0.88011014
18.0	−0.57350432	−0.22877962	1.66376055	1.04941717
17.5	−0.51839271	−0.22082777	1.65766939	1.26494878
17.0	−0.47403540	−0.21173421	1.65174064	1.52355927
16.5	−0.43780833	−0.19974272	1.64648293	1.79069446
16.0	−0.40772820	−0.18319232	1.64267289	2.00029942
15.5	−0.38229502	−0.16024582	1.64146110	2.10847978
15.0	−0.36036298	−0.12935402	1.64447911	2.13034525
14.5	−0.34104643	−0.08957419	1.65411851	2.10729233
14.0	−0.32357285	−0.04116731	1.67338326	2.07564944
13.5	−0.30754254	0.01402457	1.70569031	2.06095390
13.0	−0.29255745	0.07184162	1.75416853	2.08106117
12.5	−0.27822849	0.12611561	1.81801318	2.14552924
12.0	−0.26438258	0.16996052	1.88932264	2.24878869
11.5	−0.25084729	0.19716563	1.95587220	2.36800520
11.0	−0.23755065	0.20291371	2.01202233	2.47998261
10.5	−0.22474881	0.18211833	2.06245691	2.58195788
10.0	−0.21382875	0.12351411	2.11082164	2.69577005
9.8	0.21112323	−0.08337669	2.12929623	2.75421898
9.6	0.21046019	−0.02799753	2.14676784	2.82645677
9.4	−0.21344130	−0.05014406	2.16275036	2.91842617
9.2	−0.22273068	−0.16399574	2.17680039	3.03897360
9.0	−0.24374593	−0.33627886	2.18839444	3.19894226
8.8	−0.28626198	−0.60908417	2.19701692	3.41341916
8.6	−0.36699519	−1.05198393	2.20233520	3.70133453
8.4	−0.50465540	−1.74209978	2.20406270	4.08250014
8.2	−0.68498959	−2.61359266	2.20188070	−4.56276647
8.0	−0.84215589	−3.37804525	2.19559198	−5.10168269
7.8	−0.94493966	−3.89170236	2.18506676	−5.59483610
7.6	−1.01098728	−4.22428602	2.17023535	−5.94306778
7.4	−1.05962076	−4.45663053	2.15107714	−6.13667278

(*continued on next page*)

Table 12 (*continued*)

R	$\langle 2^1\Sigma_u^+ \lvert \mu_{x(y)}^{el} \rvert 1^1\Pi_g \rangle$	$\langle 2^1\Sigma_u^+ \lvert \mu_{x(y)}^{el} \rvert 2^1\Pi_g \rangle$	$\langle 2^3\Sigma_g^+ \lvert \mu_{x(y)}^{el} \rvert 1^3\Pi_u \rangle$	$\langle 2^3\Sigma_g^+ \lvert \mu_{x(y)}^{el} \rvert 2^3\Pi_u \rangle$
7.2	−1.10133172	−4.63339670	2.12757647	−6.22491609
7.0	−1.14129746	−4.77654483	2.09976417	−6.25514138
6.8	−1.18210720	−4.89702273	2.06775123	−6.25576663
6.6	−1.22490566	−5.00058981	2.03162245	−6.24165382
6.4	−1.26997928	−5.09050441	1.99152302	−6.22021679
6.2	−1.31774867	−5.16769563	1.94758824	−6.19529075
6.0	−1.36770043	−5.23309776	1.89997700	−6.16885951
5.8	−1.41921220	−5.28687264	1.84886634	−6.14198090
5.6	−1.47133176	−5.32885699	1.79444184	−6.11521699
5.4	−1.52285648	−5.35833559	1.73705149	−6.08884299
5.2	−1.57168829	−5.37525407	1.67651914	−6.06313539
5.0	−1.61557897	−5.37838340	1.61329790	−6.03769546
4.8	−1.65139874	−5.36647542	1.54764829	−6.01199237
4.6	−1.67506094	−5.33784896	1.47991381	−5.98498109
4.4	−1.68125814	−5.29037674	1.41053934	−5.95499323
4.2	−1.66329008	−5.22168587	1.34012867	−5.91949913
4.0	−1.61327867	−5.13008453	1.26954021	−5.87480191
3.8	−1.52348806	−5.01687893	1.20002101	−5.81562808
3.6	−1.38984502	−4.88890112	1.13341430	−5.73451403
3.4	1.21780554	−4.75668124	1.07169580	−5.62148300
3.2	1.02650422	−4.62904684	1.01908044	−5.46411575
3.0	0.84325230	−4.50971965	−0.97891075	5.24619558
2.8	0.69082983	−4.39824711	−0.95439314	4.95044776
2.6	0.57887909	−4.29320636	−0.94573790	4.55449846
2.4	0.50813797	−4.19363164	−0.94521992	4.00916828
2.2	0.48046274	−4.09234798	−0.92145620	3.22423596
2.0	0.51718005	−3.75037673	−0.82394182	−2.25056441

Table 13
Electronic transition dipole moments for the molecular excited states $3^1\Sigma_u^+$ and $3^3\Sigma_g^+$.

R	$\langle 3^1\Sigma_u^+ \lvert \mu_{x(y)}^{el} \rvert 1^1\Pi_g \rangle$	$\langle 3^1\Sigma_u^+ \lvert \mu_{x(y)}^{el} \rvert 2^1\Pi_g \rangle$	$\langle 3^3\Sigma_g^+ \lvert \mu_{x(y)}^{el} \rvert 1^3\Pi_u \rangle$	$\langle 3^3\Sigma_g^+ \lvert \mu_{x(y)}^{el} \rvert 2^3\Pi_u \rangle$
90.0	0.00015207	0.00404856	−0.00015308	−0.00404907
88.0	0.00013010	0.00429671	−0.00013390	−0.00429728
86.0	0.00013683	0.00459609	−0.00014086	−0.00459669
84.0	−0.00014475	0.00492373	−0.00014863	−0.00492434
82.0	−0.00015448	0.00528305	0.00015742	−0.00528359
80.0	−0.00016713	0.00567805	0.00016736	−0.00567833
78.0	−0.00018487	0.00611342	0.00017873	−0.00611301
76.0	−0.00014960	0.00659758	0.00019179	−0.00659277
74.0	−0.00016588	0.00712853	0.00020697	−0.00712353
72.0	−0.00018482	0.00771792	0.00022482	−0.00771220
70.0	−0.00020764	0.00837392	0.00024620	−0.00836683
68.0	−0.00023594	0.00910604	0.00027246	−0.00909682
66.0	−0.00026967	0.00992491	0.00030574	−0.00991322
64.0	−0.00031248	0.01084366	0.00027952	−0.01084311
62.0	−0.00036834	0.01187748	0.00032740	−0.01187360
60.0	−0.00044399	0.01304442	0.00039375	−0.01303702
58.0	−0.00049899	0.01438362	0.00048899	−0.01435487
56.0	−0.00063976	0.01588897	0.00062672	−0.01585238
54.0	−0.00083680	0.01760570	0.00082238	−0.01755938
52.0	−0.00110503	0.01956921	0.00103316	−0.01958269
50.0	−0.00145684	0.02182107	0.00137890	−0.02183002
48.0	0.00190663	0.02441037	0.00182115	−0.02441588
46.0	0.00240919	0.02744982	0.00239180	−0.02739988
44.0	0.00320906	0.03077970	0.00317635	−0.03085302
42.0	0.00442943	0.03478863	−0.00434491	−0.03486115
40.0	0.00640026	0.03946114	−0.00613494	−0.03952755
38.0	0.00968684	0.04492195	−0.00876943	−0.04497864
36.0	0.01576927	0.05140231	−0.01238276	−0.05147184
34.0	0.03113041	0.05904665	−0.01771422	−0.05907511
32.0	0.08516542	0.06753758	−0.02684055	−0.06825771
30.0	0.24059071	0.06514582	−0.04462200	−0.07930086
29.0	0.28455895	0.05621325	−0.05917926	−0.08567877
28.0	0.30136643	0.05126816	−0.07919762	−0.09273306
27.0	−0.32111473	0.05127119	−0.10628945	−0.10034408
26.0	−0.35524295	0.05579537	−0.14209896	−0.10894817
25.0	−0.41200444	0.06583800	−0.18802560	−0.11844199
24.0	−0.50447374	0.08452569	−0.24504659	−0.12880116
23.0	−0.65585387	0.11919283	−0.31265875	−0.13956125
22.0	0.89788476	0.18317948	−0.38889566	−0.15030609
21.0	1.21674513	0.28689267	−0.47023106	−0.16022250
20.0	1.48233963	0.41068236	−0.55285043	−0.16757571
19.5	1.56761182	0.47163127	−0.59367527	−0.16973813
19.0	1.62746938	0.53148380	−0.63382605	−0.17034762
18.5	1.66984008	0.59111102	−0.67309000	−0.16935222
18.0	1.70074456	0.65118408	−0.71126089	−0.16709035
17.5	1.72411370	0.71196783	−0.74813513	−0.16536836
17.0	1.74236030	0.77336668	−0.78328307	−0.16950084
16.5	1.75690674	0.83508589	−0.81606261	−0.19094880
16.0	1.76853374	0.89708188	−0.84545534	−0.24529526
15.5	1.77750623	0.95991133	−0.86988095	−0.34112895
15.0	1.78399047	1.02541365	−0.88692752	−0.47303972
14.5	1.78757243	1.09780129	−0.89300040	−0.62633188
14.0	1.78756509	1.18453030	−0.88277943	−0.78395318
13.5	1.78272462	1.29708704	−0.84859959	−0.92717996
13.0	1.77119082	1.45005258	−0.78137281	−1.03539153
12.5	1.75038898	1.65781794	−0.67397795	−1.09083160
12.0	1.71660086	1.93039021	−0.53342826	−1.09674117
11.5	1.66552376	2.26816847	−0.40459870	−1.12221501
11.0	1.59394205	2.65899877	0.43542703	1.37934109
10.5	1.50334815	3.07847472	0.51810007	1.27896880
10.0	1.40348964	3.49666235	−0.37211826	−0.94674967
9.8	1.36462244	3.65810109	−0.63476120	−1.13392041
9.6	1.32810282	3.81483497	−0.46892327	−0.93657097
9.4	1.29487232	3.96636353	−1.29330573	−1.61070247
9.2	1.26569958	4.11127151	−0.46611793	−0.75562987
9.0	1.24053083	4.24665162	−2.02647519	−2.25795668
8.8	1.21773599	4.36182897	−2.02914356	−2.39193811
8.6	1.19112061	4.42593765	−2.03007796	−2.57651373
8.4	1.14619580	4.36240199	−2.02957659	−2.82294404
8.2	1.07034734	4.08667244	−2.02679859	−3.13584380
8.0	0.99476373	3.70226087	−2.02190864	−3.48910576
7.8	0.96602194	3.42053847	−2.01486106	−3.81481115
7.6	0.98718092	3.29308239	−2.00564439	−4.04865579
7.4	1.04035124	3.27547009	−1.99428159	−4.18460964

(*continued on next page*)

Table 13 (*continued*)

R	$\langle 3^1\Sigma_u^+\|\mu_{x(y)}^{el}\|1^1\Pi_g\rangle$	$\langle 3^1\Sigma_u^+\|\mu_{x(y)}^{el}\|2^1\Pi_g\rangle$	$\langle 3^3\Sigma_g^+\|\mu_{x(y)}^{el}\|1^3\Pi_u\rangle$	$\langle 3^3\Sigma_g^+\|\mu_{x(y)}^{el}\|2^3\Pi_u\rangle$
7.2	1.10522880	3.31374970	−1.98077784	−4.25451352
7.0	−1.16878904	−3.37147143	−1.96509613	−4.28854946
6.8	−1.22469348	−3.42779263	−1.94729610	−4.30451315
6.6	−1.27275773	−3.47565342	−1.92745821	−4.31150375
6.4	−1.31534048	−3.51510757	−1.90564477	−4.31366378
6.2	−1.35230010	−3.54822346	−1.88188011	−4.31314431
6.0	−1.38562997	−3.57583802	−1.85619226	−4.31089897
5.8	−1.41598473	−3.59900580	−1.82860900	−4.30729243
5.6	−1.44340852	−3.61878236	−1.79914596	−4.30237580
5.4	−1.46729831	−3.63624230	−1.76784207	−4.29596881
5.2	−1.48631597	−3.65301935	−1.73461666	−4.28778364
5.0	−1.49828405	−3.67090298	−1.69947315	−4.27741007
4.8	−1.49967698	−3.69328187	−1.66241427	−4.26424906
4.6	−1.48517143	−3.72476652	−1.62347059	−4.24750058
4.4	−1.44523549	−3.77334879	−1.58271673	−4.22611214
4.2	−1.35873746	−3.85198432	−1.54032800	−4.19859659
4.0	−1.16012060	−3.95829535	−1.49663828	−4.16289452
3.8	−0.68139567	−3.78623678	−1.45224934	−4.11610776
3.6	−0.17465185	−3.01026777	−1.40817225	−4.05414622
3.4	−0.04252617	−2.36289357	−1.36565051	−3.97074455
3.2	−0.11227980	−1.94759237	−1.32748975	−3.85938894
3.0	−0.10349722	−1.72448372	−1.29594073	−3.71029431
2.8	0.02182445	−1.80118935	−1.27291826	−3.51481915
2.6	0.99465021	2.06998706	−1.25715351	−3.26834871
2.4	−0.99653233	−0.73606345	−1.23780865	−2.97959030
2.2	−0.99118398	0.10649123	−1.18840739	−2.73070354
2.0	1.00177470	−1.08786411	1.10785787	2.71533115

Table 14
Electronic transition dipole moments for the molecular excited states $1^1\Pi_g$ and $1^3\Pi_g$.

R	$\langle 1^1\Pi_g \lvert \mu_z^{el} \rvert 1^1\Pi_u\rangle$	$\langle 1^1\Pi_g \lvert \mu_z^{el} \rvert 2^1\Pi_u\rangle$	$\langle 1^3\Pi_g \lvert \mu_z^{el} \rvert 1^3\Pi_u\rangle$	$\langle 1^3\Pi_g \lvert \mu_z^{el} \rvert 2^3\Pi_u\rangle$
90.0	−0.00001078	−2.36914898	0.00000982	2.36519877
88.0	0.00002457	2.36959992	0.00002354	2.36535216
86.0	0.00002832	2.37006204	0.00002728	2.36550871
84.0	−0.00003257	−2.37056902	0.00003153	2.36568005
82.0	0.00003740	−2.37112641	−0.00003637	2.36586796
80.0	0.00004291	−2.37174062	−0.00004187	2.36607448
78.0	0.00004920	−2.37241907	−0.00004816	2.36630193
76.0	0.00005641	−2.37317036	−0.00005537	2.36655301
74.0	0.00006469	−2.37400449	−0.00006366	2.36683084
72.0	0.00007425	−2.37493318	−0.00007322	2.36713901
70.0	0.00008532	−2.37597015	−0.00008429	2.36748173
68.0	0.00009820	−2.37713159	−0.00009716	2.36786390
66.0	0.00011319	−2.37843655	−0.00011219	2.36829125
64.0	0.00013081	−2.37990790	−0.00012982	2.36877058
62.0	0.00015160	−2.38157277	−0.00015063	2.36930986
60.0	0.00017627	−2.38346389	−0.00017531	2.36991857
58.0	0.00020569	−2.38562102	−0.00020476	2.37060800
56.0	0.00024097	−2.38809255	−0.00024006	2.37139190
54.0	0.00028348	−2.39093954	−0.00028259	2.37228683
52.0	0.00033493	−2.39423715	−0.00033407	2.37331305
50.0	0.00039749	−2.39822413	−0.00039665	2.37449582
48.0	0.00047408	2.40275471	−0.00047327	2.37586494
46.0	0.00056852	2.40809739	−0.00056775	2.37745884
44.0	0.00068616	2.41444161	−0.00068543	2.37932411
42.0	0.00083431	2.42203340	0.00083362	2.38151820
40.0	0.00102325	2.43119557	0.00102257	2.38411252
38.0	0.00126746	2.44235795	0.00126703	2.38719506
36.0	0.00158720	2.45605916	0.00158736	2.39085898
34.0	0.00200930	2.47297951	0.00200973	2.39526169
32.0	0.00257470	2.49408136	0.00257497	2.40040026
30.0	0.00334693	2.52068927	0.00334698	2.40646238
29.0	0.00384923	2.53649969	0.00383960	2.40986390
28.0	0.00441817	2.55446736	0.00441940	2.41346881
27.0	−0.00511712	−2.57483880	0.00511827	2.41736306
26.0	−0.00595910	−2.59795324	0.00596004	2.42134341
25.0	−0.00698082	−2.62418638	0.00698133	2.42528305
24.0	−0.00823087	−2.65392133	0.00823061	2.42884410
23.0	−0.00976374	−2.68747783	0.00976157	2.43140601
22.0	0.01168837	2.72536980	0.01168263	2.43164888
21.0	0.01414259	2.76753233	0.01411832	2.42676936
20.0	0.01728793	2.81382172	0.01723875	2.41045008
19.5	−0.01919518	2.83839975	0.01913021	2.39374292
19.0	−0.02138204	2.86376019	0.02129589	2.36693638
18.5	−0.02390286	2.88971274	0.02378695	2.32374371
18.0	−0.02681868	2.91605980	0.02667411	2.25370109
17.5	−0.03021398	2.94248723	0.03001967	2.14004559
17.0	0.03419403	2.96860817	0.03394120	1.96127940
16.5	0.03889430	2.99390294	0.03857968	1.70705448
16.0	0.04449104	3.01762985	0.04412522	1.40795841
15.5	0.05121581	3.03864311	0.05083865	1.13029686
15.0	0.05937564	3.05504026	0.05908387	0.92021726
14.5	0.06939710	3.06344763	0.06937704	0.78311181
14.0	0.08181050	3.05784592	0.08245839	0.70544510
13.5	0.09737260	3.02796835	0.09945775	0.67242930
13.0	0.11712429	2.95936372	0.12180074	0.67330008
12.5	0.14246879	2.83996876	0.15180921	0.70100676
12.0	0.17541081	2.67652158	0.19263378	0.75155247
11.5	0.21840141	2.50079029	0.24868084	0.82263287
11.0	0.27493801	−2.34740076	0.32595395	0.91284018
10.5	0.34938008	−2.23198944	0.43169273	1.02098885
10.0	0.44690443	−2.15188269	0.57470889	1.14572593
9.8	0.49355807	−2.12711128	0.64443096	1.19998773
9.6	0.54504505	−2.10502340	0.72217992	1.25659906
9.4	0.60163004	−2.08481092	0.80867807	1.31554045
9.2	0.66343921	−2.06488432	0.90415017	1.37709411
9.0	0.73054028	−2.04441410	1.00906519	1.44176098
8.8	0.80279791	−2.02236920	1.12360020	1.51049216
8.6	0.88005834	−1.99773633	1.24768107	1.58491753
8.4	0.96185458	−1.96973170	1.38052727	1.66683263
8.2	1.04758408	−1.93780954	1.52102228	−1.75638227
8.0	1.13647361	−1.90179269	1.66717193	−1.84808378
7.8	1.22760478	−1.86198784	1.81609535	−1.93078752
7.6	1.31994236	−1.81927481	1.96404000	−1.99948744
7.4	1.41236555	−1.77509292	2.10660780	−2.06177907

(*continued on next page*)

Table 14 (*continued*)

R	$\langle 1^1\Pi_g \lvert \mu_z^{el} \rvert 1^1\Pi_u \rangle$	$\langle 1^1\Pi_g \lvert \mu_z^{el} \rvert 2^1\Pi_u \rangle$	$\langle 1^3\Pi_g \lvert \mu_z^{el} \rvert 1^3\Pi_u \rangle$	$\langle 1^3\Pi_g \lvert \mu_z^{el} \rvert 2^3\Pi_u \rangle$
7.2	1.50369863	−1.73137055	2.23912570	−2.12705579
7.0	1.59271755	−1.69091181	2.35745365	−2.19905827
6.8	1.67831933	−1.65592932	2.45821761	−2.27760888
6.6	1.75937029	−1.62915784	2.53939780	−2.36099273
6.4	1.83451363	−1.61229037	2.60029157	−2.44722707
6.2	1.90267187	−1.60685209	2.64137880	−2.53488884
6.0	1.96256218	−1.61372978	2.66398836	−2.62293691
5.8	2.01286009	−1.63318788	2.66995762	−2.71060541
5.6	2.05209499	−1.66501308	2.66136055	−2.79726959
5.4	2.07854013	−1.70854119	2.64029433	−2.88230105
5.2	2.09003950	−1.76311598	2.60895429	−2.96497804
5.0	2.08389772	−1.82766351	2.56943208	−3.04408398
4.8	2.05661236	−1.90113667	2.52393858	−3.11821511
4.6	2.00349440	−1.98262634	2.47501887	−3.18519063
4.4	1.91810253	−2.07153763	2.42601315	−3.24156355
4.2	1.79152194	−2.16767165	2.38202896	−3.28135097
4.0	1.61168903	−2.27075959	2.35220509	−3.29214837
3.8	1.36355947	−2.37840381	2.35473458	−3.24198023
3.6	1.03207057	−2.48151430	2.42333574	−3.01430509
3.4	−0.61030562	2.55892950	2.50130157	−2.18646156
3.2	−0.11351869	2.58010260	−2.30482232	0.98538839
3.0	0.41175297	2.52058886	−2.14024031	0.42425599
2.8	0.89669851	2.37959562	−2.08215980	0.24575158
2.6	1.28736508	2.18734188	−2.07648944	0.27522190
2.4	1.57115343	1.98143114	−2.09220276	0.46992893
2.2	1.76603496	1.78835605	−2.11220437	0.81991376
2.0	1.89800713	1.62427897	−2.12720649	1.33790907

Table 15
Electronic transition dipole moments for the molecular excited states $2^1\Pi_g$ and $2^3\Pi_g$.

R	$\langle 2^1\Pi_g\|\mu_z^{el}\|1^1\Pi_u\rangle$	$\langle 2^1\Pi_g\|\mu_z^{el}\|2^1\Pi_u\rangle$	$\langle 2^3\Pi_g\|\mu_z^{el}\|1^3\Pi_u\rangle$	$\langle 2^3\Pi_g\|\mu_z^{el}\|2^3\Pi_u\rangle$
90.0	−2.36519792	0.00007792	2.36915138	0.00007711
88.0	2.36535099	0.00008827	2.36960162	0.00008735
86.0	2.36550758	0.00009856	2.37006375	0.00009771
84.0	2.36567895	0.00011020	2.37057074	0.00010941
82.0	−2.36586690	0.00012338	−2.37112814	0.00012265
80.0	−2.36607346	0.00013835	−2.37174238	0.00013771
78.0	−2.36630095	0.00015543	−2.37242086	0.00015487
76.0	−2.36655207	0.00017497	−2.37317218	0.00017449
74.0	−2.36682992	0.00019741	−2.37400637	0.00019703
72.0	−2.36713810	0.00022329	−2.37493514	0.00022302
70.0	−2.36748082	0.00025323	−2.37597223	0.00025309
68.0	−2.36786294	0.00028803	−2.37713386	0.00028805
66.0	−2.36829006	0.00032865	−2.37843923	0.00032889
64.0	−2.36876898	0.00037625	−2.37991126	0.00037681
62.0	−2.36930746	0.00043226	−2.38157737	0.00043333
60.0	−2.36991491	0.00049852	−2.38347067	0.00050039
58.0	−2.37060226	0.00057728	−2.38563141	0.00058044
56.0	−2.37138287	0.00067147	−2.38810882	0.00067673
54.0	−2.37227387	0.00078541	−2.39096353	0.00079357
52.0	−2.37329572	0.00092471	−2.39427064	0.00093683
50.0	−2.37447370	0.00111655	−2.39812381	0.00111469
48.0	2.37583886	0.00133858	−2.40264011	0.00133786
46.0	2.37742911	0.00162114	−2.40816259	0.00164004
44.0	2.37937111	0.00202201	−2.41451127	0.00200930
42.0	2.38156757	0.00250849	2.42210333	0.00249232
40.0	2.38416300	0.00315412	2.43125878	0.00313351
38.0	2.38724646	0.00402607	2.44240389	0.00399895
36.0	2.39091230	0.00523075	2.45608496	0.00519623
34.0	2.39525344	0.00694627	2.47299382	0.00696540
32.0	2.40039367	0.00946419	2.49409146	0.00949053
30.0	2.40646320	0.01329109	2.52070907	0.01333546
29.0	2.40987800	0.01596068	2.53663167	0.01602735
28.0	2.41357338	0.01939112	2.55454925	0.01946910
27.0	2.41751063	0.02374610	2.57500739	0.02394811
26.0	2.42167386	0.02939552	2.59824126	0.02977083
25.0	2.42600892	0.03680415	2.62480923	0.03774245
24.0	2.43041532	0.04657495	2.65521472	0.04892653
23.0	2.43482217	0.05969196	2.69008156	0.06540941
22.0	2.43913658	0.07739302	2.73043930	0.09084449
21.0	2.44331592	0.10120629	2.77698506	0.13425724
20.0	2.44759546	0.13302638	2.83056170	0.21600207
19.5	−2.45002529	0.15263168	2.85986716	0.28542618
19.0	−2.45292509	0.17500360	2.89027038	0.38966492
18.5	−2.45664917	0.20035456	2.92055529	0.55081474
18.0	−2.46173775	0.22888544	2.94833089	0.80526366
17.5	−2.46895047	0.26080715	2.96972054	1.20827099
17.0	2.47933651	0.29648002	2.97945460	1.82447892
16.5	2.49430770	0.33664072	2.97289818	2.67650220
16.0	2.51553102	0.38308738	2.94973803	3.66648688
15.5	2.54496806	0.43939081	2.91667548	4.60435639
15.0	2.58457987	0.51245230	2.88567962	5.34929136
14.5	2.63594281	0.61467880	2.86910667	5.86099434
14.0	2.69945914	0.76615262	2.87611991	6.15634354
13.5	2.77377698	0.99486600	2.91211757	6.26896801
13.0	2.85514973	1.32922847	2.97916905	6.23159492
12.5	2.93792556	1.77613504	3.07721429	6.07065539
12.0	3.01648521	2.29516745	3.20387472	5.80544918
11.5	3.08735193	2.80744428	3.35374042	5.44923848
11.0	3.15105791	−3.24189060	3.51729304	5.01132714
10.5	3.21074074	−3.56377650	−3.67864768	−4.49980824
10.0	3.26907924	−3.77058385	−3.81677564	−3.92506123
9.8	3.29179075	−3.82478718	−3.85994830	−3.68086119
9.6	3.31370790	−3.86521304	−3.89370070	−3.43053024
9.4	3.33433081	−3.89422329	−3.91635836	−3.17598090
9.2	3.35285393	−3.91398121	−3.92632588	−2.91971814
9.0	3.36821297	−3.92750972	−3.92212831	−2.66497392
8.8	3.37935995	−3.93804199	−3.90231840	−2.41627096
8.6	3.38518831	−3.94889109	−3.86582760	−2.18002027
8.4	3.38439425	−3.96361064	−3.81139231	−1.96491230
8.2	3.37576069	−3.98563108	−3.73825251	1.78103177
8.0	3.35822681	−4.01808289	−3.64597299	1.63536920
7.8	3.33077274	−4.06338863	−3.53470597	1.52498094
7.6	3.29274239	−4.12297093	−3.40542442	1.43785530
7.4	3.24379318	−4.19836453	−3.26011360	1.36242346

(*continued on next page*)

Table 15 (*continued*)

R	$\langle 2^1\Pi_g\|\mu_z^{el}\|1^1\Pi_u\rangle$	$\langle 2^1\Pi_g\|\mu_z^{el}\|2^1\Pi_u\rangle$	$\langle 2^3\Pi_g\|\mu_z^{el}\|1^3\Pi_u\rangle$	$\langle 2^3\Pi_g\|\mu_z^{el}\|2^3\Pi_u\rangle$
7.2	3.18395492	−4.28627609	−3.10185333	1.29183110
7.0	3.11397749	−4.38398605	−2.93465259	1.22249678
6.8	3.03287173	−4.48804826	−2.76297881	1.15277185
6.6	2.94419721	−4.59557837	−2.59135275	1.08116671
6.4	2.84841726	−4.70075367	−2.42385523	1.00634178
6.2	2.74711290	−4.79989269	−2.26401462	0.92595825
6.0	2.64235198	−4.88796473	−2.11466510	0.83592048
5.8	2.53643743	−4.96053652	−1.97816078	0.72941748
5.6	2.43195607	−5.01340494	−1.85666387	0.59584843
5.4	2.33189164	−5.04257179	−1.75236153	0.42020398
5.2	2.23963889	−5.04295468	−1.66692974	0.18702964
5.0	2.15921813	−5.00968051	−1.60000776	−0.10858126
4.8	2.09521636	−4.93666634	−1.54623273	−0.43733863
4.6	2.05277193	−4.81658744	−1.49631520	−0.73872315
4.4	2.03725760	−4.64087366	−1.44150843	−0.96723331
4.2	2.05328763	−4.40091503	−1.37449046	−1.13102777
4.0	2.10242376	−4.09236237	−1.28261970	−1.28101736
3.8	2.17893921	−3.72554840	−1.13022924	−1.50069446
3.6	2.26423334	−3.34163404	−0.79856647	−1.95394519
3.4	2.32463986	−3.01676843	0.01577279	−2.84872870
3.2	2.32180725	−2.81910183	0.86918004	−3.42542328
3.0	2.23425015	−2.76293720	1.16897717	−3.48463338
2.8	2.08103445	−2.78016555	1.24571324	−3.42208447
2.6	1.90973429	−2.77938727	1.24559442	−3.32620590
2.4	1.75947853	−2.68946130	1.20933656	−3.23205428
2.2	1.65092538	−2.44074933	1.14846773	−3.16099421
2.0	1.65865541	−1.35105636	1.05959951	−3.15813166

Table 16
Electronic transition dipole moments for the molecular excited states $1^1\Delta_g$ and $1^3\Delta_u$.

R	$\langle 1^1\Delta_g \lvert \mu^{el}_{x(y)} \rvert 1^1\Pi_u\rangle$	$\langle 1^1\Delta_g \lvert \mu^{el}_{x(y)} \rvert 2^1\Pi_u\rangle$	$\langle 1^3\Delta_u \lvert \mu^{el}_{x(y)} \rvert 1^3\Pi_g\rangle$	$\langle 1^3\Delta_u \lvert \mu^{el}_{x(y)} \rvert 2^3\Pi_g\rangle$
90.0	2.35909539	−0.00000023	−2.35909453	0.00000188
88.0	−2.35881489	0.00000285	−2.35881409	0.00000474
86.0	−2.35850862	0.00000619	−2.35850783	0.00000809
84.0	−2.35817252	0.00000999	−2.35817176	0.00001190
82.0	2.35780289	0.00001429	−2.35780214	0.00001621
80.0	2.35739541	0.00001920	−2.35739469	0.00002113
78.0	2.35694514	0.00002480	−2.35694444	0.00002674
76.0	2.35644631	0.00003120	−2.35644563	0.00003315
74.0	2.35589219	0.00003855	−2.35589153	0.00004051
72.0	2.35527489	0.00004701	−2.35527427	0.00004899
70.0	2.35458517	0.00005677	−2.35458457	0.00005877
68.0	2.35381207	0.00006806	−2.35381150	0.00007010
66.0	2.35294261	0.00008119	−2.35294208	0.00008328
64.0	2.35196130	0.00009645	−2.35196080	0.00009867
62.0	2.35084953	0.00011427	−2.35084907	0.00011672
60.0	2.34956232	0.00015437	−2.34956174	0.00015713
58.0	2.34811620	0.00017806	−2.34811563	0.00018154
56.0	2.34645650	0.00020597	−2.34645594	0.00021067
54.0	2.34454230	0.00023934	−2.34454175	0.00024562
52.0	2.34232288	0.00027955	−2.34232234	0.00028776
50.0	2.33973487	0.00034241	−2.33973433	0.00033878
48.0	−2.33669811	0.00040546	−2.33669759	0.00040081
46.0	−2.33311212	0.00048174	−2.33311157	0.00047973
44.0	−2.32884605	0.00057512	−2.32884544	0.00057300
42.0	−2.32373060	0.00069046	−2.32372994	0.00068841
40.0	−2.31754323	0.00083399	−2.31754253	0.00083238
38.0	−2.30998762	0.00101373	−2.30998695	0.00101313
36.0	−2.30062904	0.00119311	−2.30063020	0.00119340
34.0	−2.28898147	0.00146527	−2.28898300	0.00146616
32.0	−2.27424982	0.00182717	−2.27425173	0.00182757
30.0	−2.25534238	0.00232184	−2.25534487	0.00231871
29.0	−2.24385866	0.00256560	−2.24386596	0.00255896
28.0	−2.23072775	0.00293461	−2.23073788	0.00290853
27.0	−2.21553780	0.00336513	−2.21555195	0.00331448
26.0	−2.19793753	0.00387901	−2.19795886	0.00378810
25.0	−2.17743322	0.00449537	−2.17746858	0.00429386
24.0	−2.15340779	0.00524197	−2.15347226	0.00479069
23.0	−2.12508834	0.00613735	−2.12520922	0.00514246
22.0	−2.09144241	0.00731504	−2.09173232	0.00503784
21.0	−2.05126428	0.00894837	−2.05188339	0.00370433
20.0	−2.00274258	0.01136828	−2.00424870	−0.00061734
19.5	1.97467527	0.01309288	−1.97697763	−0.00490927
19.0	1.94360038	0.01535995	−1.94711033	−0.01150521
18.5	1.90913179	0.01836326	−1.91442544	−0.02151815
18.0	1.87058500	0.02261968	−1.87867397	−0.03585858
17.5	1.82733760	0.02863249	−1.83956919	−0.05551589
17.0	−1.77855851	0.03723032	−1.79696978	−0.08061817
16.5	−1.72324102	0.04965697	−1.75075310	−0.10958823
16.0	−1.65990537	0.06802736	−1.70087226	−0.13877744
15.5	−1.58676614	0.09549691	−1.64738281	−0.16341122
15.0	−1.50147207	0.13709518	−1.59046260	−0.17935319
14.5	−1.40108628	0.20077254	−1.53053484	−0.18417702
14.0	−1.28209937	0.29858129	−1.46774123	−0.17671118
13.5	−1.14030590	0.44771929	−1.40253778	−0.15648211
13.0	−0.97253117	0.66664604	−1.33506007	−0.12284368
12.5	−0.77785549	0.96318484	−1.26483376	−0.07459716
12.0	−0.56009428	1.31785233	−1.19034305	−0.00966221
11.5	−0.32841283	1.68693865	−1.10807921	0.07530985
11.0	−0.09500063	−2.02988260	−1.01101999	0.18561045
10.5	0.13062411	−2.32658080	−0.88581609	−0.32950774
10.0	0.34539784	−2.57413011	−0.70812387	−0.51889458
9.8	0.42872325	−2.66051697	−0.61331884	−0.61082881
9.6	0.51098093	−2.74044715	−0.49993130	−0.71313904
9.4	0.59242468	−2.81422827	−0.36438569	−0.82524469
9.2	0.67334932	−2.88275293	−0.20370184	−0.94601226
9.0	0.75384943	−2.94624521	−0.01729888	−1.07125666
8.8	0.83398895	−3.00503195	0.19139513	−1.19414452
8.6	0.91335809	−3.05938217	0.41426780	−1.30585362
8.4	0.99168079	−3.10936110	0.64007440	−1.39776376
8.2	1.06840250	−3.15485610	0.85816190	−1.46409055
8.0	1.14281178	−3.19551478	1.06159128	−1.50298701
7.8	1.21407785	−3.23077658	1.24774645	−1.51580863
7.6	1.28129167	−3.25991191	1.41693031	−1.50567178
7.4	1.34351017	−3.28211026	1.57060577	−1.47636562

(*continued on next page*)

Table 16 (*continued*)

R	$\langle 1^1\Delta_g \lvert \mu^{el}_{x(y)} \rvert 1^1\Pi_u\rangle$	$\langle 1^1\Delta_g \lvert \mu^{el}_{x(y)} \rvert 2^1\Pi_u\rangle$	$\langle 1^3\Delta_u \lvert \mu^{el}_{x(y)} \rvert 1^3\Pi_g\rangle$	$\langle 1^3\Delta_u \lvert \mu^{el}_{x(y)} \rvert 2^3\Pi_g\rangle$
7.2	1.39979439	−3.29650546	1.71053425	−1.43181718
7.0	1.44916925	−3.30240245	1.83740685	−1.37579642
6.8	1.49113607	−3.29989706	1.95237043	−1.31171042
6.6	1.52416677	−3.28878026	2.05629978	−1.24219984
6.4	1.54766759	−3.26957180	2.15015209	−1.16925918
6.2	1.56064635	−3.24258931	2.23499097	−1.09278023
6.0	1.56193585	−3.20816435	2.31194500	−1.01107123
5.8	1.55011821	−3.16627695	2.38211230	−0.91990897
5.6	1.52336187	−3.11635163	2.44644474	−0.81169350
5.4	1.47920109	−3.05710411	2.50563276	−0.67486650
5.2	1.41436982	−2.98628308	2.56000536	−0.49597913
5.0	1.32456507	−2.90087335	2.60957423	−0.26869907
4.8	1.20446921	−2.79710110	2.65381808	−0.01082789
4.6	1.04808481	−2.67106226	2.69168589	0.23229008
4.4	0.84994451	−2.52016144	2.72122915	0.42157663
4.2	0.60763462	−2.34561548	2.73881729	0.55725409
4.0	0.32513167	−2.15478458	2.73683314	0.67465211
3.8	0.01444212	−1.95959384	2.69568563	0.83750315
3.6	−0.30722803	−1.76817433	2.54282335	1.17753797
3.4	−0.62248356	−1.57588305	1.99743143	1.88271198
3.2	−0.91565002	−1.36990047	−1.20785945	2.32397021
3.0	−1.16748442	−1.14419393	−0.94574600	2.12702193
2.8	−1.35837163	−0.91741629	−1.07521493	1.33193899
2.6	−1.48177564	−0.72633229	−1.23633364	0.41762859
2.4	−1.54908962	−0.59782211	−1.29852163	0.01773823
2.2	−1.57923098	−0.53135566	−1.32458916	−0.06025586
2.0	−1.58784614	−0.50397311	−1.33425061	0.07897827