

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.

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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])

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

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

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

where

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

and

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

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

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

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

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

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

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

Here,

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

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

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

where $\vec{\mu}_{fi}^{el}$ 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

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

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

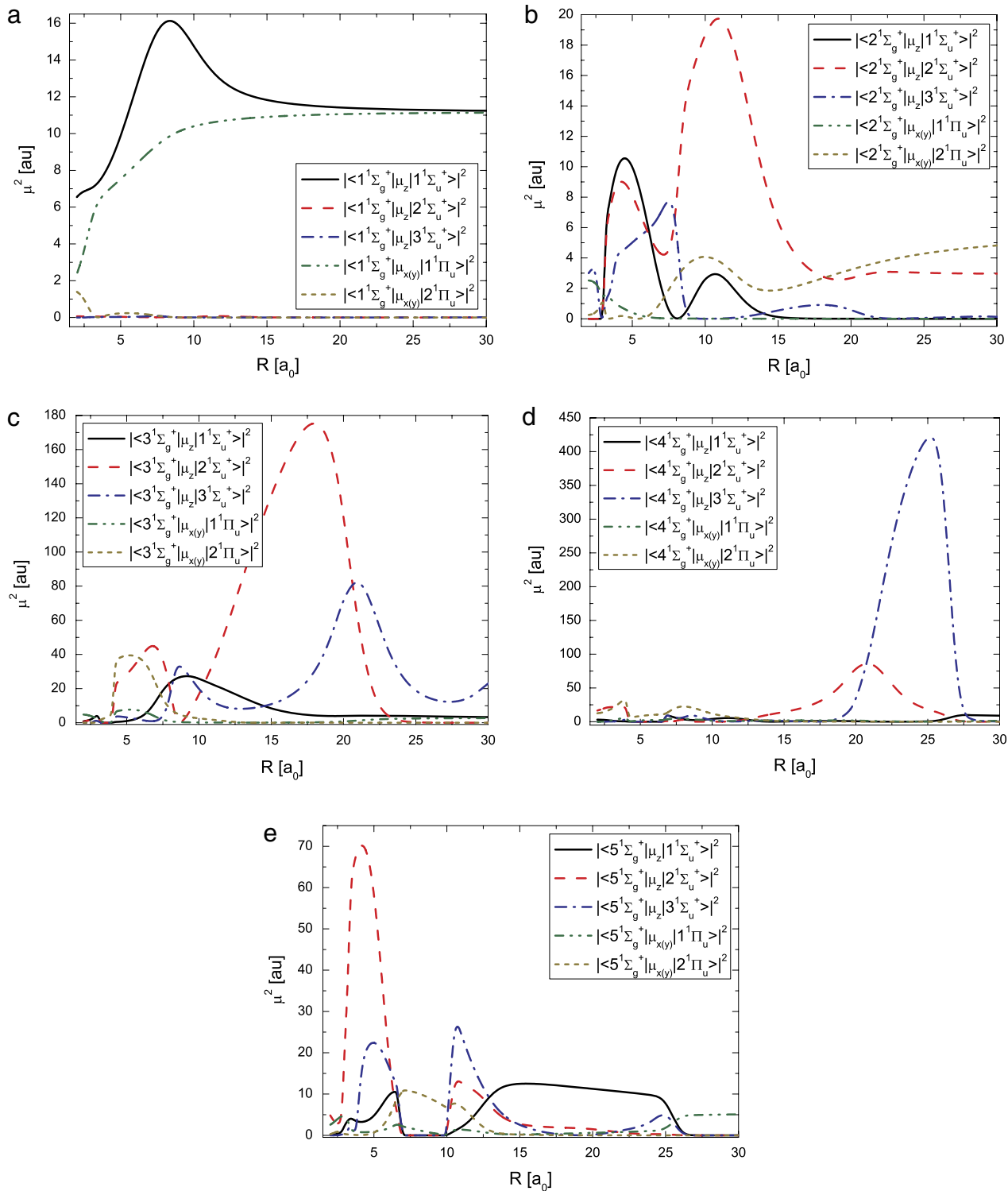


Fig. 1. The transition dipole moments for the $1^1\Sigma_g^+$ (a), $2^1\Sigma_g^+$ (b), $3^1\Sigma_g^+$ (c), $4^1\Sigma_g^+$ (d), and $5^1\Sigma_g^+$ (e) states of the lithium dimer.

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.

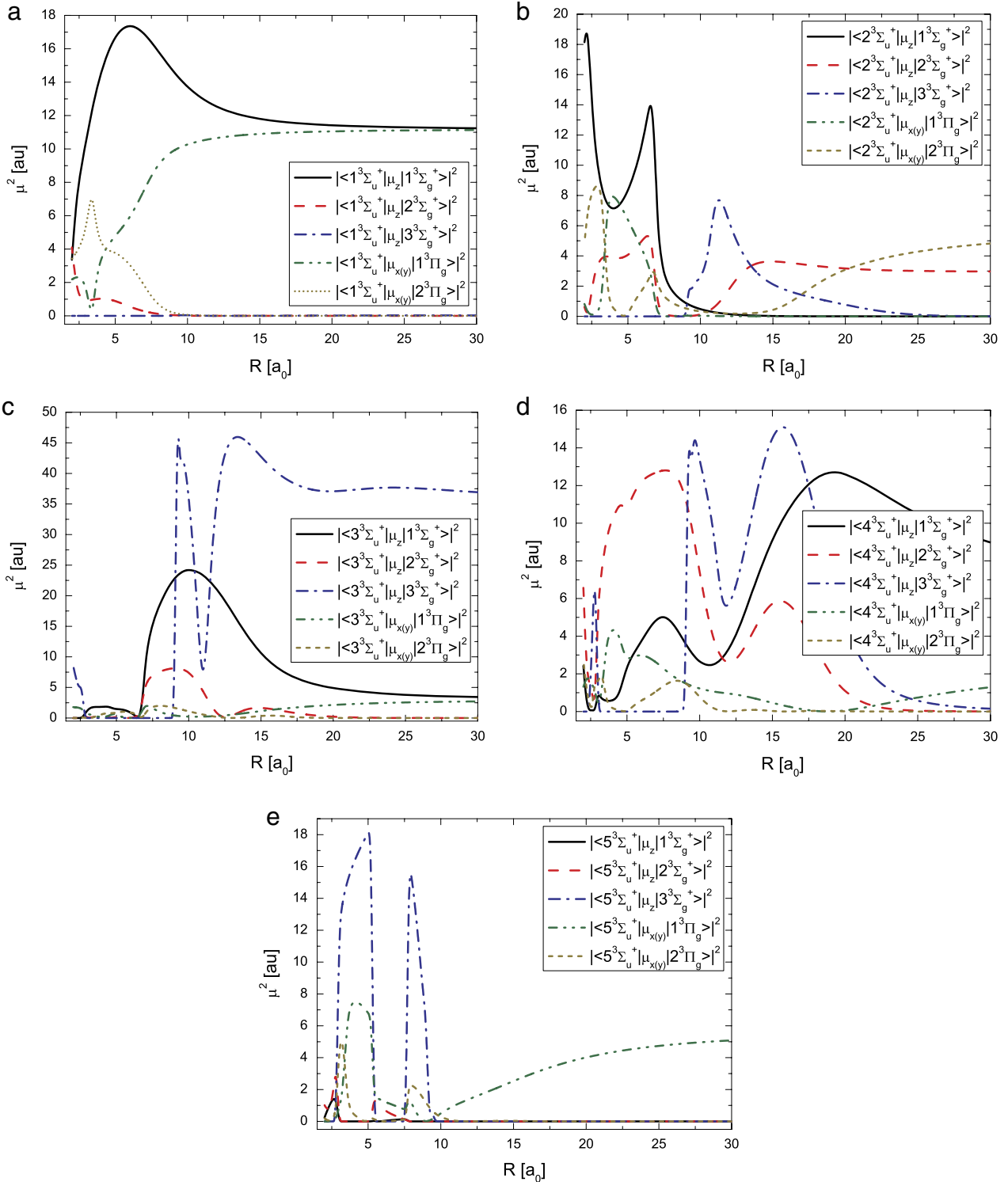


Fig. 2. The transition dipole moments for the $1^3\Sigma_u^+$ (a), $2^3\Sigma_u^+$ (b), $3^3\Sigma_u^+$ (c), $4^3\Sigma_u^+$ (d), and $5^3\Sigma_u^+$ (e) states of the lithium dimer.

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 Sheshtakov [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 $\text{Li}(2s) + \text{Li}(2s)$ and $\text{Li}(2s) + \text{Li}(2p)$ 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

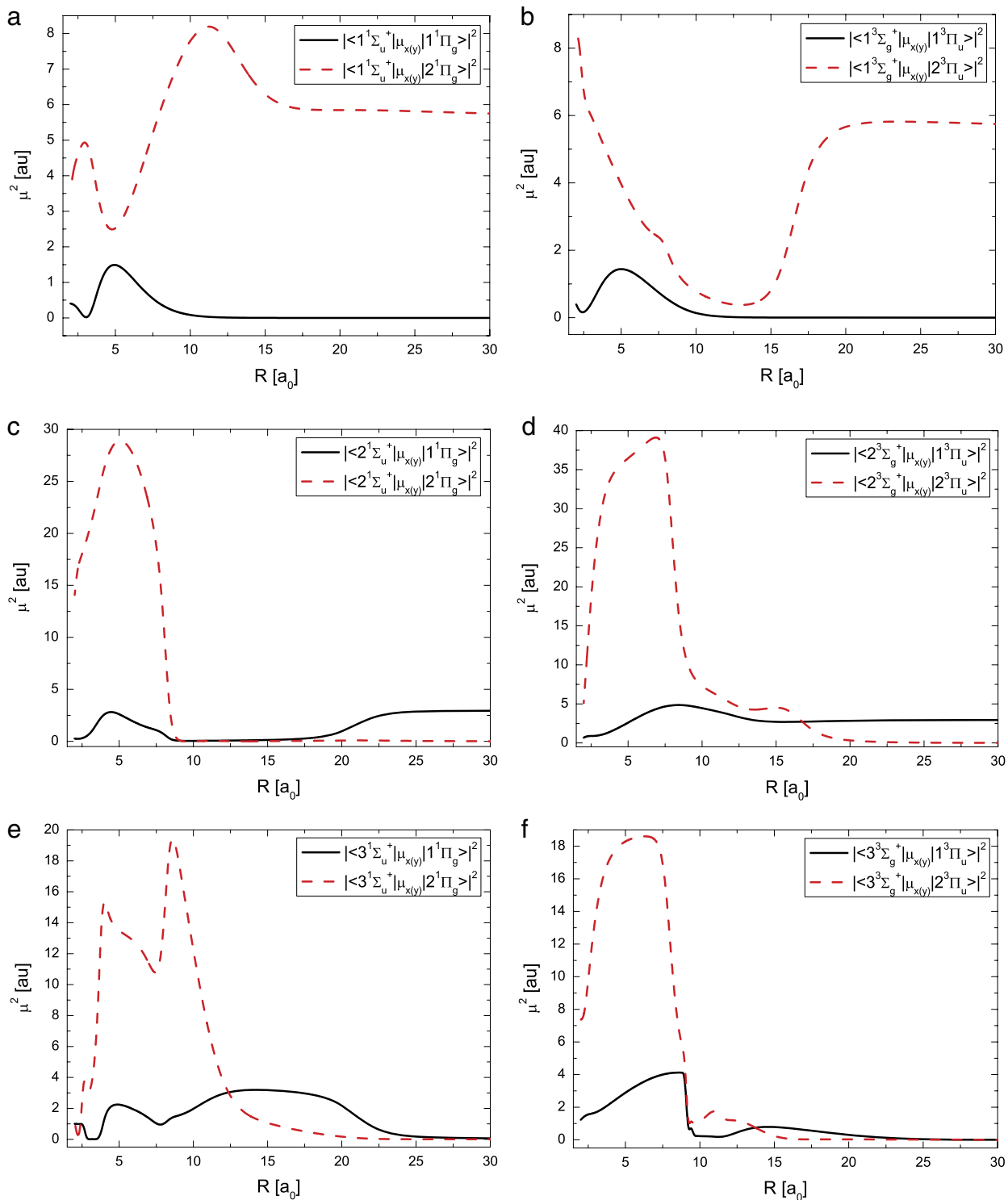


Fig. 3. The transition dipole moments for the $1^1\Sigma_u^+$ (a), $1^3\Sigma_g^+$ (b), $2^1\Sigma_u^+$ (c), $2^3\Sigma_g^+$ (d), $3^1\Sigma_u^+$ (e), and $3^3\Sigma_g^+$ (f) states of the lithium dimer.

differences between their values and the present one are 0.0244, 0.0252, and 0.0019 $e a_0$. The best agreement is obtained with Ratcliff et al. [12] for the transition between atomic asymptotes $\text{Li}(2s) + \text{Li}(2p)$ and $\text{Li}(2p) + \text{Li}(2p)$. The difference is only 0.0011 $e a_0$. We note that the biggest difference occurs for data of Schmidt-Mink et al. [14] for the transition $\text{Li}(2s) + \text{Li}(3s) \rightarrow \text{Li}(2s) + \text{Li}(3p)$ and it equals to 0.0574 $e a_0$.

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,

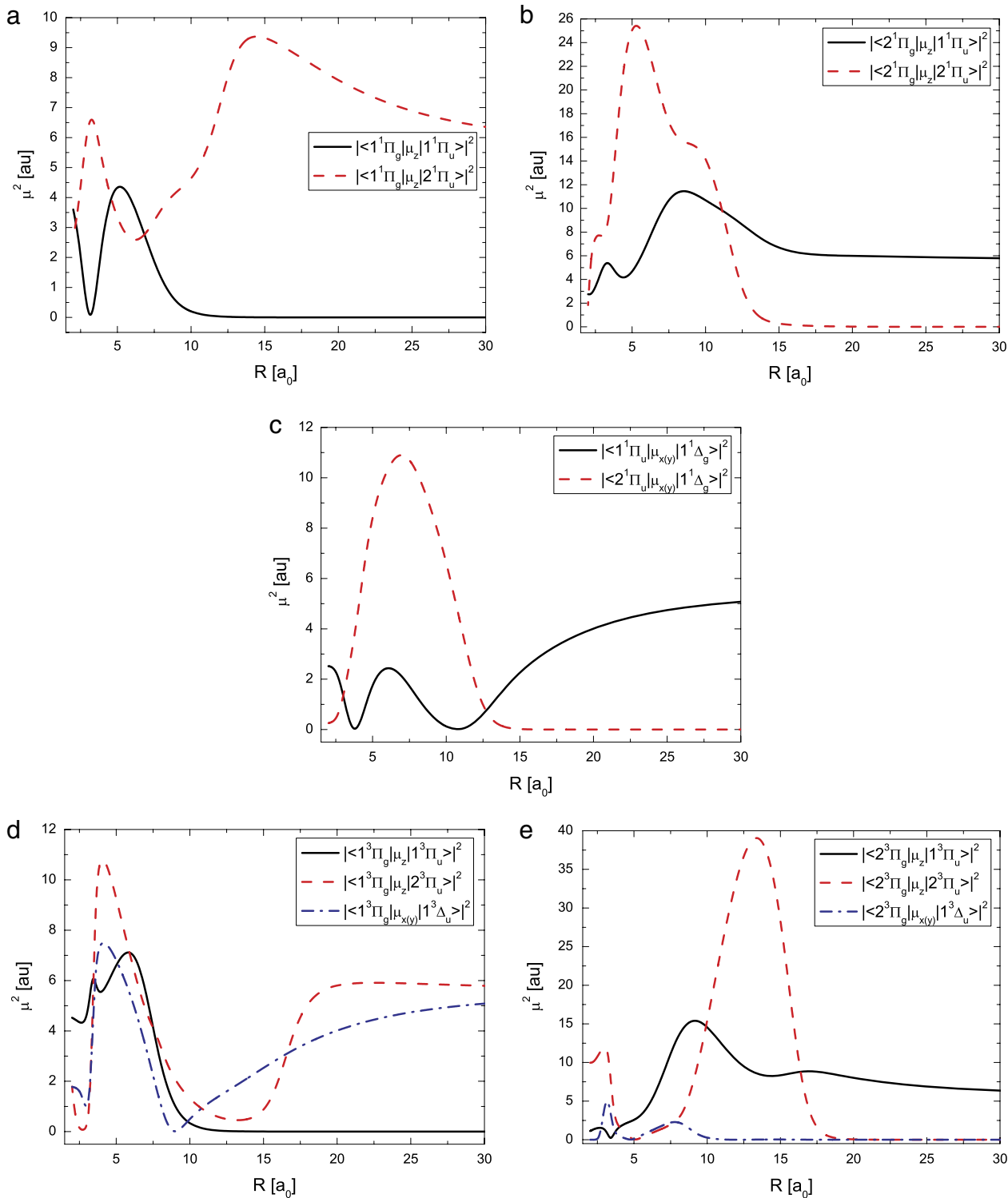


Fig. 4. The transition dipole moments for the $1^1\Pi_g$ (a), $2^1\Pi_g$ (b), $1^1\Pi_u$ (c), $1^3\Pi_g$ (d), and $2^3\Pi_g$ (e) states of the lithium dimer.

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 momenta [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} | $ \Delta\mu_{fi}^{el} $ | |
|------------------------------------|------------------------------------|-----------------------|-------------------------|--|
| Li(2s) + Li(2s) → 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) → Li(2s) + Li(3s) | Jasik and Sienkiewicz | 0.000015 | | |
| Li(2s) + Li(2s) → Li(2p) + Li(2p) | Jasik and Sienkiewicz | 0.000005 | | |
| Li(2s) + Li(2s) →* 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 | |
| | Jasik and Sienkiewicz | 0.000027 | | |
| Li(2s) + Li(2p) → Li(2s) + Li(2p) | Jasik and Sienkiewicz | 1.718163 | | |
| Li(2s) + Li(2p) →* Li(2s) + Li(3s) | 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 | |
| | Jasik and Sienkiewicz | 2.363093 | | |
| | Salihoglu et al. [9] | 2.352713 | 0.0104 | |
| | Pipin and Bishop [11] | 2.345200 | 0.0179 | |
| Li(2s) + Li(2p) → Li(2s) + Li(3p) | 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 | |
| | Jasik and Sienkiewicz | 0.000174 | | |
| | Li(2s) + Li(3s) → Li(2s) + Li(3s) | Jasik and Sienkiewicz | 0.000014 | |
| | Li(2s) + Li(3s) → Li(2p) + Li(2p) | Jasik and Sienkiewicz | 0.000611 | |
| | Li(2s) + Li(3s) →* 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) → Li(2p) + Li(2p) | Jasik and Sienkiewicz | 0.000044 | | |
| Li(2p) + Li(2p) → Li(2s) + Li(3p) | Jasik and Sienkiewicz | 0.004064 | | |

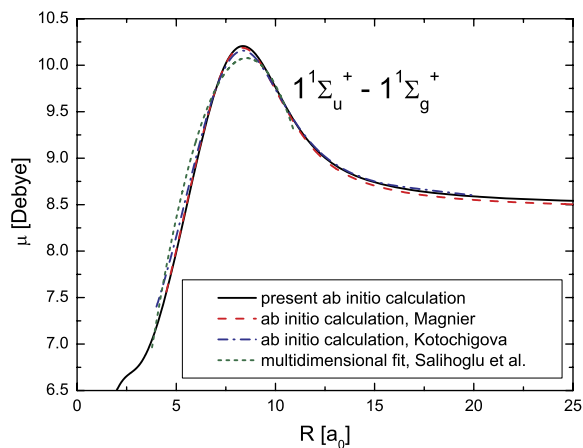


Fig. 5. The comparison between the experimental and theoretical transition dipole moments. Experimental data comes from Salihoglu et al. [9]. Theoretical results of Magnier and Kotochigova are cited in Ref. [9].

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.

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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 $\text{Li}(2s) + \text{Li}(2p)$ and first 30 vibrational levels of the $1^1\Sigma_u^+$ and $2^1\Pi_u$ states correlating, respectively, to the atomic asymptotes $\text{Li}(2s) + \text{Li}(2p)$ and $\text{Li}(2p) + \text{Li}(2p)$.

| v' | $1^1\Pi_u - 1^1\Sigma_g^+$ | | | $1^1\Sigma_u^+ - 1^1\Sigma_g^+$ | | | $2^1\Pi_u - 1^1\Sigma_g^+$ | | |
|------|----------------------------|--------------|--------------|---------------------------------|--------------|--------------|----------------------------|--------------|--------------|
| | $v'' = 0$ | $v'' = 1$ | $v'' = 2$ | $v'' = 0$ | $v'' = 1$ | $v'' = 2$ | $v'' = 0$ | $v'' = 1$ | $v'' = 2$ |
| 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 | 0.0250960000 |
| 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 | 0.0000000354 | 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 .

$$\langle \Psi_f^{el} | \mu_{x(y)}^{el} | \Psi_i^{el} \rangle = (\vec{\mu}_{fi}^{el}(\vec{R}))_{x(y)} = \int \Psi_f^{el*}(\vec{r}; \vec{R}) \vec{\mu}_{x(y)}^{el}(\vec{r}) \Psi_i^{el}(\vec{r}; \vec{R}) d\vec{r}$$

$$\langle \Psi_f^{el} | \mu_z^{el} | \Psi_i^{el} \rangle = (\vec{\mu}_{fi}^{el}(\vec{R}))_z = \int \Psi_f^{el*}(\vec{r}; \vec{R}) \mu_z^{el}(\vec{r}) \Psi_i^{el}(\vec{r}; \vec{R}) d\vec{r}$$

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

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 | -0.00002295 | -0.16916091 | 3.34145017 | -0.00003050 |
| 64.0 | -3.34301553 | -0.00002297 | -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 | -1.71844963 | 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 | 1.80139599 |
| 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 |

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Table 3 (continued)

| R | $(2^1 \Sigma_g^+ \mu_z^{el} 1^1 \Sigma_u^+)$ | $(2^1 \Sigma_g^+ \mu_z^{el} 2^1 \Sigma_u^+)$ | $(2^1 \Sigma_g^+ \mu_z^{el} 3^1 \Sigma_u^+)$ | $(2^1 \Sigma_g^+ \mu_{x(y)}^{el} 1^1 \Pi_u)$ | $(2^1 \Sigma_g^+ \mu_{x(y)}^{el} 2^1 \Pi_u)$ |
|-----|--|--|--|--|--|
| 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 | 2.31879400 |
| 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 | -0.15111568 | -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 | $(2^3 \Sigma_u^+ \mu_z^{el} 1^3 \Sigma_g^+)$ | $(2^3 \Sigma_u^+ \mu_z^{el} 2^3 \Sigma_g^+)$ | $(2^3 \Sigma_u^+ \mu_z^{el} 3^3 \Sigma_g^+)$ | $(2^3 \Sigma_u^+ \mu_{x(y)}^{el} 1^3 \Pi_g)$ | $(2^3 \Sigma_u^+ \mu_{x(y)}^{el} 2^3 \Pi_g)$ |
|-----|--|--|--|--|--|
| 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 | $\langle 3^1\Sigma_g^+ \mu_z^{el} 1^1\Sigma_u^+\rangle$ | $\langle 3^1\Sigma_g^+ \mu_z^{el} 2^1\Sigma_u^+\rangle$ | $\langle 3^1\Sigma_g^+ \mu_z^{el} 3^1\Sigma_u^+\rangle$ | $\langle 3^1\Sigma_g^+ \mu_{xy}^{el} 1^1\Pi_u\rangle$ | $\langle 3^1\Sigma_g^+ \mu_{xy}^{el} 2^1\Pi_u\rangle$ |
|------|---|---|---|---|---|
| 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 | -1.70233075 | -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 | -0.00209660 | 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 | $(3^3 \Sigma_u^+ \mu_z^{el} 1^3 \Sigma_g^+)$ | $(3^3 \Sigma_u^+ \mu_z^{el} 2^3 \Sigma_g^+)$ | $(3^3 \Sigma_u^+ \mu_z^{el} 3^3 \Sigma_g^+)$ | $(3^3 \Sigma_u^+ \mu_{x(y)}^{el} 1^3 \Pi_g)$ | $(3^3 \Sigma_u^+ \mu_{x(y)}^{el} 2^3 \Pi_g)$ |
|-----|--|--|--|--|--|
| 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 | -0.00004222 | 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 | 0.3335133 | -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 |

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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 | 0.00389200 | 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 | $\langle 5^1\Sigma_g^+ \mu_z^{el} 1^1\Sigma_u^+\rangle$ | $\langle 5^1\Sigma_g^+ \mu_z^{el} 2^1\Sigma_u^+\rangle$ | $\langle 5^1\Sigma_g^+ \mu_z^{el} 3^1\Sigma_u^+\rangle$ | $\langle 5^1\Sigma_g^+ \mu_{xy}^{el} 1^1\Pi_u\rangle$ | $\langle 5^1\Sigma_g^+ \mu_{xy}^{el} 2^1\Pi_u\rangle$ |
|------|---|---|---|---|---|
| 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 | 0.001117257 | 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 | $\langle 1^1\Sigma_u^+ \mu_{x(y)}^{el} 1^1\Pi_g \rangle$ | $\langle 1^1\Sigma_u^+ \mu_{x(y)}^{el} 2^1\Pi_g \rangle$ | $\langle 1^3\Sigma_g^+ \mu_{x(y)}^{el} 1^3\Pi_u \rangle$ | $\langle 1^3\Sigma_g^+ \mu_{x(y)}^{el} 2^3\Pi_u \rangle$ |
|------|--|--|--|--|
| 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 | 0.0107130 | 2.38061801 | -0.0106358 | -2.38057523 |
| 38.0 | 0.0131071 | 2.38309917 | -0.0130285 | -2.38305820 |
| 36.0 | 0.0161514 | 2.38601362 | -0.0160613 | -2.38597528 |
| 34.0 | 0.0201024 | 2.38941386 | -0.0201290 | -2.38942287 |
| 32.0 | 0.0253897 | 2.39336202 | -0.0254107 | -2.39336898 |
| 30.0 | 0.0326502 | 2.39789656 | -0.0326614 | -2.39789609 |
| 29.0 | 0.0374557 | 2.40037637 | -0.0373105 | -2.40036294 |
| 28.0 | 0.0430306 | 2.40302532 | -0.0430770 | -2.40293103 |
| 27.0 | -0.0496852 | 2.40572789 | -0.0497393 | -2.40559466 |
| 26.0 | -0.0576635 | 2.40845947 | -0.0577316 | -2.40814776 |
| 25.0 | -0.0672934 | 2.41112458 | -0.0673786 | -2.41042349 |
| 24.0 | -0.0789351 | 2.41358139 | -0.0787049 | -2.41203127 |
| 23.0 | -0.0931729 | 2.41566352 | -0.0934258 | -2.41230148 |
| 22.0 | 0.1109284 | 2.41716379 | -0.1113463 | -2.40978698 |
| 21.0 | 0.1329044 | 2.41791551 | -0.1336898 | -2.40165214 |
| 20.0 | 0.1605908 | 2.41798357 | -0.1620007 | -2.38150541 |
| 19.5 | 0.1770046 | 2.41794174 | -0.1790149 | -2.36265826 |
| 19.0 | 0.1960128 | 2.41805374 | -0.1983703 | -2.33362129 |
| 18.5 | 0.2169945 | 2.41863549 | -0.2204776 | -2.28817493 |
| 18.0 | 0.2407601 | 2.42014889 | -0.2460596 | -2.21597630 |
| 17.5 | 0.2677864 | 2.42327478 | -0.2754060 | -2.10063512 |
| 17.0 | 0.2986629 | 2.42896908 | -0.3095428 | -1.92112582 |
| 16.5 | 0.3341574 | 2.43853471 | -0.3495894 | -1.66756118 |
| 16.0 | 0.3752828 | 2.45353136 | -0.3970330 | -1.37026495 |
| 15.5 | 0.4234287 | 2.47579581 | -0.4538776 | -1.09425851 |
| 15.0 | 0.4805202 | 2.50716111 | -0.5228443 | -0.88431487 |
| 14.5 | 0.5492667 | 2.54900829 | -0.6081515 | -0.74493009 |
| 14.0 | 0.6335000 | 2.60152726 | -0.7138887 | -0.66236642 |
| 13.5 | 0.7385478 | 2.66274286 | -0.8480981 | -0.62127283 |
| 13.0 | 0.8718914 | 2.72771411 | -1.0189428 | -0.61017409 |
| 12.5 | 1.0421827 | 2.78864922 | -1.2393020 | -0.62127085 |
| 12.0 | 1.2610220 | 2.83631313 | -1.5247470 | -0.64941802 |
| 11.5 | 1.5413979 | 2.86286493 | -1.8937558 | -0.69119145 |
| 11.0 | 1.8976237 | 2.86404545 | -2.3668760 | -0.74431315 |
| 10.5 | 2.3433499 | 2.83966091 | -2.9605057 | -0.80749111 |
| 10.0 | 2.8911063 | 2.79196603 | -3.6846701 | -0.88094943 |
| 9.8 | 3.1412301 | 2.76700947 | -4.1046670 | -0.91379246 |
| 9.6 | 3.4098939 | 2.73893492 | -4.3555685 | -0.94916713 |
| 9.4 | 3.6975420 | 2.70778924 | -4.7184513 | -0.98772027 |
| 9.2 | 4.0045046 | 2.67390142 | -5.0974850 | -1.03034819 |
| 9.0 | 4.3310176 | 2.63720945 | -5.4905741 | -1.07836584 |
| 8.8 | 4.6770978 | 2.59785315 | -5.8958629 | -1.13344170 |
| 8.6 | 5.0426484 | 2.55581247 | -6.3109898 | -1.19752980 |
| 8.4 | 5.4273372 | 2.51116217 | -6.7320076 | -1.27183645 |
| 8.2 | 5.8306270 | 2.46392932 | -7.1571488 | 1.35422644 |
| 8.0 | 6.2517185 | 2.41411935 | -7.5837964 | 1.43492825 |
| 7.8 | 6.6894459 | 2.36175613 | -8.0093284 | 1.49795181 |
| 7.6 | 7.1421894 | 2.30684904 | -8.4311026 | 1.53582729 |
| 7.4 | 7.6077623 | 2.24948096 | -8.8464700 | 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 | -1.71790061 | 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 | $\langle 2^1 \Sigma_u^+ \mu_{x(y)}^{el} 1^1 \Pi_g \rangle$ | $\langle 2^1 \Sigma_u^+ \mu_{x(y)}^{el} 2^1 \Pi_g \rangle$ | $\langle 2^3 \Sigma_g^+ \mu_{x(y)}^{el} 1^3 \Pi_u \rangle$ | $\langle 2^3 \Sigma_g^+ \mu_{x(y)}^{el} 2^3 \Pi_u \rangle$ |
|-----|--|--|--|--|
| 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 | $\langle 3^1\Sigma_u^+ \mu_{x(y)}^{el} 1^1\Pi_g \rangle$ | $\langle 3^1\Sigma_u^+ \mu_{x(y)}^{el} 2^1\Pi_g \rangle$ | $\langle 3^3\Sigma_g^+ \mu_{x(y)}^{el} 1^3\Pi_u \rangle$ | $\langle 3^3\Sigma_g^+ \mu_{x(y)}^{el} 2^3\Pi_u \rangle$ |
|------|--|--|--|--|
| 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 | $\langle 1^1\Pi_g \mu_z^{el} 1^1\Pi_u \rangle$ | $\langle 1^1\Pi_g \mu_z^{el} 2^1\Pi_u \rangle$ | $\langle 1^3\Pi_g \mu_z^{el} 1^3\Pi_u \rangle$ | $\langle 1^3\Pi_g \mu_z^{el} 2^3\Pi_u \rangle$ |
|------|--|--|--|--|
| 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 | $\langle 1^1 \Pi_g \mu_z^{el} 1^1 \Pi_u \rangle$ | $\langle 1^1 \Pi_g \mu_z^{el} 2^1 \Pi_u \rangle$ | $\langle 1^3 \Pi_g \mu_z^{el} 1^3 \Pi_u \rangle$ | $\langle 1^3 \Pi_g \mu_z^{el} 2^3 \Pi_u \rangle$ |
|-----|--|--|--|--|
| 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 | $\langle 2^1\Pi_g \mu_z^e 1^1\Pi_u \rangle$ | $\langle 2^1\Pi_g \mu_z^e 2^1\Pi_u \rangle$ | $\langle 2^3\Pi_g \mu_z^e 1^3\Pi_u \rangle$ | $\langle 2^3\Pi_g \mu_z^e 2^3\Pi_u \rangle$ |
|------|---|---|---|---|
| 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 | $\langle 1^1\Delta_g \mu_{x(y)}^{el} 1^1\Pi_u \rangle$ | $\langle 1^1\Delta_g \mu_{x(y)}^{el} 2^1\Pi_u \rangle$ | $\langle 1^3\Delta_u \mu_{x(y)}^{el} 1^3\Pi_g \rangle$ | $\langle 1^3\Delta_u \mu_{x(y)}^{el} 2^3\Pi_g \rangle$ |
|------|--|--|--|--|
| 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 | 0.00550378 |
| 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 | $\langle 1^1 \Delta_g \mu_{x(y)}^{el} 1^1 \Pi_u \rangle$ | $\langle 1^1 \Delta_g \mu_{x(y)}^{el} 2^1 \Pi_u \rangle$ | $\langle 1^3 \Delta_u \mu_{x(y)}^{el} 1^3 \Pi_g \rangle$ | $\langle 1^3 \Delta_u \mu_{x(y)}^{el} 2^3 \Pi_g \rangle$ |
|-----|--|--|--|--|
| 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 |