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Erratum

Erratum to “Experimental study of the NaK $3^1\Pi$ state” [J. Mol. Spectrosc. (1999) 193 376–388][☆,☆☆]

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In Table 1 of Ref. [1], one intermediate state level $1(\mathrm{b})^3\Pi_0(\mathrm{v}' = 16, \mathrm{J}' = 43, \mathrm{e}) \sim 2(\mathrm{A})^1\Sigma^+(\mathrm{v}' = 17,\ \mathrm{J}' = 43,$ e) was incorrectly listed as $2(\mathrm{A})^1\Sigma^+(\mathrm{v}' = 16,\ \mathrm{J}' = 56,\ \mathrm{e})$, which is excited from $1(\mathrm{X})^1\Sigma^+(\mathrm{v}'' = 0,\ \mathrm{J}'' = 57,\ \mathrm{e})$ at the same pump frequency as the $1(\mathrm{b})^3\Pi_0(\mathrm{v}' = 16, \mathrm{J}' = 43, \mathrm{e}) \sim 2(\mathrm{A})^1\Sigma^+(\mathrm{v}' = 17,\ \mathrm{J}' = 43,\ \mathrm{e}) \leftarrow 1(\mathrm{X})^1\Sigma^+(\mathrm{v}'' = 1,$ $\mathrm{J}'' = 44$, e) transition. Here the level labeled $1(\mathrm{b})\ ^3\Pi_0(\mathrm{v}' = 16, \mathrm{J}' = 43, \mathrm{e}) \sim 2(\mathrm{A})^1\Sigma^+(\mathrm{v}' = 17, \mathrm{J}' = 43, \mathrm{e})$ is the mostly triplet component (larger triplet than singlet amplitude) of a mutually perturbing pair of levels coupled by the spin-orbit interaction. This error affects the entire last set of data in Table 1 [i.e., those levels previously listed as $3^1\Pi(\mathrm{v}, \mathrm{J} = 55, 56, 57)$]. We have corrected these assignments and carried out new measurements of the true v = 5–7, J = 55–57 levels. These have been listed in a corrected version of Table 1, which is available electronically in the JMS supplementary materials [2] or directly from the authors.

As previously, we fit the molecular $3^1\Pi$ rovibrational level energies to a Dunham expansion,

$$E(\mathrm{v},\mathrm{J}) = \sum_{i,k} (Y_{i,k} + \delta y_{i,k}) \left(\mathrm{v} + \tfrac{1}{2}\right)^i [\mathrm{J}(\mathrm{J}+1) - \Lambda^2]^k, \qquad (1)$$

where the $Y_{i,k}$ are the standard Dunham coefficients, the $y_{i,k}$ constants describe the Λ-doubling of the $^1\Pi$ state ($y_{i,k} = 0$ for $k = 0$), and $\delta = -1$ or $+1$ for the f and e parity levels, respectively. The corrected coefficients are listed here in the revised Table 2. Correcting the assignment error primarily affects the centrifugal distortion constants, and higher order rotational constants (above $k = 2$) are no longer needed. Vibrational constants ($Y_{i,0}$) and inertial rotational constants ($Y_{i,1}$) are not strongly affected by this correction. However, it is now possible to obtain the first lambda doubling constant $y_{0,1}$. The new constants also satisfy the Kratzer relation $[Y_{02} \approx -4(Y_{01})^3/(Y_{10})^2 = -3.57\mathrm{E}-7\ \mathrm{cm}^{-1}$ compared to the fitted value $-3.62\mathrm{E}{-}7\ \mathrm{cm}^{-1}]$ much better than the previous set. In addition, these new constants are in much better agreement with those of Pashov *et al.* [6].

The revised Dunham coefficients were then used to determine a new RKR potential curve that is listed here in the corrected Table 3 and plotted in the corrected Fig. 3. The new potential energy curve is found to be virtually indistinguishable by eye from the previous curve.

Finally, the new RKR curve was used to calculate relative intensities of $3^1\Pi(\mathrm{v},\ \mathrm{J} = 30,\ \mathrm{f}) \rightarrow 1(\mathrm{X})^1\Sigma^+(\mathrm{v}'',$ $\mathrm{J} = 30$, e) transitions using a constant transition dipole moment function (revised Fig. 4, supplementary materials [2]) and a fitted R dependent dipole moment function $M_e(R)$, where R is the internuclear separation (revised Fig. 5, supplementary materials [2]). Best agreement was obtained using an expansion in inverse powers of R^{-2}:

$$M_e(R) = p_1 R^{-2} + p_2 R^{-4} + p_3 R^{-6} + p_4 R^{-8} + p_5 R^{-10}. \qquad (2)$$

The parameters were fit by the least squares method and the best fit values are $p_2/p_1 = -78.4\ (\mathrm{Å})^2$, $p_3/p_1 = 2233.1\ (\mathrm{Å})^4$, $p_4/p_1 = -26001\ (\mathrm{Å})^6$, and $p_5/p_1 = 108087\ (\mathrm{Å})^8$.

In the revised Fig. 6, we show the fitted $3^1\Pi \rightarrow 1(\mathrm{X})^1\Sigma^+$ relative transition dipole moment function. This experimental $M_e(R)$ is very little changed from that reported in the original article. It should be considered to be valid for $R = 3.65$–6.03 Å (the turning points of the $3^1\Pi(\mathrm{v} = 12)$ level). In Fig. 6 we also show the recent theoretical dipole moment function of Magnier, Aubert-Frécon, and Millié [8] as well as the earlier calculation of Ratcliff *et al.* [9]. Since only a relative transition dipole

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Table 2 Revised. The molecular constants of the NaK $3^1\Pi$ state obtained in this work along with the theoretical constants of Ref. 3

	Experiment (this work)	Theory (Ref. 3)
R_e	4.4587 ± 0.003	4.51
D_e	1290.95 ± 0.58	1155
$Y_{0,0}$	25520.696 ± 0.079	25568
$Y_{1,0}$	47.546 ± 0.033	47.20
$Y_{2,0}$	-0.1688 ± 0.0036	
$Y_{3,0}$	$-7.93\text{E}-3 \pm 1.3\text{E}-4$	
$Y_{0,1}$	$0.058646 \pm .000083$	
$Y_{1,1}$	$-5.725\text{E}-4 \pm 1.5\text{E}-5$	
$Y_{2,1}$	$-1.080\text{E}-5 \pm 6.3\text{E}-7$	
$Y_{0,2}$	$-3.62\text{E}-7 \pm 2.2\text{E}-8$	
$Y_{1,2}$	$5.0\text{E}-9 \pm 3.0\text{E}-9$	
$y_{0,1}$	$1.00\text{E}-5 \pm 3.9\text{E}-6$	

Note: All values are given in cm^{-1} except for the equilibrium internuclear separation R_e, which is in Å. The dissociation energy D_e was obtained from the expression $D_e = [D_e(\text{X}^1\Sigma^+) + \Delta\text{E}_{\text{atomic}} - Y_{0,0}]$ with $D_e(\text{X}^1\Sigma^+) = (5274.9 \pm 0.5)\ \text{cm}^{-1}$ from Ref. 4 and $\Delta\text{E}_{\text{atomic}} = \text{E}[\text{Na}(3\text{S}_{1/2}) + \text{K}(3\text{D}_{3/2})] - \text{E}[\text{Na}(3\text{S}_{1/2}) + \text{K}(4\text{S}_{1/2})] = 21536.75\ \text{cm}^{-1}$ from Ref. 5. Quoted uncertainties represent 95% confidence limits.

Table 3 Revised. RKR turning points for the NaK $3^1\Pi$ state obtained in this work

v	R_1(Å)	R_2(Å)	E(cm^{-1})
−0.5	4.4587		0.0000
−0.4	4.3619	4.5608	4.7896
−0.2	4.2945	4.6384	14.2850
0	4.2496	4.6936	23.7665
0.2	4.2140	4.7395	33.2334
0.4	4.1839	4.7801	42.6855
0.6	4.1575	4.8169	52.1224
0.8	4.1338	4.8512	61.5438
1	4.1122	4.8833	70.9491
2	4.0250	5.0241	117.7227
3	3.9586	5.1456	164.0399
4	3.9044	5.2565	209.8528
5	3.8584	5.3607	255.1141
6	3.8186	5.4606	299.7761
7	3.7834	5.5577	343.7912
8	3.7520	5.6530	387.1118
9	3.7237	5.7472	429.6905
10	3.6980	5.8412	471.4795
11	3.6745	5.9353	512.4313
12	3.6530	6.0301	552.4984
13	3.6330	6.1261	591.6331
14	3.6146	6.2236	629.7879
15	3.5973	6.3231	666.9151
16	3.5812	6.4251	702.9673
17	3.5660	6.5299	737.8968
18	3.5515	6.6381	771.6561
19	3.5378	6.7502	804.1975
20	3.5245	6.8668	835.4735
21	3.5116	6.9886	865.4365
22	3.4989	7.1164	894.0390

Includes Y_{00} correction = 0.03665 cm^{-1}.

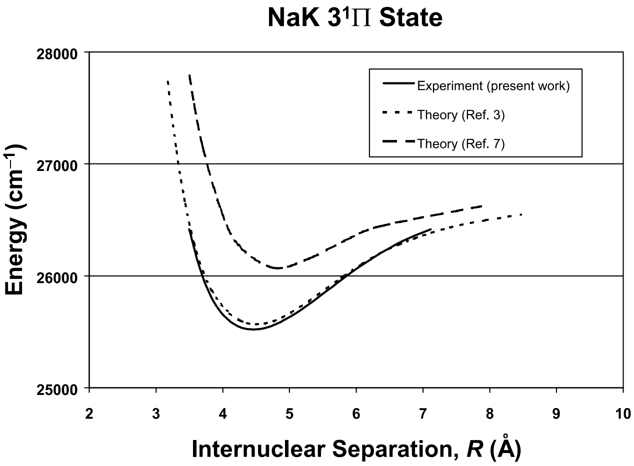

Fig. 3. **Revised.** Comparison of the experimental NaK $3^1\Pi$ state RKR potential curve (solid line), obtained in the present work, with the theoretical $3^1\Pi$ state potentials of Ref. 3 (dotted line) and Ref. 7 (dashed line).

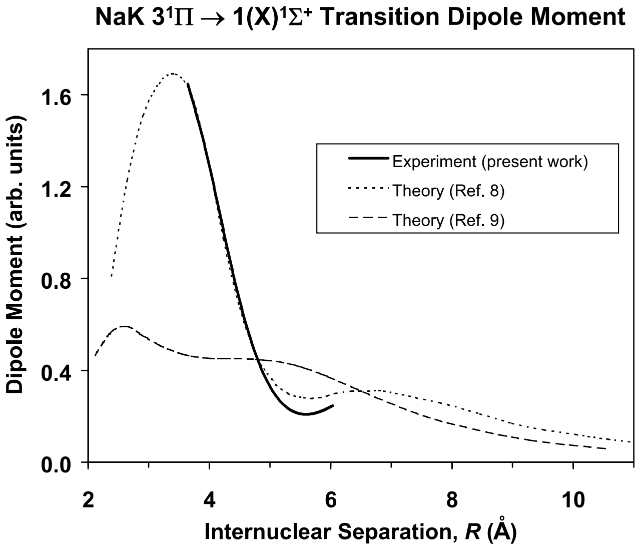

Fig. 6. **Revised.** Solid line: experimental NaK $3^1\Pi \rightarrow X^1\Sigma^+$ relative transition dipole moment vs. internuclear separation obtained in this work $[M_e(R) = p_1R^{-2} + p_2R^{-4} + p_3R^{-6} + p_4R^{-8} + p_5R^{-10}$ with $p_2/p_1 = -78.4$ (Å)^2, $p_3/p_1 = 2233.1$ (Å)^4, $p_4/p_1 = -26001$ (Å)^6, and $p_5/p_1 = 108087$ (Å)^8]. Dotted line: theoretical transition dipole moment from Ref. 8. Long dashed line: theoretical transition dipole moment from Ref. 9. The experimental curve has been normalized to the theoretical curve of Ref. 8 at $R = 4.76$ Å (9.0 au).

moment can be determined from the data, we have normalized the experimental curve to the theoretical curve of Magnier at $R = 4.76$ Å (9 au). It can be seen that the most recent calculated dipole moment function is overall in excellent agreement with the experimental data. In the near future, we hope to be able to extend our measurements of the dipole moment function to larger and smaller values of R in order to test the predicted behavior in these regions.

Acknowledgments

We thank Pat Burns for discovering the misassignment of the $2(\text{A})^1\Sigma^+(\text{v}' = 17, \text{J}' = 43, \text{e})$ energy level.

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[2] Supplementary materials for this article include one table and two figures (revised Table 1 and revised Figs. 4 and 5). These materials may be retrieved from ScienceDirect.

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