ERRATUM

Erratum: Internal rotation, Stark effect, and rotational magnetic moments in CH_3CD_3

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An error was made in the analysis of the internal rotation data. Owing to a mistake in the input file to the least squares calculation discussed in Sect. 7, the value of V_3 was iterated only where it appears explicitly in the energy; for the determination of the matrix elements it was held fixed at the starting value, thereby shifting some of the resulting parameters. The corrected torsional and rotational constants from Table 1 are given in Table 1a below. The changes are small, but in some cases significant. The new value for V_3 of 1005.01(21) cm^{-1} should also be entered in the Abstract. The differences (observed − calculated) in Table 3 do not change.

As a further consequence, the constants in [7] must be modified by ~2.5 times the error limits:

[7] $V_3' = 1012.85(24) - 2.65(13)n_D\ cm^{-1}$

The intercept is the predicted barrier height for C_2H_6 and the slope is the change per deuteron in the barrier height. The latter should also be noted in the Abstract. For Table 6, the corrected values of V_3' can be obtained from the current [7]; the agreement remains good.

None of the discussion in the text needs to be altered.

The recently reported frequency of 32 948.805(10) MHz for the pure rotational transition ($J_K = 1_0 \leftarrow 0_0$) for the ground torsional state (1) agrees very well with the value predicted by the current model.

TABLE 1a. Molecular constants for CH_3CD_3

Quantity	Units	Value[a]
A	MHz	53 499(11)[b]
B	MHz	16 503.84(8)
D_J	kHz	19.6(1.4)
D_{JK}	kHz	50.0(6.6)
D_K	kHz	142.1[c]
ρ		0.3339792(22)[b]
s		55.6762(18)
V_3	cm^{-1}	1 005.01(21)
F_{3J}	MHz	−134(9)
D_{Jm}	MHz	2.62(9)
d_J	MHz	6.88(27)
I_α	amu Å^2	3.1549(12)[b]

[a]Unless otherwise noted, the value has changed from the original. None of the errors has changed.
[b]The value did not change.
[c]This was held fixed at the same value as was used in the original.

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1. W. HÜTTNER, H. HÄUSSLER, and W. MAJER. Chem. Phys. Lett. **109**, 359 (1984).