Supplementary material to

The υ_{10} = 1 level of Propyne, $H_3C-C\equiv CH$, and Its Interactions with υ_9 = 1 and υ_{10} = 2

by

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This file contains data obtained with Pickett's SPFIT program which was written to fit general asymmetric top molecules. **Table 1** contains the υ = 0 constants. Options exist to fit *l*-doubled states of a symmetric rotor and to consider vibration-rotation interaction. The fit differs slightly from that presented in the paper which was obtained employing a program written by Dr. Petr Pracna to fit general symmetric top molecules. First, instead of fitting rotational and centrifugal distortion constants for all states, in the present case differences of these constants from those of the υ = 0 state have been fit. This is a rather technical difference with no effect on the quality of the fit. However, there are also slight differences in the type and number of parameters determined as well as in the weighting scheme. **Table 2** presents the υ_9 = 1 and υ_{10} = 2 constants used in the combined fit while **Table 3** gives the resulting constants for the υ_{10} = 1 state. As can be seen in the second part of this file (**Tables 5** to **7**), the resulting differences are usually small but not always insignificant. In the υ_{10} = 1 fit, the υ = 0 constants were kept fixed, and the uncertainties of the ground state parameters have not been propagated. This is a usually done. **Table 4** demonstrates that inclusion of the ground states lines in the fit and release of the ground state constants mostly changes both the constants and their uncertainties only slightly. The uncertainties of the υ_{10} = 1 parameters $A-B$, $A\zeta$, and η_K increase by a larger amount. Only the value of L_{KKJ} changes by more than 1σ.

IMPORTANT NOTE: The υ_{10} = 1 files provided in the DATA or FITTING SPECTRA sections will work only with the 7 July 2001 and 26 Sept. 2001 versions of the program !! In previous versions there was a bug that allowed one *l*-doubled state to be fit only.

Table 1

Spectroscopic constants (MHz) of propyne, $H_3C{-}C{\equiv}CH$, in its ground vibrational state.

Parameter	Value
$A-B$	150 594.45 (46)
B	8 545.876 862 1 (217)
$D_J \cdot 10^3$	2.939 241 0 (251)
$D_{JK} \cdot 10^3$	163.414 49 (209)
D_K	2.907 2 (122)
$H_J \cdot 10^{12}$	−63.2 (61)
$H_{JK} \cdot 10^9$	914.08 (89)
$H_{KJ} \cdot 10^6$	5.302 1 (114)
$L_{JJK} \cdot 10^{12}$	−6.313 (148)
$L_{JK} \cdot 10^{12}$	−41.81 (189)
$L_{KKJ} \cdot 10^{12}$	−419.4 (203)

Table 2

Spectroscopic constants[a] (MHz) of propyne, $H_3C-C\equiv CH$, in its $\upsilon_9 = 1$ and $\upsilon_{10} = 2$ vibrationally excited states used for the global $\upsilon_{10} = 1$ fit.

	$\upsilon_9 = 1$	$\upsilon_{10} = 2, l = 0$	$\upsilon_{10} = 2, l = \pm 2$
$E_v \cdot 10^{-6}$	19.143 863 85	19.512 354 46	20.126 227 48
$\Delta(A-B)$	−45.181	−140.787	−206.169
ΔB	5.181 79	47.826 59	47.383 37
$\Delta D_J \cdot 10^6$	12.39	161.8	153.08
$\Delta D_{JK} \cdot 10^6$	91.3	686.6	884.7
$\Delta D_K \cdot 10^3$	23.3	86.2	79.7
q_{22}	−9.019 00	−16.784 49[b]	[b]
$q^J_{22} \cdot 10^6$	19.31	54.633[b]	[b]
$q^K_{22} \cdot 10^3$	−10.158	4.292[b]	[b]
$A\zeta \cdot 10^{-3}$	159.92 059		141.908 28
$\eta_J \cdot 10^3$	466.883		336.179
η_K	12.009 9		11.312 2
$\eta_{JK} \cdot 10^6$	−32.74		−51.9
$\eta_{KK} \cdot 10^3$	1.03		5.11
$F_{9/22} \cdot 10^{-3}$	8.502 8[c]		[c]
$F^J_{9/22} \cdot 10^3$	25.9[c]		[c]

[a] $\Delta X := X_\upsilon - X_{\upsilon=0}$.

[b] Between $\upsilon_{10} = 2, l = 0$ and $\upsilon_{10} = 2, l = \pm 2$.

[c] Between $\upsilon_9 = 1$ and $\upsilon_{10} = 2, l = \pm 2$.

Table 3

Spectroscopic constants[a] (MHz) of propyne, $H_3C{-}C{\equiv}CH$, in its $\upsilon_{10} = 1$ vibrationally excited state, taking into account the interactions with $\upsilon_9 = 1$ and $\upsilon_{10} = 2$.

	$\upsilon_{10} = 1$
$E_v \cdot 10^{-6}$	9.921 549 62 (78)
$\Delta(A-B)$	−85.840 3 (108)
ΔB	23.939 204 (93)
$\Delta D_J \cdot 10^6$	77.173 (42)
$\Delta D_{JK} \cdot 10^6$	609.25 (109)
$\Delta D_K \cdot 10^3$	8.585 (117)
$\Delta H_J \cdot 10^{12}$	216.8 (79)
$\Delta H_{JK} \cdot 10^9$	−2.002 (186)
$\Delta H_{KJ} \cdot 10^9$	75.9 (80)
q_{22}	−16.786 365 (111)
$q^J_{22} \cdot 10^6$	53.619 4 (295)
$q^K_{22} \cdot 10^3$	4.634 1 (35)
$A\zeta \cdot 10^{-3}$	141.920 464 (31)
$\eta_J \cdot 10^3$	334.765 3 (82)
η_K	10.927 31 (185)
$\eta_{JK} \cdot 10^6$	−33.490 (151)
$\eta_{KK} \cdot 10^3$	−
$C_{9/10}$	20.127 (233)[b]
$F_{10/22} \cdot 10^{-3}$	52.274 (76)[c]
$F^J_{10/22} \cdot 10^3$	−300.7 (67)[c]

[a] $\Delta X := X_\upsilon - X_{\upsilon=0}$.

[b] Between $\upsilon_{10} = 1$ and $\upsilon_9 = 1$.

[c] Between $\upsilon_{10} = 1$ and $\upsilon_{10} = 2$, $l = \pm 2$.

Table 4

Spectroscopic constants[a] (MHz) of propyne, $H_3C-C\equiv CH$, in its $\upsilon = 0$ and $\upsilon_{10} = 1$ states, taking into account the interactions with $\upsilon_9 = 1$ and $\upsilon_{10} = 2$.

$\upsilon = 0$		$\upsilon_{10} = 1$	
Parameter	Value	Value	Parameter
		9.921 549 57 (91)	$E_v \cdot 10^{-6}$
$A-B$	150 594.45 (46)	−85.840 (74)	$\Delta(A-B)$
B	8 545.876 861 1 (214)	23.939 182 (103)	ΔB
$D_J \cdot 10^3$	2.939 241 4 (240)	77.171 (50)	$\Delta D_J \cdot 10^6$
$D_{JK} \cdot 10^3$	163.414 05 (172)	609.54 (138)	$\Delta D_{JK} \cdot 10^6$
D_K	2.907 2 (122)	8.576 (117)	$\Delta D_K \cdot 10^3$
$H_J \cdot 10^{12}$	−63.8 (58)	216.9 (98)	$\Delta H_J \cdot 10^{12}$
$H_{JK} \cdot 10^9$	914.12 (67)	−2.048 (242)	$\Delta H_{JK} \cdot 10^9$
$H_{KJ} \cdot 10^6$	5.295 8 (101)	75.6 (83)	$\Delta H_{KJ} \cdot 10^9$
$L_{JJK} \cdot 10^{12}$	−6.288 (112)		
$L_{JK} \cdot 10^{12}$	−42.70 (157)		
$L_{KKJ} \cdot 10^{12}$	−395.6 (188)		
		−16.786 365 (111)	q_{22}
		53.619 8 (295)	$q^J_{22} \cdot 10^6$
		4.633 8 (36)	$q^K_{22} \cdot 10^3$
		141.920 46 (44)	$A\zeta \cdot 10^{-3}$
		334.765 7 (84)	$\eta_J \cdot 10^3$
		10.927 (49)	η_K
		−33.447 (155)	$\eta_{JK} \cdot 10^6$
		−	$\eta_{KK} \cdot 10^3$
		20.081 (237)[b]	$C_{9/10}$
		52.269 (76)[c]	$F_{10/22} \cdot 10^{-3}$
		−302.7 (70)[c]	$F^J_{10/22} \cdot 10^3$

[a] $\Delta X := X_\upsilon - X_{\upsilon=0}$. [b] Between $\upsilon_{10} = 1$ and $\upsilon_9 = 1$. [c] Between $\upsilon_{10} = 1$ and $\upsilon_{10} = 2$, $l = \pm 2$.

Table 5

Spectroscopic constants (cm^{-1}) of propyne, $H_3C-C\equiv CH$, in its ground vibrational state.

Parameter	Value
A	5.308 350 0 (155)
B	0.285 059 768 32 (72)
$D_J \cdot 10^9$	98.042 53 (84)
$D_{JK} \cdot 10^6$	5.450 921 (70)
$D_K \cdot 10^6$	96.97 (41)
$H_J \cdot 10^{15}$	−2.107 (203)
$H_{JK} \cdot 10^{12}$	30.490 5 (296)
$H_{KJ} \cdot 10^{12}$	176.86 (38)
$L_{JJK} \cdot 10^{18}$	−210.6 (49)
$L_{JK} \cdot 10^{15}$	−1.394 (63)
$L_{KKJ} \cdot 10^{15}$	−13.99 (68)

Table 6

Spectroscopic constants[a] (cm^{-1}) of propyne, $H_3C{-}C{\equiv}CH$, in its $\upsilon_9 = 1$ and $\upsilon_{10} = 2$ vibrationally excited states used for the global $\upsilon_{10} = 1$ fit.

	$\upsilon_9 = 1$	$\upsilon_{10} = 2, l = 0$	$\upsilon_{10} = 2, l = \pm 2$
E_v	638.570 562	650.862 086	671.338 686
A	5.307 015 8	5.305 249 2	5.303 053 5
B	0.285 232 61	0.286 655 09	0.286 640 31
$D_J \cdot 10^9$	98.455 8	103.439 6	103.148 7
$D_{JK} \cdot 10^6$	5.453 97	5.473 82	5.480 43
$D_K \cdot 10^6$	97.75	99.84	99.63
$q_{22} \cdot 10^6$	−300.84	−559.87[b]	[b]
$q^J_{22} \cdot 10^9$	0.644 2	1.822 4[b]	[b]
$q^K_{22} \cdot 10^9$	−338.8	143.2[b]	[b]
$A\zeta$	5.306 740		4.733 551
$\eta_J \cdot 10^6$	15.573 5		11.213 7
$\eta_K \cdot 10^6$	400.61		377.33
$\eta_{JK} \cdot 10^9$	−1.092		−1.731
$\eta_{KK} \cdot 10^9$	34.3		171.
$F_{9/22} \cdot 10^3$	283.62[c]		[c]
$F^J_{9/22} \cdot 10^9$	964.[c]		[c]

[a]Sextic and octic centrifugal distortion constants fixed to ground state values.

[b]Between $\upsilon_{10} = 2, l = 0$ and $\upsilon_{10} = 2, l = \pm 2$.

[c]Between $\upsilon_9 = 1$ and $\upsilon_{10} = 2, l = \pm 2$.

Table 7

Spectroscopic constants[a] (cm^{-1}) of propyne, $H_3C{-}C{\equiv}CH$, in its $\upsilon_{10} = 1$ vibrationally excited state, taking into account the interactions with $\upsilon_9 = 1$ and $\upsilon_{10} = 2$.

	$\upsilon_{10} = 1$
E_v	330.947 272 (26)
A	5.306 285 2 (4)
B	0.285 858 294 2 (31)
$D_J \cdot 10^9$	100.616 73 (141)
$D_{JK} \cdot 10^6$	5.471 243 (35)
$D_K \cdot 10^6$	96.688 (4)
$H_J \cdot 10^{15}$	5.125 (264)
$H_{JK} \cdot 10^{12}$	30.423 7 (62)
$H_{KJ} \cdot 10^{12}$	179.39 (27)
$q_{22} \cdot 10^6$	−559.932 9 (37)
$q^J_{22} \cdot 10^9$	1.788 55 (98)
$q^K_{22} \cdot 10^9$	154.576 (116)
$A\zeta$	4.733 957 12 (102)
$\eta_J \cdot 10^6$	11.166 568 (274)
$\eta_K \cdot 10^6$	364.496 (62)
$\eta_{JK} \cdot 10^9$	−1.117 1 (50)
$\eta_{KK} \cdot 10^9$	−
$C_{9/10} \cdot 10^6$	671.4 (78)[b]
$F_{10/22}$	1.743 69 (255)[c]
$F^J_{10/22} \cdot 10^6$	−10.029 (225)[c]

[a]Octic centrifugal distortion constants fixed to ground state values.

[b]Between $\upsilon_{10} = 1$ and $\upsilon_9 = 1$.

[c]Between $\upsilon_{10} = 1$ and $\upsilon_{10} = 2$, $l = \pm 2$.