

Supporting Informations - table S1

Table S1: Molecular constants in the RAM system of 2-methylfuran obtained by a global fit using program BELGI-C_s.

Operator ^a	Constant ^b	Unit	Present work ^c
P_a^2	A	cm ⁻¹	0.29308980(67)
P_b^2	B	cm ⁻¹	0.11841455(81)
P_c^2	C	cm ⁻¹	0.08558655(30)
$\{P_a, P_b\}$	D _{ab}	cm ⁻¹	-0.005714(10)
$-P^4$	Δ_J	cm ⁻¹	0. 877042(31)*10 ⁻⁸
$-P^2 P_a^2$	Δ_{JK}	cm ⁻¹	0.4673(24)*10 ⁻⁷
$-P_a^4$	Δ_K	cm ⁻¹	0.35765(32)*10 ⁻⁷
$-2P^2(P_b^2 - P_c^2)$	δ_J	cm ⁻¹	0.238514(17)*10 ⁻⁷
$-\{P_a^2, (P_b^2 - P_c^2)\}$	δ_K	cm ⁻¹	0.35765(32)*10 ⁻⁷
P_α^2	F	cm ⁻¹	5.64 ^{fixed}
$(1/2)(1 - \cos(3\alpha))$	V ₃	cm ⁻¹	420.3157(35)
$(1/2)(1 - \cos(6\alpha))$	V ₆	cm ⁻¹	-9.010(11)
$P_a P_\gamma$	ρ	unitless	0.0551544(10)
$(1 - \cos 3\alpha)P_a^2$	k ₅	cm ⁻¹	0.1363(14)*10 ⁻³
$(1 - \cos 3\alpha)P^2$	F _v	cm ⁻¹	-0.168(25)*10 ⁻³
$(1 - \cos 3\alpha)(P_b^2 - P_c^2)$	c ₂	cm ⁻¹	-0.48350(37)*10 ⁻⁴
$P_\alpha^2 \{P_a, P_b\}$	Δ_{ab}	cm ⁻¹	-0.5554(40)*10 ⁻⁵
$P_a P_\alpha P^2$	L _v	cm ⁻¹	0.1226(71)*10 ⁻⁶
$P_\alpha^2 P^2$	G _v	cm ⁻¹	-0.1087(56)*10 ⁻⁵
P_α^4	k ₄	cm ⁻¹	-0.2702(27)*10 ⁻³
$(1 - \cos 6\alpha)P^2$	N _v	cm ⁻¹	0.296(20)*10 ⁻⁴
P_a^6	H _K	cm ⁻¹	0.35(10)*10 ⁻¹³
$N_{\nu t=0}/N_{\nu t=1}/N_{tot}$			14152/ 3742/ 17894
$\sigma_{\nu t=0}/\sigma_{\nu t=1}/\sigma_{tot}$		kHz	107.3/ 114.3/ 108.8

^a All constants refer to a rho-axis system, therefore the inertia tensor is not diagonal and the constants cannot be directly compared to those of a principal axis system. P_a, P_b, P_c are the components of the overall rotation angular momentum, P_γ is the angular momentum of the internal rotor rotating around the internal rotor axis by an angle γ. {u,v} is the anti commutator uv + vu.

^b The product of the parameter and operator from a given row yields the term actually used in the vibration-rotation-torsion Hamiltonian, except for F, ρ and A, which occur in the Hamiltonian in the form $F(P_\gamma - \rho P_a)^2 + AP_a^2$.

$N_{\nu t=0}/N_{\nu t=1}/N_{tot}$ are the numbers of $\nu_t = 0$ transitions, $\nu_t = 1$ transitions and the total number of transitions.

$\sigma_{\nu t=0}/\sigma_{\nu t=1}/\sigma_{tot}$ are the respective standard deviations.

^c Values of the parameters from the present fit. Statistical uncertainties are shown as one standard uncertainty in the last digit.