Supplementary Table 3 - $^{13}CH_3OD$ Molecular Parameters used in the Energy Calculation

First column shows the (n l m) order of the torsion-rotation terms.
[n = total order, l = torsional order, m = rotational order, with n = l + m]
Second column gives the torsion-rotation operator in the Hamiltonian.
Current and prior parameter names are as given in Table 2 of Ref. [16],
Xu et al., J. Mol. Spectrosc. 303 (2104) 1-7.

Term Order (n l m)	T-R Operator	Parameter Name	Prior Name	Value (cm-1) [ρ is unitless]
(2 2 0)	P_γ^2	F	F	17.4186877
	$(1-\cos 3\gamma)/2$	V_3	V_3	366.0335657
(2 1 1)	$P_\gamma P_a$	ρ	ρ	0.695925575
(2 0 2)	P_a^2	A	A	3.675258735
	P_b^2	B	B	0.762473926
	P_c^2	C	C	0.715377077
	$\{P_a, P_b\}$	D_{ab}	D_{ab}	2.68334E-02
(4 4 0)	P_γ^4	F_m	k_4	-2.80112E-03
	$(1-\cos 6\gamma)/2$	V_6	V_6	4.16790E-02
(4 3 1)	$P_\gamma^3 P_a$	ρ_m	k_3	-1.07868E-02
	$\{(1-\cos 3\gamma), P_\gamma P_a\}$	ρ_3	k6	5.82369E-02
(4 2 2)	$P_\gamma^2 P2$	F_J	G_v	-8.00367E-05
	$P_\gamma^2 P_a^2$	F_K	k_2	-1.60923E-02
	$2P_\gamma^2(P_b^2-P_c^2)$	F_{bc}	c_1	-2.19992E-05
	$P_\gamma^2\{P_a,P_b\}$	F_{ab}	Δ_{ab}	2.62381E-04
	$\sin 3\gamma\{P_a,P_c\}$	D_{3ac}	D_{ac}	1.85342E-02
	$(1-\cos 3\gamma)P^2$	V_{3J}	F_v	-2.16646E-03
	$(1-\cos 3\gamma)P_a^2$	V_{3K}	k_5	9.44716E-02
	$(1-\cos 3\gamma)(P_b^2-P_c^2)$	V_{3bc}	c_2	-1.27212E-04
	$(1-\cos 3\gamma)\{P_a,P_b\}$	V_{3ab}	d_{ab}	7.71976E-03
(4 1 3)	$P_\gamma P_a P^2$	ρ_J	L_v	-1.48812E-04
	$P_\gamma P_a^3$	ρ_K	k_1	-1.14948E-02
	$P_\gamma\{P_a,(P_b^2-P_c^2)\}$	ρ_{bc}	c_4	-5.80500E-05
	$P_\gamma(P_a^2P_b+P_bP_a^2)$	ρ_{ab}	δ_{ab}	3.77768E-04
(4 0 4)	$-P^4$	Δ_J	Δ_J	1.38946E-06
	$-P^2P_a^2$	Δ_{JK}	Δ_{JK}	6.92328E-05
	$-P_a^4$	Δ_K	Δ_K	3.24104E-03
	$-2P^2(P_b^2-P_c^2)$	δ_J	δ_J	9.19784E-08
	$-\{P_a^2,(P_b^2-P_c^2)\}$	δ_K	δ_K	3.59818E-05

	$\{P_a,P_b\}P^2$	D_{abJ}	D_{abJ}	-3.99135E-07
	$\{P_a^3,P_b\}$	D_{abK}	D_{abK}	1.20840E-04
(6 6 0)	$(1-\cos 9\gamma)/2$	V_9	V_9	-4.52771E+00
	P_γ^6	F_{mm}	k_{4B}	1.44564E-05
(6 5 1)	$P_\gamma^5 P_a$	ρ_{mm}	k_{3B}	6.75954E-05
(6 4 2)	$P_\gamma^4 P^2$	F_{mJ}	M_v	2.98775E-08
	$P_\gamma^4 P_a^2$	F_{mK}	K_1	1.50244E-04
	$(1-\cos 6\gamma)P^2$	V_{6J}	N_v	-1.53113E-05
	$(1-\cos 6\gamma)P_a^2$	V_{6K}	K_2	-2.73029E-03
	$(1-\cos 6\gamma)(P_b^2-P_c^2)$	V_{6bc}	c_{11}	-5.60345E-05
	$(1-\cos 6\gamma)\{P_a,P_b\}$	V_{6ab}	dd_{ab}	-1.38133E-04
(6 3 3)	$P_\gamma^3 P_a^3$	ρ_{mK}	K_3	1.92141E-04
	$P_\gamma^3 P_a P^2$	ρ_{mJ}	k_{3J}	9.76955E-08
	$P_\gamma^3\{P_a,(P_b^2-P_c^2)\}$	ρ_{mbc}	c_{12}	8.33830E-09
	$P_\gamma^3\{P_a^2,P_b\}$	ρ_{mab}	$\delta\delta_{ab}$	2.08199E-09
	$\{(1-\cos 3\gamma),P^2P_aP_\gamma\}$	ρ_{3J}	k_{6J}	1.74026E-05
	$\{(1-\cos 3\gamma),P_a^3P_\gamma\}$	ρ_{3K}	k_{6K}	4.25102E-04
(6 2 4)	$P_\gamma^2 P_a^2 P^2$	F_{JK}	k_{2J}	1.11338E-07
	$P_\gamma^2 P_a^4$	F_{KK}	k_{2K}	1.46876E-04
	$2P_\gamma^2\{P_a^2,(P_b^2-P_c^2)\}$	F_{Kbc}	c_8	-2.41937E-08
	$(1-\cos 3\gamma)P^4$	V_{3JJ}	f_v	9.34411E-09
	$(1-\cos 3\gamma)P_a^2P^2$	V_{3JK}	k_{5J}	2.25458E-05
	$(1-\cos 3\gamma)P_a^4$	V_{3KK}	f_k	5.90899E-04
	$(1-\cos 3\gamma)\{P_a,P_b\}P^2$	V_{3Jab}	d_{abJ}	-7.12608E-08
	$(1-\cos 3\gamma)\{P_a^3,P_b\}$	V_{3Kab}	d_{abK}	1.75551E-06
	$(1-\cos 3\gamma)(P_b^2-P_c^2)P^2$	V_{3Jbc}	c_{2J}	7.91492E-09
	$(1-\cos 3\gamma)\{P_a^2,(P_b^2-P_c^2)\}$	V_{3Kbc}	c_9	5.50081E-07
	$\sin 3\gamma P^2\{P_a,P_c\}$	d_{3acJ}		-1.52918E-07
(6 1 5)	$P_\gamma P_a^5$	ρ_{KK}	l_k	6.25915E-05
	$P_\gamma P_a^3P^2$	ρ_{JK}	λ_v	4.81530E-08
	$P_\gamma\{P_a^3,(P_b^2-P_c^2)\}$	ρ_{Kbc}	c_{7K}	-2.96363E-08
(6 0 6)	$P^4P_a^2$	H_{JK}	H_{JK}	7.64126E-11
	$P_a^4P^2$	H_{KJ}	H_{KJ}	5.81438E-09
	P_a^6	H_K	H_K	1.17317E-05