Supplementary material: Expansion coefficients (see Eqs.(2-5)) for the CCSD(T)/cc-pVTZ potential energy surface of propane, $V(\alpha,\theta_1,\theta_2)$, the vibrationally corrected $V^{EF}(\alpha,\theta_1,\theta_2)$ (V^{EF}=V+ V'+V^{ZPVE}) and the refined V^{ADJ} surfaces (in cm^{-1}/degrees^M)

Propane G_{36} species					
		CH_3-CH_2-CH_3		**CH_3-$^{13}CH_2$-CH_3**	
Coeff.	V	V^{EF}	V^{ADJ}	V^{EF}	V^{ADJ}
A_{000}	1161.901	1198.911	1198.911	1197.242	1199.364
A_{100}	-16.540	-13.942	-13.398	-14.173	-13.475
A_{200}	9.148	9.098	8.506	9.105	8.511
A_{300}	-0.101	-0.099	-0.090	-0.099	-0.090
A_{030}	-608.397	-624.819	-599.710	-624.050	-599.999
A_{130}	13.092	12.979	12.549	12.978	12.564
A_{230}	-0.821	-0.808	-0.755	-0.807	-0.755
A_{330}	0.016	0.015	0.014	0.015	0.014
A_{033}	63.484	60.790	60.790	61.033	60.894
A_{133}	-8.599	-8.524	-8.241	-8.546	-8.251
A_{233}	0.430	0.424	0.396	0.425	0.397
A_{333}	-0.008	-0.008	-0.007	-0.008	-0.007
A_{060}	-8.122	-8.201	-8.207	-8.264	-8.195
A_{160}	0.809	0.754	0.728	0.759	0.728
A_{260}	-0.062	-0.055	-0.051	-0.055	-0.051
A_{360}	0.003	0.002	0.002	0.002	0.002
A_{063}	3.155	2.836	2.830	2.845	2.826
A_{163}	-0.349	-0.337	-0.326	-0.338	-0.326
A_{263}	0.020	0.025	0.023	0.024	0.023
A_{363}	-0.001	-0.001	-0.001	-0.001	-0.001
A_{066}	1.215	0.758	0.758	0.765	0.760
A_{166}	0.027	0.066	0.065	0.061	0.065
A_{266}	-0.022	-0.017	-0.015	-0.017	-0.015
A_{366}	0.001	0.001	0.001	0.001	0.001
$A_{0\text{-}3\text{-}3}$	-42.207	-36.667	-48.437	-37.482	-48.538
$A_{1\text{-}3\text{-}3}$	10.658	10.766	10.415	10.8	10.425
$A_{2\text{-}3\text{-}3}$	-0.540	-0.537	-0.503	-0.54	-0.503
$A_{3\text{-}3\text{-}3}$	0.013	0.013	0.012	0.013	0.012
A_{000} ($B_{\alpha\alpha}$)		1.4580	1.4085	1.4326	1.3839

Propane G_{18} species					
$^{13}CH_3$-CH_2-CH_3					
Coeff.	V^{EF}	V^{ADJ}	*Coeff.*	V^{EF}	V^{ADJ}
A_{000}	1199.344	1199.344	A_{260}	-0.055	-0.051
A_{100}	-13.958	-13.415	A_{206}	-0.055	-0.051
A_{200}	9.100	8.508	A_{360}	0.002	0.002
A_{300}	-0.099	-0.090	A_{306}	0.002	0.002
A_{030}	-625.282	-600.172	A_{063}	2.821	2.821
A_{003}	-624.911	-599.801	A_{036}	2.818	2.818
A_{130}	12.995	12.564	A_{163}	-0.336	-0.324
A_{103}	12.987	12.556	A_{136}	-0.336	-0.325
A_{230}	-0.808	-0.755	A_{263}	0.024	0.023
A_{203}	-0.808	-0.755	A_{236}	0.025	0.024
A_{330}	0.015	0.014	A_{363}	-0.001	-0.001
A_{303}	0.015	0.014	A_{336}	-0.001	-0.001
A_{033}	60.884	60.884	A_{066}	0.761	0.761
A_{133}	-8.532	-8.250	A_{166}	0.066	0.065
A_{233}	0.424	0.397	A_{266}	-0.017	-0.015
A_{333}	-0.008	-0.007	A_{366}	0.001	0.001
A_{060}	-8.167	-8.167	$A_{0\text{-}3\text{-}3}$	-36.725	-48.495
A_{006}	-8.208	-8.208	$A_{1\text{-}3\text{-}3}$	10.772	10.422
A_{160}	0.752	0.726	$A_{2\text{-}3\text{-}3}$	-0.538	-0.503
A_{106}	0.755	0.728	$A_{3\text{-}3\text{-}3}$	0.013	0.012
A_{000} ($B_{\alpha\alpha}$)				1.4320	1.3833
CH_3-CHD-CH_3					
Coeff.	V^{EF}	V^{ADJ}	*Coeff.*	V^{EF}	V^{ADJ}
A_{000}	1197.213	1199.310	A_{063}	2.840	2.820
A_{100}	-14.174	-13.416	A_{163}	-0.336	-0.325
A_{200}	9.105	8.508	A_{263}	0.025	0.023
A_{300}	-0.099	-0.090	A_{363}	-0.001	-0.001
A_{030}	-624.061	-599.987	A_{066}	0.768	0.761
A_{130}	12.975	12.560	A_{166}	0.061	0.065
A_{230}	-0.807	-0.755	A_{266}	-0.017	-0.015
A_{330}	0.015	0.014	A_{366}	0.001	0.001
A_{033}	61.033	60.884	$A_{0\text{-}3\text{-}3}$	-37.470	-48.494
A_{133}	-8.546	-8.250	$A_{1\text{-}3\text{-}3}$	10.801	10.422
A_{233}	0.424	0.397	$A_{2\text{-}3\text{-}3}$	-0.540	-0.503
A_{333}	-0.008	-0.007	$A_{3\text{-}3\text{-}3}$	0.013	0.012
A_{060}	-8.273	-8.188	$A_{0\text{-}30}$	1.092	0.004
A_{160}	0.759	0.727	$A_{0\text{-}33}$	-0.096	0.009
A_{260}	-0.055	-0.051	$A_{1\text{-}30}$	0.085	
A_{360}	0.002	0.002	$A_{1\text{-}33}$	-0.012	
A_{000} ($B_{\alpha\alpha}$)				1.4223	1.3739

Propane G_6 species								
CH_2D-CH_2-CH_3								
Coeff.	V^{EF}	V^{ADJ}	*Coeff.*	V^{EF}	V^{ADJ}	*Coeff.*	V^{EF}	V^{ADJ}
A_{000}	1195.737	1195.737	A_{040}	0.858	0.858	A_{253}	0.005	0.005
A_{100}	-13.970	-13.426	A_{050}	0.129	0.129	A_{263}	0.025	0.024
A_{200}	9.096	8.504	A_{060}	-7.814	-7.814	A_{216}	0.003	0.003
A_{300}	-0.100	-0.090	A_{006}	-8.004	-8.004	A_{226}	-0.001	-0.001
A_{010}	-1.761	-1.761	A_{140}	0.075	0.075	A_{236}	0.020	0.019
A_{020}	0.169	0.169	A_{150}	0.044	0.044	A_{353}	-0.001	-0.001
A_{030}	-620.969	-595.859	A_{160}	0.811	0.785	A_{363}	-0.001	-0.001
A_{003}	-624.637	-599.527	A_{106}	0.735	0.709	A_{046}	-0.161	-0.161
A_{110}	-0.672	-0.672	A_{240}	-0.005	-0.005	A_{056}	-0.117	-0.117
A_{120}	0.321	0.321	A_{250}	0.003	0.003	A_{066}	0.665	0.665
A_{130}	12.881	12.450	A_{260}	-0.058	-0.054	A_{146}	0.015	0.015
A_{103}	13.004	12.574	A_{206}	-0.057	-0.053	A_{156}	0.007	0.007
A_{210}	0.014	0.014	A_{350}	-0.001	-0.001	A_{166}	0.073	0.072
A_{220}	-0.006	-0.006	A_{360}	0.003	0.002	A_{246}	0.003	0.003
A_{230}	-0.805	-0.752	A_{306}	0.003	0.002	A_{256}	0.002	0.002
A_{203}	-0.811	-0.758	A_{043}	0.048	0.048	A_{266}	-0.016	-0.015
A_{330}	0.016	0.014	A_{053}	-0.027	-0.027	A_{366}	0.001	0.000
A_{303}	0.016	0.014	A_{063}	2.965	2.965	$A_{0\text{-}1\text{-}3}$	0.634	0.634
A_{013}	-0.577	-0.577	A_{016}	-0.092	-0.092	$A_{0\text{-}2\text{-}3}$	-0.553	-0.553
A_{023}	0.019	0.019	A_{026}	0.104	0.104	$A_{0\text{-}3\text{-}3}$	-36.902	-48.672
A_{033}	60.539	60.539	A_{036}	2.986	2.986	$A_{1\text{-}1\text{-}3}$	-0.004	-0.004
A_{113}	0.048	0.048	A_{143}	-0.027	-0.027	$A_{1\text{-}2\text{-}3}$	0.069	0.069
A_{123}	-0.041	-0.041	A_{153}	0.013	0.013	$A_{1\text{-}3\text{-}3}$	10.763	10.413
A_{133}	-8.479	-8.196	A_{163}	-0.368	-0.357	$A_{2\text{-}1\text{-}3}$	0.006	0.006
A_{213}	-0.001	-0.001	A_{116}	0.006	0.006	$A_{2\text{-}2\text{-}3}$	-0.005	-0.005
A_{223}	0.001	0.001	A_{126}	-0.008	-0.008	$A_{2\text{-}3\text{-}3}$	-0.530	-0.496
A_{233}	0.419	0.392	A_{136}	-0.351	-0.339	$A_{3\text{-}1\text{-}3}$	-0.001	-0.001
A_{333}	-0.007	-0.007	A_{243}	0.003	0.003	$A_{3\text{-}3\text{-}3}$	0.012	0.011
A_{000} ($B_{\alpha\alpha}$)				1.4027	1.3550			