HINDERED INTERNAL ROTATION

I. Ozier and N. Moazzen-Ahmadi

In asymmetric tops like methyl alcohol, CH_3OH, and symmetric rotors like CH_3SiH_3, the methyl group can undergo internal rotation relative to the rest of the molecule, traditionally called the frame (LS59, OM07). Although various different tops are considered here, all have three-fold symmetry. In such cases, the potential V hindering the internal rotation can be written:

$$V(\alpha) = V_3(\tfrac{1}{2})(1-\cos 3\alpha) + V_6(\tfrac{1}{2})(1-\cos 6\alpha) + V_9(\tfrac{1}{2})(1-\cos 9\alpha) + \ldots ,$$

where α is the deviation from equilibrium of the angle between the top and frame that measures the torsional motion. If only the first two terms are retained, then V_3 is the height of the hindering potential and V_6 is the shape parameter. For symmetric tops like CH_3CH_3 where the top and frame are identical, α is replaced by 2γ and the origin for γ is often taken as the eclipsed configuration. In the expansion, $-\cos 6n\gamma$ is then replaced by $(-1)^{n+1}\cos 6n\gamma$, where $n = 1,2,\ldots$ In cases where different forms of the expansion have been used in the original works, the values of the parameters published there have been converted to the conventions defined here.

In Tables 1 and 2, values are given for V_3 for a selection of asymmetric and symmetric tops, respectively. In cases where the higher order parameters have been determined, these are given in the Comments column. Where appropriate, this column also indicates the specific top, isomer, state, and/or isotopomer that has been studied. For ethane, three symmetric top isotopomer are listed to illustrate the isotopic dependence of V_3 and V_6. In all other cases, only one isotopomer is listed, even if several have been studied. In all but one of these cases, the isotopomer reported is the one with the highest natural abundance. However, CH_3OCDO is listed because the results obtained are more precise than for CH_3OCHO. The molecules are listed alphabetically in Hill order according to the molecular formula.

The determinations listed for the potential parameters are effective values that incorporate to varying degrees effects from other molecular parameters. For example, the apparent value of V_3 can be changed significantly if the reduced rotational constant F is calculated from the structure, rather than being determined independently (LS59). Other examples include such mechanisms as coupling to excited skeletal vibrations (OM07) and redundancies connecting some of the torsional parameters (LB68, MO87). The experimental uncertainties quoted are taken from the original works; no attempt has been made to standardize the definitions. All the potential parameters are given in cm^{-1}. Where the original work has reported these values in other units, the conversion to cm^{-1} has been carried out using standard factors (LB02):

1 calorie = 4.1868 joules;
1 calorie/mole = 0.34998915 cm^{-1}.

A variety of different methods have been used to measure V_3, V_6, and V_9 (LS59, OM07); only a few of the more important will be discussed here. *For asymmetric rotors*, both the pure rotational spectrum and its torsion-rotation counterpart are electric dipole allowed and are affected in lowest order by the leading terms in the torsional Hamiltonian. Both types of spectra have been used extensively to determine V_3 (LS59). *For symmetric tops* with a single torsional degree of freedom, either the permanent electric dipole moment vanishes, as in CH_3CH_3, or the normal rotational spectrum is independent of V_3 in lowest order, as in CH_3SiH_3. In the latter case, the molecular beam avoided crossing method can often be used (OM07). The torsion-rotation spectrum is forbidden in lowest order, but becomes weakly allowed through interactions with the infrared active skeletal vibrations (OM07). By employing long absorption path lengths, this spectrum has been used to determine V_3 in a number of molecules. For both asymmetric and symmetric tops, the most precise determinations of the molecular parameters have been made in cases where both rotational and torsion-rotation spectra have been investigated.

References

ALA97 Antolínez, S., López, J. C., and Alonso, J. L., *J. Chem. Soc., Faraday Trans.* 93, 1291, 1997.

ALB97 Alonso, J. L., López, J. C., Blanco, S., and Guarnieri, A., *J. Mol. Spectrosc.* 182, 148, 1997.

ALL97 Alonso, J. L., Lesarri, A., López, J. C., Blanco, S., Kleiner, I., and Demaison, *J., Molec. Phys*. 91, 731, 1997.

BL85 Bestmann, G., Lalowski, W., and Dreizler, H., *Z. Naturforsch.* A 40, 271, 1985.

BM07 Borvayeh, L., Moazzen-Ahmadi, N., and Horneman, V.-M., *J. Mol. Spectrosc.* 242, 77, 2007.

BW64 Butcher, S. S., and Wilson, E. B., *J. Chem. Phys.* 40, 1671, 1964.

CA96 Charro, M. E., and Alonso, J. L., *J. Mol. Spectrosc.* 176, 251, 1996.

CB61 Cahill, P., and Butcher, S., *J. Chem. Phys.* 35, 2255, 1961.

DG87 Durig, J. R., Guirgis, G. A., and Van Der Veken, B. J., *J. Raman Spectrosc.* 18, 549, 1987.

DL73 Durig, J. R., Li, Y. S., Carreira, L. A., and Odom, J. D., *J. Amer. Chem. Soc*. 95, 2491, 1973.

DM87 Demaison, J., Maes, H., van Eijck, B. P., Wlodarczak, G., and Lasne, M. C., *J. Mol. Spectrosc.* 125, 214, 1987.

DS81 Dreizler, H., and Scappini, F., *Z. Naturforsch*. A 36, 1187, 1981.

EG96 Eltayeb, S., Guirgis, G. A., Fanning, A. R., and Durig, J. R., *J. Raman Spectrosc*. 27, 111, 1996.

FD83 Fliege, E., Dreizler, H., Demaison, J., Boucher, D., Burie, J., and Dubrulle A., *J. Chem. Phys.* 78, 3541, 1983.

G00 Groner, P., *J. Mol. Structure* 550–551, 473, 2000.

GA89 Groner, P., Attia, G. M., Mohamad, A. B., Sullivan, J. F., Li, Y. S., and Durig, J. R., *J. Chem. Phys.* 91, 1434, 1989.

GG04 Groner, P., Gillies, C. W., Gillies, J. Z., Zhang, Y., and Block, E., *J. Mol. Spectrosc.* 226, 169, 2004.

GH02 Grabow, J.-U., Hartwig, H., Heineking, N., Jäger, W., Mäder, H., Nicolaisen, H. W., and Stahl, W., *J. Mol. Structure* 612, 349, 2002.

IA03 Ilyushin, V. V., Alekseev, E. A., Dyubko, S. F., and Kleiner, I., *J. Mol. Spectrosc.* 220, 170, 2003.

K60 Krisher, L. C., *J. Chem. Phys.* 33, 1237, 1960.

KD86 Kasten, W., and Dreizler, H., *Z. Naturforsch*. A 41, 944, 1986.

KH96 Kleiner, I., Hougen, J. T., Grabow, J.-U., Belov, S. P., Tretyakov, M. Yu., and Cosléou, J., *J. Mol. Spectrosc.* 179, 41, 1996.

KL67 Kuczkowski, R. L., and Lide, D. R., *J. Chem. Phys.* 46, 357, 1967.

KW74 Krisher, L. C., Watson, W. A., and Morrison, J. A., *J. Chem. Phys*. 61, 3429, 1974.

L59 Laurie, V. W., *J. Chem. Phys.* 30, 1210, 1959.

LB68 Lees, R. M., and Baker, J. G., *J. Chem. Phys.* 48, 5299, 1968.

LB97 di Lauro, C., Bunker, P. R., Johns, J. W. C., and McKellar, A. R. W., *J. Mol. Spectrosc.* 184, 177, 1997.

LB02 Demaison, J., and Wlodarczak, G., Hindered rotation-Asymmetric top molecules, in: Hüttner, W. (Ed), *Landolt-Börnstein Numerical Data and Functional Relationships in Science and Technology, New Series: Group II: Molecules and Radicals, volume 24, subvolume C, Molecular Constants Mostly from Microwave, Molecular Beam, and Sub-Doppler Laser Spectroscopy*, Springer-Verlag, Heidelberg, 2002.

LE97 de Luis, A., Eugenia Sanz, M., Lorenzo, F. J., López, J. C., and Alonso, J. L., *J. Mol. Spectrosc.* 184, 60, 1997.

LJ72 Lide, D. R., Johnson, D. R., Sharp, K. G., and Coyle, T. D., *J. Chem. Phys.* 57, 3699, 1972.
LS59 Lin, C. C., and Swalen, J. D., *Rev. Mod. Phys*. 31, 841 1959.
MK66 Moloney, M. J., and Krisher, L. C., *J. Chem. Phys.* 45, 3277, 1966.
MM96 Marstokk, K.-M., Møllendal, H., and Samdal, S., *J. Mol. Structure* 376, 11, 1996.
MM01 Marstokk, K.-M., Mollendal, H., Samdal, S., and Steinborn, D., *J. Mol. Structure* 567, 41, 2001.
MO87 Moazzen-Ahmadi, N., and Ozier, I., *J. Mol. Spectrosc.* 126, 99, 1987.
MS02 Merke, I., Stahl, W., Kassi, S., Petitprez, D., and Wlodarczak, G., *J. Mol. Spectrosc.* 216, 437, 2002.
ND06 Nair, K. P. R., Demaison, J., Wlodarczak, G., and Merke, I., *J. Mol. Spectrosc.* 237, 137, 2006.
NH02 Niide, Y., and Hayashi, M., *J. Mol. Spectrosc.* 216, 61, 2002.
NH04 Niide, Y., and Hayashi, M., *J. Mol. Spectrosc.* 223, 152, 2004.
NY85 Nakagawa, J., Yamada, K., Bester, M., and Winnewisser, G., *J. Mol. Spectrosc.* 110, 74, 1985.
OH07 Ohashi, N., and Hougen, J. T., *J. Mol. Spectrosc.* 243, 162, 2007.
OK75 Odom, J. D., Kalasinsky, V. F., and Durig, J. R., *Inorg. Chem.*14, 2837, 1975.
OM07 Ozier, I., and Moazzen-Ahmadi, N., Internal rotation in symmetric tops, in: Arimondo, E., Berman, P. R., and Lin, C. C., (Eds.), *Advances in Atomic, Molecular and Optical Physics*, vol. 54, p. 423, Elsevier, Amsterdam, 2007.
PK59 Pierce, L., and Krisher, L. C., *J. Chem. Phys.* 31, 875, 1959.
S75 Stiefvater, O. L., *J. Chem. Phys.* 62, 233, 1975.
SD04 Suenram, R. D., DaBell, R. S., Hight Walker, A. R., Lavrich, R. J., Plusquellic, D. F., Ellzy, M. W., Lochner, J. M., Cash, L., Jensen, J. O., and Samuels, A. C., *J. Mol. Spectrosc.* 224, 176, 2004.
SG05 Schnell, M., Grabow, J.-U., Hartwig, H, Heineking, N., Meyer, M., Stahl, W., and Caminati, W., *J. Mol. Spectrosc.* 229, 1, 2005.
SH82 Shiki, Y., Hasegawa, A., and Hayashi, M., *J. Mol. Structure* 78, 185, 1982.
SH86 Sastry, K. V. L. N., Herbst, E., Booker, R. A., and De Lucia, F. C., *J. Mol. Spectrosc.* 116, 120, 1986.
SL02 Suenram, R. D., Lovas, F. J., Plusquellic, D. F., Lesarri, A., Kawashima, Y., Jensen, J. O., and Samuels, A. C., *J. Mol. Spectrosc*. 211, 110, 2002.
SL06 Suenram, R. D., Lovas, F. J., Plusquellic, D. F., Ellzy, M. W., Lochner, J. M., Jensen, J. O., and Samuels, A. C., *J. Mol. Spectrosc*. 235, 18, 2006.
ST06 Styger, C., Ozier, I., Wang, S.-X., and Bauder, A., *J. Mol. Spectrosc.* 239, 115, 2006.
TB86 Typke, V., Botskor, I., and Wiedenmann, K.-H., *J. Mol. Spectrosc.* 120, 435, 1986.
TH86 Tyblewksi, M., Ha, T.-K., and Bauder, A., *J. Mol. Spectrosc.* 115, 353, 1986.
VD88 Vormann, K., and Dreizler, H., *Z. Naturforsch*. A 43, 338, 1988.
VG96 Voges, K., Gripp, J., Hartwig, H., and Dreizler, H., *Z. Naturforsch.* A 51, 299, 1996.
VR75 Varma, R., Ramaprasad, K. R., and Nelson, J. F., *J. Chem. Phys.* 63, 915, 1975.
WA02 Wang, S.-X., Schroderus, J., Ozier, I., Moazzen-Ahmadi, N., Horneman, V.-M., Ilyushyn, V. V., Alekseev, E. A., Katrich, A. A., and Dyubko, S. F., *J. Mol. Spectrosc.* 214, 69, 2002.

TABLE 1. Asymmetric Top Potential Parameters

	Name	Molecular Formula	Line Formula	Ref.	V_3/cm^{-1}	Comments
1	Trifluoromethanethiol	CHF_3S	CF_3SH	LB02	500.83 ± 0.03	
2	Methylphosphonic difluoride	CH_3F_2OP	$CH_3P(=O)F_2$	SL06	676 ± 25	
3	Methanol	CH_4O	CH_3OH	LB02	373.594 ± 0.007	V_6 = −1.597 ± 0.051
						V_9 = 1.04 ± 0.20
4	Methanethiol	CH_4S	CH_3SH	SH86	443.029 ± 0.070	V_6 = −1.6451 ± 0.0144
5	Methyldisulfane	CH_4S_2	CH_3SSH	TH86	609.0 ± 14.0	
6	Trifluoromethyl isocyanate	C_2F_3NO	$CF_3N{=}C{=}O$	LB02	47.8769 ± 0.0051	
7	Trifluoroacetaldehyde	C_2HF_3O	$CF_3C(H){=}O$	DG87	298 ± 10	
8	Pentafluoroethane	C_2HF_5	CF_3CHF_2	EG96	1190 ± 4	
9	Acetyl bromide	C_2H_3BrO	$CH_3C(Br){=}O$	K60	456.7 ± 10.5	
10	1-Chloro-1,1-difluoroethane	$C_2H_3ClF_2$	CH_3CClF_2	ALB97	1311.8 ± 1.4	
11	Acetyl chloride	C_2H_3ClO	$CH_3C(Cl){=}O$	LB02	442.74 ± 1.05	^{35}Cl
12	Acetyl fluoride	C_2H_3FO	$CH_3C(F){=}O$	PK59	364.3 ± 2.1	
13	Methyl fluoroformate	$C_2H_3FO_2$	$CH_3OC(F){=}O$	LB02	374.1 ± 0.2	
14	Methyl trifluoromethyl ether	$C_2H_3F_3O$	CH_3OCF_3	LB02	382 ± 10	CH_3
15	Acetyl iodide	C_2H_3IO	$CH_3C(=O)I$	MK66	455.3 ± 10.5	
16	Methyl cyanate	C_2H_3NO	$CH_3OC{\equiv}N$	LB02	399.0 ± 17.5	
17	1-Chloro-1-fluoroethane	C_2H_4ClF	CH_3CHClF	LB02	1334.9 ± 3.8	
18	1,1-Difluoroethane	$C_2H_4F_2$	CH_3CHF_2	LB02	1163.0 ± 2.5	
19	Acetaldehyde	C_2H_4O	$CH_3C(H){=}O$	KH96	407.716 ± 0.010	V_6 =−12.068 ± 0.037
20	Thioacetaldehyde *S*-oxide	C_2H_4OS	$CH_3C(H){=}S{=}O$	LB02	285.6 ± 0.3	*Z* isomer
21	Acetic acid	$C_2H_4O_2$	CH_3COOH	IA03	170.1742 ± 0.0002	V_6 = −6.4725 ± 0.0001
22	Methyl formate	$C_2H_3DO_2$	$CH_3OC(D){=}O$	LB02	400.60 ± 0.03	deuterated
23	Fluoroethane	C_2H_5F	CH_3CH_2F	FD83	1172.1 ± 1.4	
24	Nitrosoethane	C_2H_5NO	$CH_3CH_2N{=}O$	LB02	903 ± 25	*gauche* conformer
		C_2H_5NO	$CH_3CH_2N{=}O$	LB02	911 ± 25	*cis* conformer
25	Acetamide	C_2H_5NO	$CH_3C(NH_2){=}O$	LB02	24.949 ± 0.008	
26	Difluorodimethylsilane	$C_2H_6F_2Si$	$(CH_3)_2SiF_2$	SG05	439.4 ± 2.5	

	Name	Molecular Formula	Line Formula	Ref.	V_3/cm^{-1}	Comments
27	*N*-Nitrosodimethylamine	$C_2H_6N_2O$	$(CH_3)_2NN{=}O$	LB02	145.8 ± 0.25	*cis* CH_3
		$C_2H_6N_2O$	$(CH_3)_2NN{=}O$	LB02	737.4 ± 13.3	*trans* CH_3
28	Ethanol	C_2H_6O	CH_3CH_2OH	LB02	1173.76 ± 2.20	*trans* isomer
29	Dimethyl ether	C_2H_6O	$(CH_3)_2O$	NH04	926.0 ± 3.5	
30	Dimethyl sulfide	C_2H_6S	$(CH_3)_2S$	NH04	751.1 ± 4.8	
31	Vinylsilane	C_2H_6Si	$SiH_3C(H){=}CH_2$	SH82	520.1 ± 1.8	
32	Dimethyl disulfide	$C_2H_6S_2$	CH_3SSCH_3	LB02	535.1 ± 1.8	
33	Dimethyl diselenide	$C_2H_6Se_2$	$CH_3SeSeCH_3$	GG04	395 ± 2	
34	Dimethylsilane	C_2H_8Si	$(CH_3)_2SiH_2$	NH04	578.0 ± 3.5	
35	3,3,3-Trifluoropropene	$C_3H_3F_3$	$CF_3C(H){=}CH_2$	ALL97	653.06 ± 0.83	
36	Methyl cyanoformate	$C_3H_3NO_2$	$CH_3OC(C{\equiv}N){=}O$	LB02	406.6 ± 1.1	*s-trans* conformer
37	(Methylthio)acetylene	C_3H_4S	$CH_3SC{\equiv}CH$	DM87	592.0 ± 3.3	
38	1,1,1-Trifluoropropane	$C_3H_5F_3$	$CH_3CH_2CF_3$	ALA97	922.2 ± 1.4	
39	2-Iodopropene	C_3H_5I	$CH_3C(I){=}CH_2$	LB02	905.8 ± 4.2	
40	Ethyl isocyanide	C_3H_5N	$CH_3CH_2N{\equiv}C$	LB02	1167.6 ± 18.2	
41	Propene	C_3H_6	$CH_3C(H){=}CH_2$	LB02	697.499 ± 0.048	V_6 = −13.0 (fixed)
42	Propanal	C_3H_6O	$CH_3CH_2C(H){=}O$	BW64	798 ± 39	*cis* conformer
43	Acetone	C_3H_6O	$(CH_3)_2C{=}O$	G00	251.4 ± 2.6	V_6 = −6.92 ± 0.65
44	(Methylthio)ethene	C_3H_6S	$CH_3SC(H){=}CH_2$	MM01	1138 ± 13	
45	Propanoic acid	$C_3H_6O_2$	CH_3CH_2COOH	S75	819.0 ± 10.5	*cis* conformer
46	Methyl mercaptoacetate	$C_3H_6O_2S$	$CH_3OC(=O)C(H_2)SH$	LB02	411 ± 8	state 0^+
		$C_3H_6O_2S$	$CH_3OC(=O)C(H_2)SH$	LB02	412 ± 9	state 0^-
47	2-Bromopropane	C_3H_7Br	$(CH_3)_2CHBr$	LB02	1437.0 ± 2.5	^{79}Br
48	1-Chloropropane	C_3H_7Cl	$CH_3C(H_2)C(H_2)Cl$	LE97	1017.8 ± 1.4	*gauche* conformer
		C_3H_7Cl	$CH_3C(H_2)C(H_2)Cl$	LE97	966.0 ± 7.0	*trans* conformer
49	2-Chloropropane	C_3H_7Cl	$(CH_3)_2CHCl$	LB02	1374.03 ± 1.00	^{35}Cl
50	1-Fluoropropane	C_3H_7F	$CH_3C(H_2)C(H_2)F$	KD86	965.3 ± 12.2	*gauche* conformer
		C_3H_7F	$CH_3C(H_2)C(H_2)F$	KD86	948.5 ± 2.8	*trans* conformer
51	2-Fluoropropane	C_3H_7F	$(CH_3)_2CHF$	LB02	1162.79 ± 0.84	
52	Butanenitrile	C_4H_7N	$CH_3C(H_2)C(H_2)C{\equiv}N$	VD88	1087.4 ± 8.4	*gauche* conformer
		C_4H_7N	$CH_3C(H_2)C(H_2)C{\equiv}N$	VD88	1088.5 ± 13.3	*trans* conformer
53	Propanamide	C_3H_7NO	$CH_3CH_2C(=O)NH_2$	MM96	761 ± 42	*syn* conformer
54	*N,N*-Dimethylformamide	C_3H_7NO	$(CH_3)_2NC(H){=}O$	LB02	366.04 ± 0.26	*cis* CH_3
		C_3H_7NO	$(CH_3)_2NC(H){=}O$	LB02	772.4 ± 7.4	*trans* CH_3
55	Propane	C_3H_8	$(CH_3)_2CH_2$	BL85	1108.1 ± 9.5	
56	Cyclopropylgermane	C_3H_8Ge	$\underbrace{C(H_2)C(H_2)C}(H)(GeH_3)$	LB02	466.6 ± 16.7	GeH_3
57	*N*-Nitrosoethylmethylamine	$C_3H_8N_2O$	$CH_3CH_2N(CH_3)N{=}O$	LB02	310 ± 30	*N*-methyl top, OGM conformer
58	1-Propanol	C_3H_8O	$CH_3C(H_2)C(H_2)OH$	DS81	956 ± 21	*trans* conformer
59	Cyclopropylsilane	C_3H_8Si	$\underbrace{C(H_2)C(H_2)C}(H)(SiH_3)$	TB86	670.9 ± 1.5	
60	Dimethyl(methylene)silane	C_3H_8Si	$(CH_3)_2Si{=}CH_2$	LB02	351.4 ± 5.9	
61	Dimethyl methylphosphonate	$C_3H_9O_3P$	$(OCH_3)_2P(=O)CH_3$	SL02	662 ± 6	*P*-methyl top
		$C_3H_9O_3P$	$(OCH_3)_2P(=O)CH_3$	OH07	278.82 ± 0.06	*O*-methyl top #1
		$C_3H_9O_3P$	$(OCH_3)_2P(=O)CH_3$	OH07	181.82 ± 0.01	*O*-methyl top #2
62	But-2-ynoyl fluoride	C_4H_3FO	$CH_3C{\equiv}CC(F){=}O$	LB02	2.20 ± 0.12	
63	*cis*-2-Butenenitrile	C_4H_5N	$CH_3C(H){=}C(H)C{\equiv}N$	LB02	485.50 ± 0.25	
64	2-Methylacrylonitrile	C_4H_5N	$CH_2{=}C(CH_3)C{\equiv}N$	LB02	695.2 ± 2.1	
65	2-Methyloxazole	C_4H_5NO	$\underbrace{N{=}C(CH_3)OC(H){=}C}(H)$	LB02	251.70 ± 1.17	
66	4-Methyloxazole	C_4H_5NO	$\underbrace{N{=}C(H)OC(H){=}C}(CH_3)$	LB02	429.44 ± 0.33	

	Name	Molecular Formula	Line Formula	Ref.	V_3/cm^{-1}	Comments
67	5-Methyloxazole	C_4H_5NO	N=C(H)OC(CH_3)=C(H)	LB02	477.90 ± 1.34	
68	5-Methylisoxazole	C_4H_5NO	C(H)=NOC(CH_3)=C(H)	LB02	272.05 ± 1.00	
69	2-Methylthiazole	C_4H_5NS	N=C(CH_3)SC(H)=C(H)	GH02	34.938 ± 0.020	
70	4-Methylisothiazole	C_4H_5NS	N=C(H)C(CH_3)=C(H)S	LB02	105.767 ± 0.043	
71	4-Methyl-2-oxetanone	$C_4H_6O_2$	OC(=O)C(H_2)C(H)(CH_3)	LB02	1256.5 ± 10.5	
72	*trans*-1-Fluoro-2-butene	C_4H_7F	CH_3C(H)=C(H)CH_2F	LB02	596 ± 7	anticlinal conformer
73	1-Isocyanopropane	C_4H_7N	CH_3C(H_2)C(H_2)N≡C	LB02	1012.3 ± 8.4	*gauche* conformer
		C_4H_7N	CH_3C(H_2)C(H_2)N≡C	LB02	1033.8 ± 7.7	*trans* conformer
74	Isobutene	C_4H_8	(CH_3)$_2$C=CH_2	LB02	761.58 ± 1.05	
75	*cis*-2-Butene	C_4H_8	CH_3CH=CHCH_3	LB02	259.89 ± 0.42	
76	3-Methoxy-1-propene	C_4H_8O	CH_3OC(H_2)C(H)=CH_2	LB02	728.0 ± 10.5	*skew-gauche* conformer
		C_4H_8O	CH_3OC(H_2)C(H)=CH_2	LB02	829.5 ± 10.5	*syn-trans* conformer
77	2,2-Dimethyloxirane	C_4H_8O	OC(CH_3)(CH_3)C(H_2)	LB02	945.61 ± 0.75	
78	*cis*-2,3-Dimethyloxirane	C_4H_8O	OC(H)(CH_3)C(H)(CH_3)	LB02	577.80 ± 1.84	*cis* conformer
		C_4H_8O	OC(H)(CH_3)C(H)(CH_3)	LB02	862.52 ± 1.84	*trans* conformer
79	2-Methyloxetane	C_4H_8O	OC(H_2)C(H_2)C(H)(CH_3)	LB02	1166.5 ± 4.9	
80	3-Methyloxetane	C_4H_8O	OC(H_2)C(H)(CH_3)C(H_2)	LB02	1149.4 ± 4.2	
81	3-Methoxythietane	C_4H_8OS	SC(H_2)C(H)(OCH_3)C(H_2)	LB02	1071.0 ± 10.5	
82	3-(Methylthio)-1-propene	C_4H_8S	CH_3SC(H_2)C(H)=CH_2	LB02	619 ± 28	
83	2,2-Dimethylthiirane	C_4H_8S	SC(CH_3)(CH_3)C(H_2)	LB02	1268.3 ± 3.0	
84	Butane	C_4H_{10}	CH_3C(H_2)C(H_2)CH_3	LB02	948 ± 24	
85	*N*-Methyl-*N*-nitrosopropylamine	$C_4H_{10}N_2O$	CH_3C(H_2)C(H_2)N(CH_3)N=O	LB02	320 ± 30	*N*-methyl top, conformer OMGA
86	Dihydro-3-methyl-2(3*H*)-furanone	$C_5H_8O_2$	OC(=O)C(H)(CH_3)C(H_2)C(H_2)	LB02	913.8 ± 2.5	
87	Dihydro-4-methyl-2(3*H*)-furanone	$C_5H_8O_2$	OC(=O)C(H_2)C(H)(CH_3)C(H_2)	CA96	1437.8 ± 8.4	
88	Dihydro-5-methyl-2(3*H*)-furanone	$C_5H_8O_2$	OC(=O)C(H_2)C(H_2)C(H)(CH_3)	CA96	1233.0 ± 4.2	
89	*tert*-Butyl isocyanate	C_5H_9NO	(CH_3)$_3$C≡N=C=O	LB02	41.510 ± 0.015	(CH_3)$_3$ C group
90	Methyl *tert*-butyl ether	$C_5H_{12}O$	(CH_3)$_3$COCH_3	LB02	498.6 ± 1.5	*O*-methyl top
91	2-Methylcyclopentanone	$C_6H_{10}O$	C(=O)C(H)(CH_3)C(H_2)C(H_2)C(H_2)	LB02	844.2 ± 2.4	
92	3-Methylcyclopentanone	$C_6H_{10}O$	C(=O)C(H_2)C(H)(CH_3)C(H_2)C(H_2)	LB02	1233.8 ± 1.7	
93	*tert*-Butyl ethyl ether	$C_6H_{14}O$	(CH_3)$_3$COC(H_2)CH_3	LB02	1025 ± 3	ethyl CH_3
94	2,4-Difluorotoluene	$C_7H_6F_2$	C(H)=C(CH_3)C(F)=C(H)C(F)=C(H)	LB02	204.04 ± 0.23	
95	2-Chlorotoluene	C_7H_7Cl	C(H)=C(H)C(Cl)=C(CH_3)C(H)=C(H)	ND06	513.8 ± 2.7	^{35}Cl
96	2,6-Dimethylpyridine	C_7H_9N	C(H)=C(H)C(CH_3)=NC(CH_3)=C(H)	LB02	98.24 ± 0.27	
97	1,2,2-Trimethylpropyl methylphosphonofluoridate	$C_7H_{16}FO_2P$	(CH_3)$_3$CC(H)(CH_3)OP(O)(F)CH_3	SD04	821 ± 5	*P*-methyl top, conformer GD-I
		$C_7H_{16}FO_2P$	(CH_3)$_3$CC(H)(CH_3)OP(O)(F)CH_3	SD04	738 ± 5	*P*-methyl top, conformer GD-II
98	Germyl azide	GeH_3N_3	GeH_3-N=N≡N	GA89	86.598 ± 0.062	
99	Silylphospine	H_5PSi	SiH_3PH_2	VR75	537.2 ± 14.0	

TABLE 2. Symmetric Top Potential Parameters

	Name	Molecular Formula	Line Formula	Ref.	V_3/cm^{-1}	Comments
1	Phosphine-trifluoroborane	BF_3H_3P	H_3PBF_3	OK75	1169 ± 123	
2	Trihydro(phosphorus trifluoride)boron	BF_3H_3P	F_3PBH_3	KL67	1134 ± 53	
3	Trihydro(phosphine)boron	BH_6P	H_3PBH_3	DL73	864.5 ± 17.5	
4	Trifluoro(trifluoromethyl)silane	CF_6Si	CF_3SiF_3	LJ72	489 ± 50	
5	Trifluoromethylgermane	CH_3F_3Ge	CF_3GeH_3	KW74	448 ± 53	
6	Trifluoromethylsilane	CH_3F_3Si	CH_3SiF_3	ST06	414.147 ± 0.030	
7	Methylgermane	CH_6Ge	CH_3GeH_3	L59	433.6 ± 8.8	
8	Methylsilane	CH_6Si	CH_3SiH_3	OM07	603.3878 ± 0.0037	
9	Methylstannane	CH_6Sn	CH_3SnH_3	CB61	227 ± 10	
10	1,1,1-Trifluoroethane	$C_2H_3F_3$	CH_3CF_3	WA02	1112.24 ± 0.16	
11	Ethane	C_2H_6	CH_3CH_3	OM07	1013.28 ± 0.10	V_6 = 8.798 ± 0.041
12	Ethane-1,1,1-d_3	$C_2H_3D_3$	CH_3CD_3	OM07	1001.876 ± 0.023	V_6 = 9.328 ± 0.018
13	Ethane-d_6	C_2D_6	CD_3CD_3	OM07	989.946 ± 0.090	V_6 = 9.51 ± 0.10
14	1-Silylpropyne	C_3H_6Si	$CH_3C{\equiv}CSiH_3$	NY85	3.77 ± 0.70	
15	Trimethylchlorosilane	C_3H_9ClSi	$(CH_3)_3SiCl$	MS02	576.9 ± 0.9	
16	2-Butyne	C_4H_6	$CH_3C{\equiv}CCH_3$	LB97	6.067 ± 0.040	V_6 = 0.1240 ± 0.0144 V_9 = –0.0916 ± 0.0180
17	Ethynyltrimethylgermane	$C_5H_{10}Ge$	$(CH_3)_3GeC{\equiv}CH$	VG96	376.2 ± 16.7	
18	Disilane	H_6Si_2	SiH_3SiH_3	BM07	412.033 ± 0.010	