Supplementary Material

Barrier to Methyl Internal Rotation and Equilibrium Structure Determined from the Microwave Spectrum of 2-Methylthiophene

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Table S1: Nuclear coordinates of 2MTP in the principal axis system calculated at the MP2/6-311++G(d,p) level of theory. The atoms are numbered according to Figure 1.

	a / Å	b / Å	c / Å
S1	−0.193422	−1.148581	0.000000
C2	0.815087	0.250550	−0.000001
C3	−0.046599	1.400304	0.000000
C4	−1.352303	1.140712	−0.000000
C5	−1.631006	−0.211041	0.000001
H6	−2.598140	−0.696395	−0.000001
H7	−2.120970	1.905565	0.000001
H8	0.485457	2.392801	−0.000000
C9	2.312266	0.144727	0.000000
H10	2.681240	−0.381503	−0.885957
H11	2.681237	−0.381518	0.885950
H12	2.743714	1.149342	0.000009

Table S2: Equilibrium rotational constants *A*, *B*, *C* and the V_3 torsional barrier for 2MTP calculated at different levels of theory and their deviations to the experimental values *ΔA, ΔB, ΔC*. Σ*Δ* is the sum of the absolute values of *ΔA, ΔB, ΔC*.

	A	*ΔA*	*B*	*ΔB*	*C*	*ΔC*	Σ*Δ*	V_3	ΔV_3
Method/Basis Set	MHz	MHz	MHz	MHz	MHz	MHz	MHz	cm^{-1}	cm^{-1}
MP2/6-31G(d,p)	5269.9	30.0	3119.3	–5.2	1983.5	1.7	36.9	208.1	10.4
MP2/6-31+G(d,p)	5260.4	39.5	3113.8	0.3	1980.0	5.2	45.0	183.7	–14.0
MP2/6-31++G(d,p)	5260.2	39.6	3113.7	0.4	1980.0	5.3	45.3	183.0	–14.7
MP2/6-311G(d,p)	5265.0	34.9	3115.9	–1.8	1981.7	3.5	40.2	208.0	10.3
MP2/6-311+G(d,p)	5265.2	34.7	3110.6	3.5	1979.6	5.6	43.8	183.7	–14.1
MP2/6-311++G(d,p)	5265.2	34.7	3110.6	3.5	1979.6	5.6	43.8	183.0	–14.7
MP2/6-311G(df,pd)	5311.3	–11.5	3134.0	–19.9	1995.5	–10.2	41.7	210.0	12.3
MP2/6-311+G(df,pd)	5308.5	–8.7	3130.0	–15.9	1993.5	–8.2	32.8	184.6	–13.1
MP2/6-311++G(df,pd)	5307.9	–8.1	3129.7	–15.6	1993.3	–8.0	31.7	181.0	–16.7
MP2/6-311G(2d,2p)	5276.9	22.9	3118.3	–4.2	1984.0	1.3	28.4	168.7	–29.0
MP2/6-311+G(2d,2p)	5275.4	24.4	3117.1	–3.0	1983.3	2.0	29.4	173.6	–24.1
MP2/6-311++(G2d,2p)	5275.2	24.6	3117.1	–3.0	1983.3	2.0	29.6	171.2	–26.5
MP2/6-311G(2df,2pd)	5320.6	–20.8	3133.3	–19.2	1996.3	–11.0	51.0	151.5	–46.2
MP2/6-311+G(2df,2pd)	5318.6	–18.7	3131.4	–17.3	1995.3	–10.0	46.0	157.7	–40.0
MP2/6-311++G(2df,2pd)	5318.1	–18.3	3131.4	–17.3	1995.2	–9.9	45.5	159.9	–37.8
MP2/6-311G(3df,3pd)	5336.5	–36.6	3135.0	–20.9	1999.3	–14.0	71.5	121.9	–75.8
MP2/6-311+G(3df,3pd)	5334.2	–34.3	3133.9	–19.8	1998.5	–13.2	67.3	135.2	–62.5
MP2/6-311++G(3df,3pd)	5334.0	–34.1	3133.8	–19.7	1998.5	–13.2	67.0	137.0	–60.7
MP2/cc-pVDZ	5198.3	101.6	3081.3	32.8	1958.6	26.7	161.0	203.3	5.5
MP2/cc-pVTZ	5305.9	–6.0	3126.8	–12.7	1991.6	–6.4	25.1	169.2	–28.5
MP2/aug-cc-pVDZ	5185.7	114.2	3072.7	41.4	1953.3	31.9	187.5	188.2	–9.6
MP2/aug-cc-pVTZ	5305.3	–5.5	3124.6	–10.5	1990.7	–5.5	21.5	149.1	–48.7
M06-2X/6-31G(d,p)	5287.9	11.9	3113.8	0.3	1984.0	1.3	13.5	254.5	56.7
M06-2X/6-31+G(d,p)	5282.1	17.7	3110.9	3.2	1982.1	3.2	24.1	250.0	52.3
M06-2X/6-31++G(d,p)	5282.1	17.8	3111.0	3.1	1982.1	3.2	24.1	248.6	50.9
M06-2X/6-311G(d,p)	5298.3	1.5	3119.9	–5.8	1987.9	–2.6	10.0	236.0	38.3
M06-2X/6-311+G(d,p)	5299.0	0.9	3118.0	–3.9	1987.2	–2.0	6.8	241.3	43.6
M06-2X/6-311++G(d,p)	5298.7	1.1	3118.0	–3.9	1987.2	–1.9	6.9	245.2	47.5
M06-2X/6-311G(df,pd)	5315.6	–15.7	3127.7	–13.6	1993.4	–8.2	37.5	234.7	37.0
M06-2X/6-311+G(df,pd)	5316.5	–16.6	3125.8	–11.7	1992.8	–7.5	35.8	237.3	39.6
M06-2X/6-311++G(df,pd)	5316.3	–16.4	3125.8	–11.7	1992.7	–7.5	35.6	240.6	42.8
M06-2X/6-311G(3df,3pd)	5355.6	–55.7	3136.1	–22.0	2002.4	–17.1	94.9	194.1	–3.6
M06-2X/6-311+G(3df,3pd)	5354.9	–55.0	3135.7	–21.7	2002.1	–16.9	93.6	204.6	6.8
M06-2X/6-311++G(3df,3pd)	5354.7	–54.9	3135.7	–21.6	2002.1	–16.8	93.3	205.3	7.5
M06-2X/cc-pVDZ	5267.9	31.9	3106.9	7.2	1978.6	6.6	45.8	233.5	35.7
M06-2X/cc-pVTZ	5336.8	–36.9	3130.9	–16.8	1997.6	–12.3	66.0	212.4	14.6
M06-2X/aug-cc-pVDZ	5269.7	30.1	3105.8	8.3	1978.4	6.9	45.2	235.6	37.9
M06-2X/aug-cc-pVTZ	5338.5	–38.7	3130.9	–16.8	1997.9	–12.6	68.2	216.2	18.5
MP2-CCSD/cc-pVDZ	5168.0	131.8	3066.5	47.6	1948.4	36.9	216.3	242.8	45.1
MP2-CCSD/cc-pVTZ	5305.9	–6.0	3126.8	–12.7	1991.6	–6.4	25.1		
ωB97X-D/6-31G(d,p)	5286.4	13.4	3108.8	5.3	1981.8	3.5	22.2	247.8	50.0
ωB97X-D/6-31+G(d,p)	5281.1	18.7	3106.5	7.6	1980.1	5.1	31.5	246.0	48.3
ωB97X-D/6-31++G(d,p)	5281.0	18.8	3106.6	7.5	1980.2	5.1	31.5	245.4	47.7
ωB97X-D/6-311G(d,p)	5300.3	–0.5	3117.7	–3.6	1987.3	–2.1	6.1	230.2	32.5

	A	*ΔA*	*B*	*ΔB*	*C*	*ΔC*	Σ*Δ*	V_3	ΔV_3
ωB97X-D/6-311+G(d,p)	5301.0	−1.1	3115.7	−1.6	1986.6	−1.3	4.1	234.1	36.4
ωB97X-D/6-311++G(d,p)	5300.7	−0.8	3115.6	−1.5	1986.5	−1.3	3.6	237.6	39.8
ωB97X-D/6-311G(df,pd)	5318.7	−18.8	3126.7	−12.6	1993.5	−8.2	39.7	228.4	30.7
ωB97X-D/6-311+G(df,pd)	5319.7	−19.9	3124.7	−10.6	1992.8	−7.6	38.1	229.4	31.6
ωB97X-D/6-311++G(df,pd)	5319.5	−19.6	3124.7	−10.6	1992.8	−7.5	37.7	232.2	34.4
ωB97X-D/6-311G(2d,2p)	5329.6	−29.8	3126.0	−11.9	1994.7	−9.4	51.1	200.1	2.3
ωB97X-D/6-311+G(2d,2p)	5329.5	−29.7	3125.4	−11.3	1994.4	−9.1	50.1	207.7	10.0
ωB97X-D/6-311++G(2d,2p)	5329.2	−29.4	3125.4	−11.3	1994.4	−9.1	49.8	208.2	10.4
ωB97X-D/6-311G(2df,2pd)	5349.4	−49.6	3132.2	−18.1	1999.9	−14.7	82.3	188.5	−9.2
ωB97X-D/6-311+G(2df,2pd)	5349.7	−49.8	3131.3	−17.2	1999.6	−14.3	81.4	194.7	−3.1
ωB97X-D/6-311++G(2df,2pd)	5349.4	−49.5	3131.3	−17.2	1999.6	−14.3	81.0	196.5	−1.3
ωB97X-D/6-311G(3df,3pd)	5363.4	−63.6	3136.3	−22.2	2003.6	−18.3	104.1	180.5	−17.3
ωB97X-D/6-311+G(3df,3pd)	5362.7	−62.8	3135.9	−21.8	2003.3	−18.0	102.6	191.0	−6.7
ωB97X-D/6-311++G(3df,3pd)	5362.5	−62.7	3135.8	−21.7	2003.3	−18.0	102.4	191.5	−6.3
ωB97X-D/cc-pVDZ	5262.0	37.9	3099.3	14.8	1974.7	10.5	63.2	225.8	28.1
ωB97X-D/cc-pVTZ	5342.2	−42.3	3129.7	−15.6	1997.9	−12.6	70.6	201.7	4.0
ωB97X-D/aug-cc-pVDZ	5264.0	35.8	3098.7	15.4	1974.7	10.5	61.8	224.8	27.0
ωB97X-D/aug-cc-pVTZ	5343.4	−43.6	3129.5	−15.4	1998.0	−12.7	71.7	202.9	5.2
B3LYP-D3/6-31G(d,p)	5229.1	70.8	3087.0	27.1	1964.8	20.5	118.3	274.6	76.8
B3LYP-D3/6-31+G(d,p)	5222.6	77.3	3083.5	30.6	1962.5	22.7	130.7	270.4	72.7
B3LYP-D3/6-31++G(d,p)	5222.5	77.3	3083.5	30.6	1962.5	22.7	130.6	268.0	70.3
B3LYP-D3/6-311G(d,p)	5242.6	57.2	3095.5	18.6	1970.1	15.1	91.0	250.2	52.5
B3LYP-D3/6-311+G(d,p)	5243.2	56.7	3093.6	20.5	1969.5	15.8	92.9	251.4	53.7
B3LYP-D3/6-311++G(d,p)	5242.9	57.0	3093.5	20.6	1969.4	15.9	93.4	255.7	57.9
B3LYP-D3/6-311G(df,pd)	5261.1	38.8	3105.7	8.4	1976.8	8.5	55.7	248.0	50.3
B3LYP-D3/6-311+G(df,pd)	5262.0	37.9	3103.8	10.3	1976.2	9.1	57.2	247.0	49.3
B3LYP-D3/6-311++G(df,pd)	5261.7	38.1	3103.7	10.3	1976.1	9.2	57.6	250.8	53.1
B3LYP-D3/6-311G(2d,2p)	5272.5	27.3	3104.9	9.2	1978.0	7.3	43.8	220.9	23.2
B3LYP-D3/6-311+G(2d,2p)	5274.5	25.3	3103.8	10.3	1977.8	7.4	43.1	224.3	26.6
B3LYP-D3/6-311++G(2d,2p)	5274.2	25.6	3103.8	10.3	1977.8	7.5	43.4	225.7	28.0
B3LYP-D3/6-311G(2df,2pd)	5294.3	5.6	3110.9	3.2	1983.5	1.8	10.5	208.6	10.9
B3LYP-D3/6-311+G(2df,2pd)	5294.5	5.4	3110.1	4.0	1983.2	2.1	11.4	211.6	13.9
B3LYP-D3/6-311++G(2df,2pd)	5294.2	5.6	3110.1	4.0	1983.2	2.1	11.7	214.2	16.5
B3LYP-D3/6-311G(3df,3pd)	5308.6	−8.7	3114.9	−0.8	1987.1	−1.9	11.4	196.3	−1.5
B3LYP-D3/6-311+G(3df,3pd)	5307.9	−8.1	3114.5	−0.5	1986.9	−1.6	10.2	207.3	9.6
B3LYP-D3/6-311++G(3df,3pd)	5307.8	−7.9	3114.5	−0.4	1986.9	−1.6	10.0	207.9	10.2
B3LYP-D3/cc-pVDZ	5202.7	97.2	3079.0	35.1	1958.1	27.1	159.4	248.1	50.4
B3LYP-D3/cc-pVTZ	5285.3	14.6	3108.6	5.5	1981.3	4.0	24.1	222.9	25.1
B3LYP-D3/aug-cc-pVDZ	5203.9	96.0	3078.0	36.1	1957.8	27.4	159.5	249.5	51.7
B3LYP-D3/aug-cc-pVTZ	5286.4	13.5	3108.2	5.9	1981.3	4.0	23.4	222.1	24.3
B3LYP-D3BJ/6-31G(d,p)	5231.6	68.3	3091.7	22.4	1967.1	18.2	108.9	255.7	58.0
B3LYP-D3BJ/6-31+G(d,p)	5225.2	74.6	3088.2	25.9	1964.8	20.4	120.9	252.0	54.3
B3LYP-D3BJ/6-31++G(d,p)	5225.2	74.7	3088.3	25.8	1964.8	20.4	120.9	249.4	51.7
B3LYP-D3BJ/6-311G(d,p)	5244.7	55.1	3100.2	13.9	1972.3	12.9	81.9	231.0	33.3
B3LYP-D3BJ/6-311+G(d,p)	5245.3	54.5	3098.4	15.7	1971.7	13.6	83.8	232.2	34.4
B3LYP-D3BJ/6-311++G(d,p)	5245.0	54.8	3098.3	15.8	1971.6	13.7	84.3	236.4	38.6
B3LYP-D3BJ/6-311G(df,pd)	5262.6	37.2	3110.4	3.7	1978.9	6.3	47.3	228.6	30.9
B3LYP-D3BJ/6-311+G(df,pd)	5263.5	36.3	3108.6	5.5	1978.3	6.9	48.8	195.4	−2.4
B3LYP-D3BJ/6-311++G(df,pd)	5263.3	36.6	3108.5	5.6	1978.2	7.0	49.2		

	A	ΔA	B	ΔB	C	ΔC	$\Sigma\Delta$	V_3	ΔV_3
B3LYP-D3BJ/6-311G(2d,2p)	5276.0	23.9	3108.9	5.1	1980.1	5.2	34.2	200.4	2.7
B3LYP-D3BJ/6-311+G(2d,2p)	5275.9	23.9	3108.5	5.6	1979.9	5.3	34.8	204.0	6.3
B3LYP-D3BJ/6-311++G(2d,2p)	5275.7	24.2	3108.5	5.6	1979.9	5.4	35.1	205.3	7.6
B3LYP-D3BJ/6-311G(2df,2pd)	5295.1	4.7	3115.5	−1.4	1985.5	−0.2	6.4	188.1	−9.6
B3LYP-D3BJ/6-311+G(2df,2pd)	5295.4	4.5	3114.7	−0.6	1985.2	0.1	5.2	191.1	−6.6
B3LYP-D3BJ/6-311++G(2df,2pd)	5295.1	4.7	3114.7	−0.6	1985.2	0.1	5.5	193.7	−4.1
B3LYP-D3BJ/6-311G(3df,3pd)	5309.2	−9.3	3119.4	−5.3	1989.1	−3.8	18.4	175.5	−22.2
B3LYP-D3BJ/6-311+G(3df,3pd)	5308.6	−8.7	3119.1	−5.0	1988.8	−3.6	17.3	186.7	−11.1
B3LYP-D3BJ/6-311++G(3df,3pd)	5308.5	−8.6	3119.0	−4.9	1988.8	−3.5	17.1	187.3	−10.5
B3LYP-D3BJ/cc-pVDZ	5205.7	94.1	3083.8	30.3	1960.5	24.8	149.2	228.3	30.6
B3LYP-D3BJ/cc-pVTZ	5286.3	13.5	3113.3	0.8	1983.3	1.9	16.3	202.4	4.6
B3LYP-D3BJ/aug-cc-pVDZ	5206.9	92.9	3082.8	31.3	1960.2	25.1	149.3	230.2	32.5
B3LYP-D3BJ/aug-cc-pVTZ	5287.4	12.4	3112.9	1.2	1983.3	1.9	15.6	201.5	3.8
CAM-B3LYP-D3BJ/6-311G(d,p)	5303.5	−3.7	3122.6	−8.5	1989.7	−4.4	16.6	229.4	31.6
CAM-B3LYP-D3BJ/6-311+G(d,p)	5304.3	−4.5	3120.7	−6.6	1989.0	−3.7	14.8	233.3	35.5
CAM-B3LYP-D3BJ/6-311++G(d,p)	5304.0	−4.2	3120.6	−6.5	1988.9	−3.7	14.3	239.1	41.4
CAM-B3LYP-D3BJ/cc-pVDZ	5263.1	36.8	3105.7	8.4	1977.4	7.8	53.0	231.7	34.0
CAM-B3LYP-D3BJ/cc-pVTZ	5343.5	−43.6	3135.6	−21.6	2000.4	−15.2	80.4	205.9	8.2
CAM-B3LYP-D3BJ/aug-cc-pVDZ	5264.7	35.2	3104.8	9.3	1977.3	8.0	52.5	233.9	36.2
B3PW91-D3/6-31G(d,p)	5268.4	31.5	3105.6	8.5	1977.9	7.4	47.4	251.4	53.7
B3PW91-D3/6-31+G(d,p)	5262.5	37.4	3103.4	10.7	1976.2	9.0	57.1	248.6	50.9
B3PW91-D3/6-31++G(d,p)	5262.4	37.4	3103.4	10.7	1976.2	9.0	57.1	248.9	51.2
B3PW91-D3/6-311G(d,p)	5282.8	17.1	3115.4	−1.3	1984.0	1.4	19.7	230.7	33.0
B3PW91-D3/6-311+G(d,p)	5282.8	17.0	3113.4	0.7	1983.1	2.2	20.0	233.1	35.3
B3PW91-D3/6-311++G(d,p)	5282.5	17.4	3113.3	0.8	1983.0	2.3	20.5	237.4	39.6
B3PW91-D3/6-311G(df,pd)	5299.9	−0.1	3124.3	−10.2	1989.9	−4.6	14.9	228.9	31.2
B3PW91-D3/6-311+G(df,pd)	5300.4	−0.5	3122.3	−8.2	1989.1	−3.8	12.5	228.8	31.0
B3PW91-D3/6-311++G(df,pd)	5300.1	−0.2	3122.2	−8.1	1989.0	−3.8	12.1	232.5	34.8
B3PW91-D3/6-311G(2d,2p)	5313.2	−13.3	3123.4	−9.3	1991.3	−6.0	28.6	198.4	0.7
B3PW91-D3/6-311+G(2d,2p)	5312.6	−12.8	3122.8	−8.7	1991.0	−5.7	27.2	203.3	5.6
B3PW91-D3/6-311++G(2d,2p)	5312.3	−12.4	3122.9	−8.8	1990.9	−5.7	26.9	204.4	6.7
B3PW91-D3/6-311G(2df,2pd)	5331.3	−31.4	3129.2	−15.2	1996.2	−10.9	57.5	186.2	−11.5
B3PW91-D3/6-311+G(2df,2pd)	5331.0	−31.2	3128.4	−14.3	1995.8	−10.5	56.0	190.4	−7.4
B3PW91-D3/6-311++G(2df,2pd)	5330.8	−30.9	3128.4	−14.3	1995.8	−10.5	55.7	192.8	−4.9
B3PW91-D3/6-311G(3df,3pd)	5344.5	−44.7	3133.1	−19.0	1999.6	−14.4	78.1	178.8	−18.9
B3PW91-D3/6-311+G(3df,3pd)	5343.8	−43.9	3132.8	−18.7	1999.4	−14.2	76.8	188.8	−8.9
B3PW91-D3/6-311++G(3df,3pd)	5343.6	−43.8	3132.8	−18.7	1999.4	−14.1	76.5	189.4	−8.3
B3PW91-D3/cc-pVDZ	5245.4	54.5	3098.2	15.9	1971.9	13.3	83.6	225.1	27.3
B3PW91-D3/cc-pVTZ	5321.5	−21.6	3126.3	−12.2	1993.6	−8.4	42.2	201.6	3.9
B3PW91-D3/aug-cc-pVDZ	5246.1	53.7	3097.5	16.6	1971.7	13.6	83.9	224.0	26.3
B3PW91-D3/aug-cc-pVTZ	5322.4	−22.6	3126.0	−11.9	1993.7	−8.4	42.9		
B3PW91-D3BJ/6-31G(d,p)	5269.2	30.6	3109.9	4.2	1979.7	5.5	40.4	235.3	37.5
B3PW91-D3BJ/6-31+G(d,p)	5263.6	36.3	3107.7	6.4	1978.1	7.2	49.8	232.8	35.1
B3PW91-D3BJ/6-31++G(d,p)	5263.5	36.4	3107.8	6.3	1978.1	7.1	49.8	233.0	35.2
B3PW91-D3BJ/6-311G(d,p)	5283.1	16.7	3119.7	−5.6	1985.7	−0.4	22.8	213.9	16.2
B3PW91-D3BJ/6-311+G(d,p)	5283.2	16.6	3117.7	−3.6	1984.9	0.4	20.6	216.3	18.5
B3PW91-D3BJ/6-311++G(d,p)	5282.9	16.9	3117.6	−3.5	1984.8	0.5	20.9	220.5	22.8
B3PW91-D3BJ/6-311G(df,pd)	5299.8	0.0	3128.6	−14.5	1991.6	−6.3	20.8	212.1	14.3
B3PW91-D3BJ/6-311+G(df,pd)	5300.3	−0.4	3126.6	−12.5	1990.8	−5.6	18.4	211.9	14.2

	A	*ΔA*	*B*	*ΔB*	*C*	*ΔC*	Σ*Δ*	V_3	ΔV_3
B3PW91-D3BJ/6-311++G(df,pd)	5300.0	−0.1	3126.5	−12.4	1990.7	−5.5	18.0	215.6	17.8
B3PW91-D3BJ/6-311G(2d,2p)	5312.9	−13.1	3127.6	−13.5	1992.9	−7.7	34.3	180.3	−17.4
B3PW91-D3BJ/6-311+G(2d,2p)	5312.4	−12.6	3127.1	−13.0	1992.7	−7.4	32.9	185.2	−12.5
B3PW91-D3BJ/6-311++G(2d,2p)	5312.1	−12.2	3127.1	−13.0	1992.6	−7.4	32.6	186.3	−11.4
B3PW91-D3BJ/6-311G(2df,2pd)	5330.6	−30.8	3133.4	−19.3	1997.8	−12.5	62.7	168.1	−29.7
B3PW91-D3BJ/6-311+G(2df,2pd)	5330.5	−30.6	3132.6	−18.5	1997.4	−12.2	61.2	172.2	−25.5
B3PW91-D3BJ/6-311++G(2df,2pd)	5330.2	−30.3	3132.6	−18.5	1997.4	−12.1	60.9	174.6	−23.1
B3PW91-D3BJ/6-311G(3df,3pd)	5343.6	−43.8	3137.3	−23.2	2001.2	−15.9	82.9	160.6	−37.1
B3PW91-D3BJ/6-311+G(3df,3pd)	5343.0	−43.1	3137.0	−22.9	2001.0	−15.7	81.7	170.7	−27.0
B3PW91-D3BJ/6-311++G(3df,3pd)	5342.8	−42.9	3136.9	−22.8	2001.0	−15.7	81.5	171.3	−26.4
B3PW91-D3BJ/cc-pVDZ	5246.7	53.2	3102.6	11.5	1973.9	11.4	76.0	207.5	9.7
B3PW91-D3BJ/cc-pVTZ	5321.0	−21.2	3130.5	−16.5	1995.3	−10.0	47.7	183.4	−14.4
B3PW91-D3BJ/aug-cc-pVDZ	5247.4	52.4	3101.9	12.2	1973.6	11.6	76.3	206.7	8.9
B3PW91-D3BJ/aug-cc-pVTZ	5322.0	−22.1	3130.3	−16.2	1995.3	−10.0	48.4	182.8	−15.0
MN15/6-31G(d,p)	5308.8	−8.9	3113.0	1.1	1986.6	−1.3	11.4		
MN15/6-31+G(d,p)	5303.4	−3.6	3109.6	4.5	1984.5	0.8	8.8	253.1	55.4
MN15/6-31++G(d,p)	5303.4	−3.6	3109.6	4.5	1984.5	0.8	8.8	247.6	49.9
MN15/6-311G(d,p)	5323.5	−23.6	3124.8	−10.7	1993.4	−8.1	42.5	228.8	31.0
MN15/6-311+G(d,p)	5325.0	−25.1	3122.7	−8.6	1992.8	−7.5	41.3	229.6	31.9
MN15/6-311++G(d,p)	5324.8	−24.9	3122.6	−8.5	1992.7	−7.4	40.9	234.4	36.7
MN15/6-311G(df,pd)	5344.3	−44.5	3135.1	−21.0	2000.4	−15.2	80.6	228.1	30.4
MN15/6-311+G(df,pd)	5345.7	−45.8	3132.5	−18.4	1999.6	−14.3	78.5	226.7	29.0
MN15/6-311++G(df,pd)	5345.7	−45.8	3132.5	−18.4	1999.6	−14.3	78.5	229.5	31.8
MN15/6-311G(2d,2p)	5356.0	−56.1	3132.9	−18.8	2001.1	−15.8	90.7	189.3	−8.4
MN15/6-311+G(2d,2p)	5356.0	−56.2	3132.1	−18.0	2000.8	−15.5	89.7	197.3	−0.4
MN15/6-311++G(2d,2p)	5355.8	−55.9	3132.1	−18.0	2000.8	−15.5	89.5	198.0	0.3
MN15/6-311G(2df,2pd)	5376.1	−76.3	3138.7	−24.6	2006.3	−21.0	121.9	178.4	−19.3
MN15/6-311+G(2df,2pd)	5376.6	−76.7	3137.6	−23.6	2005.9	−20.6	120.9	187.6	−10.1
MN15/6-311++G(2df,2pd)	5376.3	−76.5	3137.7	−23.6	2005.9	−20.6	120.7	189.5	−8.2
MN15/6-311G(3df,3pd)	5387.8	−88.0	3142.9	−28.8	2009.6	−24.4	141.2	176.8	−20.9
MN15/6-311+G(3df,3pd)	5386.9	−87.0	3142.2	−28.1	2009.2	−23.9	139.0	186.2	−11.5
MN15/6-311++G(3df,3pd)	5386.8	−86.9	3142.2	−28.1	2009.2	−23.9	138.9	185.4	−12.4
MN15/cc-pVDZ	5289.2	10.6	3107.4	6.7	1981.8	3.5	20.9	218.8	21.0
MN15/cc-pVTZ	5371.2	−71.4	3138.2	−24.1	2005.4	−20.1	115.6	196.1	−1.7
MN15/aug-cc-pVDZ	5291.5	8.4	3107.4	6.7	1982.1	3.2	18.3		
MN15/aug-cc-pVTZ	5379.1	−79.3	3140.3	−26.2	2007.3	−22.1	127.5	214.6	16.8
PBE0/6-31G(d,p)	5200.3	99.6	3072.1	42.0	1955.0	30.3	171.8	223.1	25.4
PBE0/6-31+G(d,p)	5193.2	106.7	3068.8	45.3	1952.7	32.5	184.5	219.0	21.3
PBE0/6-31++G(d,p)	5193.1	106.7	3068.9	45.2	1952.7	32.5	184.5	217.9	20.2
PBE0/6-311G(d,p)	5214.3	85.6	3081.6	32.5	1960.8	24.4	142.5	198.7	0.9
PBE0/6-311+G(d,p)	5214.6	85.3	3079.7	34.4	1960.1	25.2	144.8	198.3	0.6
PBE0/6-311++G(d,p)	5214.3	85.6	3079.6	34.5	1960.0	25.3	145.3	202.4	4.7
PBE0/6-311G(df,pd)	5232.3	67.6	3090.7	23.4	1967.0	18.3	109.2	196.9	−0.8
PBE0/6-311+G(df,pd)	5232.4	67.4	3088.6	25.5	1966.2	19.1	112.0	194.3	−3.4
PBE0/6-311++G(df,pd)	5232.4	67.4	3088.6	25.5	1966.2	19.1	112.0	197.8	0.1
PBE0/6-311G(2d,2p)	5243.8	56.1	3088.8	25.3	1967.8	17.5	98.9	164.7	−33.0
PBE0/6-311+G(2d,2p)	5244.1	55.8	3087.9	26.2	1967.4	17.8	99.8	166.5	−31.3
PBE0/6-311++G(2d,2p)	5243.7	56.1	3087.9	26.2	1967.4	17.9	100.2	168.1	−29.7
PBE0/6-311G(2df,2pd)	5263.3	36.6	3094.7	19.4	1972.9	12.4	68.4	153.8	−43.9

	A	*ΔA*	*B*	*ΔB*	*C*	*ΔC*	*ΣΔ*	V_3	*Δ*V_3
PBE0/6-311+G(2df,2pd)	5263.3	36.6	3093.8	20.3	1972.5	12.7	69.6	155.3	–42.4
PBE0/6-311++G(2df,2pd)	5263.0	36.9	3093.8	20.3	1972.5	12.8	69.9	157.9	–39.8
PBE0/6-311G(3df,3pd)	5278.1	21.7	3099.0	15.1	1976.7	8.5	45.3	144.3	–53.4
PBE0/6-311+G(3df,3pd)	5277.5	22.3	3098.7	15.4	1976.5	8.7	46.5	153.9	–43.9
PBE0/6-311++G(3df,3pd)	5277.4	22.5	3098.6	15.5	1976.5	8.8	46.8	154.5	–43.2
PBE0/cc-pVDZ	5178.7	121.2	3066.4	47.7	1949.9	35.4	204.2	189.8	–7.9
PBE0/cc-pVTZ	5254.0	45.8	3092.6	21.5	1970.7	14.5	81.9	167.3	–30.5
PBE0/aug-cc-pVDZ	5178.5	121.3	3065.0	49.1	1949.2	36.0	206.5	191.6	–6.1
PBE0/aug-cc-pVTZ	5254.9	45.0	3092.0	22.1	1970.6	14.6	81.7	167.2	–30.5
PBE0-D3/6-31G(d,p)	5197.4	102.5	3072.7	41.4	1954.8	30.4	174.3	227.0	29.2
PBE0-D3/6-31+G(d,p)	5190.3	109.5	3069.3	44.7	1952.6	32.7	187.0	222.6	24.9
PBE0-D3/6-31++G(d,p)	5190.3	109.6	3069.4	44.7	1952.6	32.7	187.0	221.5	23.8
PBE0-D3/6-311G(d,p)	5211.4	88.5	3082.2	31.9	1960.6	24.6	145.1	202.7	5.0
PBE0-D3/6-311+G(d,p)	5211.7	88.2	3080.3	33.8	1959.9	25.3	147.3	202.3	4.6
PBE0-D3/6-311++G(d,p)	5211.4	88.5	3080.2	33.9	1959.8	25.4	147.9	206.5	8.7
PBE0-D3/6-311G(df,pd)	5229.4	70.5	3091.2	22.9	1966.8	18.5	111.8	201.1	3.3
PBE0-D3/6-311+G(df,pd)	5229.5	70.4	3089.2	24.9	1966.0	19.3	114.6	198.5	0.8
PBE0-D3/6-311G(2d,2p)	5240.9	59.0	3089.3	24.8	1967.6	17.7	101.5	169.2	–28.6
PBE0-D3/6-311+G(2d,2p)	5241.2	58.7	3088.4	25.7	1967.2	18.0	102.4	171.0	–26.8
PBE0-D3/6-311++G(2d,2p)	5240.8	59.0	3088.4	25.7	1967.2	18.1	102.8	172.6	–25.2
PBE0-D3/6-311G(2df,2pd)	5260.3	39.5	3095.2	18.9	1972.7	12.6	71.0	158.3	–39.4
PBE0-D3/6-311+G(2df,2pd)	5260.3	39.5	3094.3	19.8	1972.3	12.9	72.2	169.9	–37.8
PBE0-D3/6-311++G(2df,2pd)	5260.0	39.8	3094.3	19.8	1972.3	13.0	72.6	162.5	–35.3
PBE0-D3/6-311G(3df,3pd)	5275.2	24.7	3099.5	14.6	1976.5	8.7	48.0	149.0	–48.8
PBE0-D3/6-311+G(3df,3pd)	5274.6	25.3	3099.2	14.9	1976.3	8.9	49.2	158.5	–39.2
PBE0-D3/6-311++G(3df,3pd)	5274.4	25.5	3099.1	15.0	1976.3	9.0	49.4	159.1	–38.6
PBE0-D3/cc-pVDZ	5175.8	124.0	3067.0	47.1	1949.7	35.5	206.7	194.0	–3.8
PBE0-D3/cc-pVTZ	5251.1	48.8	3093.1	21.0	1970.5	14.7	84.5	171.9	–25.8
PBE0-D3/aug-cc-pVDZ	5175.7	124.2	3065.5	48.6	1949.1	36.2	209.0	195.7	–2.0
PBE0-D3/aug-cc-pVTZ	5291.9	47.9	3092.5	21.6	1970.4	14.8	84.3	172.0	–25.8
Experimental	5299.9		3114.1		1985.3			197.7	

Table S3: Coefficients of the Fourier expansion for the potential energy curves of the methyl internal rotation of 2MTP given in Figure 2. The potential is expanded as

$$V(\alpha) = a_0 + a_3\cos(3\alpha) + a_6\cos(6\alpha) + a_9\cos(9\alpha).$$

Coef.	MP2	B3LYP
a_0	–591.244957593	–592.422045454
a_3	–0.000402718	–0.000534224
a_6	0.000108369	0.000042608
a_9	–0.000011819	–0.000003690

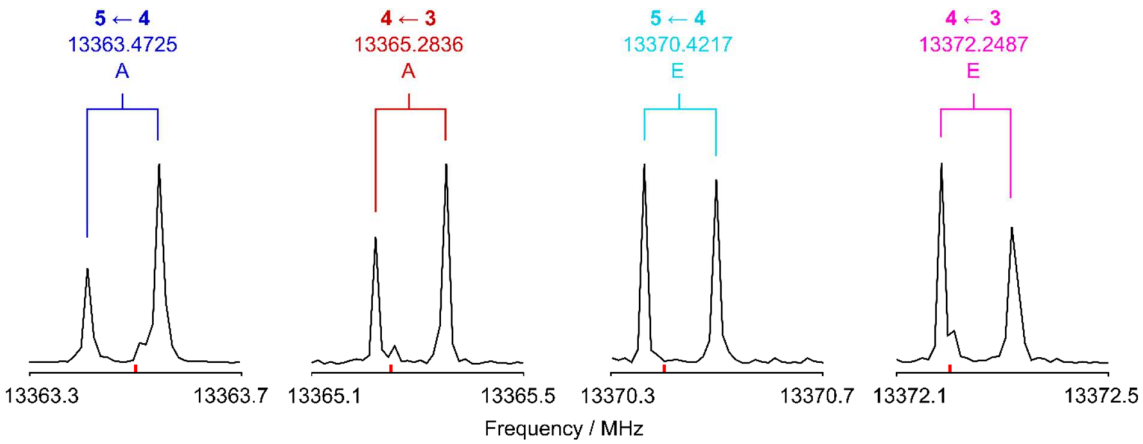

Figure S1: Four spectra of the *b*-type R-branch $3_{13} \leftarrow 2_{02}$ transition of the ^{33}S isotopologue of 2MTP, featuring the A- and E-species from methyl internal rotation and some components of the quadrupole hyperfine structure. The polarization frequencies are marked with red lines. Intensities are given in arbitrary units and are normalized for all spectra.

Table S4. Rotational constants of 2MTP for all observed isotopologues obtained with the *XIAM* program when $D_{p_i^2 J}$, $D_{p_i^2 K}$, and $D_{p_i^2 -}$ are fitted. For all ^{13}C isotopologue fits, the values of D_K and d_2 were fixed to those of the parent species.

Par[a]	Unit	Parent	^{34}S	$^{13}C(2)$	$^{13}C(3)$	$^{13}C(4)$	$^{13}C(5)$	$^{13}C(9)$
A_0	MHz	5299.85002(45)	5161.33031(63)	5296.4757(13)	5194.5222(15)	5232.1892(13)	5297.7182(11)	5298.8303(36)
B_0	MHz	3114.09632(30)	3112.72380(44)	3101.70154(90)	3114.13351(92)	3078.91353(80)	3064.14099(72)	3015.8671(23)
C_0	MHz	1985.26582(21)	1964.94486(32)	1979.75498(21)	1970.31204(18)	1961.46901(20)	1964.55462(19)	1944.73199(30)
N[b]		148	127	51	47	55	54	42
σ[c]	kHz	4.4	5.6	2.8	2.4	2.9	2.6	3.6

[a] All parameters refer to the principal axis system. Watson's S reduction in I^r representation was used. Standard error in parentheses is in the units of the last significant digits.
[b] Number of lines.
[c] Standard deviation of the fit.

Table S5. A section of Table 2 showing the rotational constants of 2MTP for all observed isotopologues obtained with the *XIAM* program when $D_{p_i^2 J}$, $D_{p_i^2 K}$, and $D_{p_i^2 -}$ are fitted for the parent species and the ^{34}S isotopologue fits. For all ^{13}C isotopologue fits, the values of D_K, d_2, and $D_{p_i^2 -}$ were fixed to those of the parent species.

Par[a]	Unit	Parent	^{34}S	$^{13}C(2)$	$^{13}C(3)$	$^{13}C(4)$	$^{13}C(5)$	$^{13}C(9)$
A_0	MHz	5299.85002(45)	5161.33031(63)	5296.47565(86)	5194.52016(96)	5232.18924(71)	5297.71936(65)	5298.8233(15)
B_0	MHz	3114.09632(30)	3112.72380(44)	3101.70161(38)	3114.13512(38)	3078.91352(30)	3064.14021(29)	3015.87188(63)
C_0	MHz	1985.26582(21)	1964.94486(32)	1979.75497(20)	1970.31198(19)	1961.46901(20)	1964.55468(18)	1944.73180(31)
N[b]		148	127	51	47	55	54	42
σ[c]	kHz	4.4	5.6	2.8	2.5	2.9	2.6	3.8

[a] All parameters refer to the principal axis system. Watson's S reduction in I^r representation was used. Standard error in parentheses is in the units of the last significant digits.
[b] Number of lines.
[c] Standard deviation of the fit.

Table S6. Rotational constants of 2MTP for all observed isotopologues obtained with the *XIAM* program when only $D_{p_i^2 J}$ and $D_{p_i^2 K}$ are fitted. For all ^{13}C isotopologue fits, the values of D_K and d_2 were fixed to those of the parent species.

Par[a]	Unit	Parent	^{34}S	$^{13}C(2)$	$^{13}C(3)$	$^{13}C(4)$	$^{13}C(5)$	$^{13}C(9)$
A_0	MHz	5299.84640(74)	5161.32794(71)	5296.47261(98)	5194.5169(12)	5232.18578(80)	5297.71590(70)	5298.8205(20)
B_0	MHz	3114.09953(42)	3112.72640(43)	3101.70431(43)	3114.13765(48)	3078.91594(33)	3064.14274(31)	3015.87348(79)
C_0	MHz	1985.26548(38)	1964.94443(40)	1979.75479(23)	1970.31188(23)	1961.46889(21)	1964.55452(19)	1944.73171(40)
N[b]		148	127	51	47	55	54	42
σ[c]	kHz	7.9	6.9	3.1	3.0	3.2	2.7	4.8

[a] All parameters refer to the principal axis system. Watson's S reduction in I^r representation was used. Standard error in parentheses is in the units of the last significant digits.

[b] Number of lines.

[c] Standard deviation of the fit.

Table S7: Observed frequencies (ν_{obs}) of the parent species of 2MTP. *J*, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective A or E torsional species. Observed-minus-calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	*J*	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.8627525	−0.4
2	0	2	1	0	1	E	9.8604369	1.2
3	0	3	2	0	2	A	14.1126908	0.2
3	0	3	2	0	2	E	14.1066432	0.9
4	0	4	3	0	3	A	18.0301213	−0.9
4	0	4	3	0	3	E	18.0227677	0.0
5	0	5	4	0	4	A	21.8966401	−0.6
5	0	5	4	0	4	E	21.8902762	0.3
6	0	6	5	0	5	A	25.8065567	0.0
6	0	6	5	0	5	E	25.8013001	−0.1
1	1	1	0	0	0	A	7.2947448	1.7
1	1	1	0	0	0	E	7.2302205	0.3
2	1	2	1	0	1	A	11.2654171	1.4
2	1	2	1	0	1	E	11.2336638	0.2
3	1	3	2	0	2	A	14.8214765	0.2
3	1	3	2	0	2	E	14.7993557	1.7
4	1	4	3	0	3	A	18.3292738	0.3
4	1	4	3	0	3	E	18.3140482	1.1
5	1	5	4	0	4	A	22.0093474	−0.8
5	1	5	4	0	4	E	21.9995821	1.4
6	1	6	5	0	5	A	25.8461342	−0.7
6	1	6	5	0	5	E	25.8395306	−0.3
1	1	0	1	0	1	A	3.3240657	2.3
1	1	0	1	0	1	E	3.3597833	−1.0
2	1	1	2	0	2	A	4.7887479	2.2
2	1	1	2	0	2	E	4.7939375	−1.0
3	1	2	3	0	3	A	7.4150065	−0.4
3	1	2	3	0	3	E	7.4161364	−0.9
4	1	3	4	0	4	A	11.1502758	1.1
4	1	3	4	0	4	E	11.1492974	−1.6
5	1	4	5	0	5	A	15.4905892	2.2
5	1	4	5	0	5	E	15.4808332	−1.6
6	1	5	6	0	6	A	19.8865604	3.1
6	1	5	6	0	6	E	19.8621726	−4.0
7	1	6	7	0	7	A	24.1027713	3.9
7	1	6	7	0	7	E	24.0634546	−6.3
2	0	2	1	1	1	A	7.6673807	−4.2
2	0	2	1	1	1	E	7.7295349	−0.4
3	0	3	2	1	2	A	12.7100285	0.7
3	0	3	2	1	2	E	12.7334150	0.6
4	0	4	3	1	3	A	17.3213371	0.6
4	0	4	3	1	3	E	17.3300565	0.5
5	0	5	4	1	4	A	21.5974908	1.3

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
5	0	5	4	1	4	E	21.5989968	0.4
2	1	1	2	1	2	A	3.3860849	2.0
2	1	1	2	1	2	E	3.4207088	−1.7
2	1	1	1	1	0	A	11.3274298	−5.3
3	1	2	2	1	1	A	16.7389523	0.5
2	1	2	1	1	1	A	9.0700418	−5.9
2	1	2	1	1	1	E	9.1027639	0.7
3	1	3	2	1	2	A	13.4188141	0.6
3	1	3	2	1	2	E	13.4261268	0.8
4	1	4	3	1	3	A	17.6204876	−0.1
4	1	4	3	1	3	E	17.6213367	1.3
5	1	5	4	1	4	A	21.7101971	0.1
5	1	5	4	1	4	E	21.7083018	0.5
2	2	1	1	1	0	A	17.9134875	7.3
2	2	1	1	1	0	E	17.4826894	−0.4
2	2	1	2	1	2	A	9.9721357	7.7
2	2	1	2	1	2	E	9.6088075	−2.9
3	2	2	3	1	3	A	11.8514015	3.9
3	2	2	3	1	3	E	11.6934375	−0.1
4	2	3	4	1	4	A	14.3612045	−0.5
4	2	3	4	1	4	E	14.2809844	−1.0
5	2	4	5	1	5	A	17.4069032	1.7
5	2	4	5	1	5	E	17.3497286	−1.5
6	2	5	6	1	6	A	20.8428224	2.4
6	2	5	6	1	6	E	20.7915100	−3.2
7	2	6	7	1	7	A	24.5198440	4.5
7	2	6	7	1	7	E	24.4670829	−5.9
4	2	2	4	1	3	A	7.3881670	−1.0
4	2	2	4	1	3	E	7.4055401	−1.5
5	2	3	5	1	4	A	9.4255523	−4.0
5	2	3	5	1	4	E	9.4340706	−0.3
6	2	4	6	1	5	A	12.8427814	−0.7
6	2	4	6	1	5	E	12.8549893	0.0
7	2	5	7	1	6	A	17.2458424	0.2
7	2	5	7	1	6	E	17.2553205	−1.0
8	2	6	8	1	7	A	21.9693908	1.5
8	2	6	8	1	7	E	21.9643763	−1.3
3	2	1	2	2	0	A	16.4834931	−4.3
3	2	1	2	2	0	E	16.2766391	1.3
4	2	2	3	2	1	A	22.4869773	2.2
4	2	2	3	2	1	E	22.4123978	0.7
3	2	2	2	2	1	A	15.2980804	−2.7
3	2	2	2	2	1	E	15.5107554	2.2
4	2	3	3	2	2	A	20.1302950	−0.2
4	2	3	3	2	2	E	20.2088846	1.3
5	2	4	4	2	3	A	24.7558935	0.0
5	2	4	4	2	3	E	24.7770456	−0.4
4	1	3	3	2	2	A	16.6202069	−6.6
4	1	3	3	2	2	E	16.7859179	0.5

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
5	1	4	4	2	3	A	22.7268725	1.0
5	1	4	4	2	3	E	22.7988445	−1.3
4	3	2	3	3	1	A	20.9169580	−6.6
4	3	2	3	3	1	E	21.0900728	7.4
4	3	1	3	3	0	E	21.1218262	−1.6
3	3	0	3	2	1	A	12.5290723	10.2
3	3	0	3	2	1	E	13.0126501	3.9
4	3	1	4	2	2	A	11.3288895	−8.2
4	3	1	4	2	2	E	11.7220751	−1.7
5	3	2	5	2	3	A	10.3037722	−4.5
5	3	2	5	2	3	E	10.4630188	−3.9
6	3	3	6	2	4	A	10.1751023	−1.7
6	3	3	6	2	4	E	10.2136144	−1.7
7	3	4	7	2	5	A	11.4444999	−3.6
7	3	4	7	2	5	E	11.4591556	0.5
8	3	5	8	2	6	A	14.3095361	−5.9
8	3	5	8	2	6	E	14.3321981	2.3
9	3	6	9	2	7	A	18.5435509	−6.3
9	3	6	9	2	7	E	18.5737497	1.8
3	3	1	3	2	2	A	13.9845438	9.9
3	3	1	3	2	2	E	13.3518580	−0.1
4	3	2	4	2	3	A	14.7712035	0.2
4	3	2	4	2	3	E	14.2330388	−1.4
5	3	3	5	2	4	A	16.1494262	−0.2
5	3	3	5	2	4	E	15.8610002	2.6
6	3	4	6	2	5	A	18.1832263	0.6
6	3	4	6	2	5	E	18.0420238	4.0
7	3	5	7	2	6	A	20.8413528	−1.2
7	3	5	7	2	6	E	20.7555261	2.4
8	3	6	8	2	7	A	24.0111625	0.6
8	3	6	8	2	7	E	23.9461906	−0.3
4	4	1	4	3	2	A	18.8784859	−9.4
4	4	1	4	3	2	E	18.3418855	−16.9
5	4	2	5	3	3	A	18.9818512	−0.7
5	4	2	5	3	3	E	18.2304124	−10.5
6	4	3	6	3	4	A	19.4163791	3.5
6	4	3	6	3	4	E	18.6897685	0.6
7	4	4	7	3	5	A	20.3660599	2.8
7	4	4	7	3	5	E	19.9004442	10.3
8	4	5	8	3	6	A	21.9557996	−2.6
8	4	5	8	3	6	E	21.7199211	12.8
9	4	6	9	3	7	A	24.2167969	−4.3
9	4	6	9	3	7	E	24.0860738	9.8
4	4	0	4	3	1	A	18.4533510	−10.8
4	4	0	4	3	1	E	18.7822010	12.8
5	4	1	5	3	2	A	17.5232971	−2.2
5	4	1	5	3	2	E	18.0624679	7.9
6	4	2	6	3	3	A	16.0087865	1.0
6	4	2	6	3	3	E	16.5239639	−0.9

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
7	4	3	7	3	4	A	14.3522632	0.8
7	4	3	7	3	4	E	14.6232102	−7.6
8	4	4	8	3	5	A	13.3481835	−2.5
8	4	4	8	3	5	E	13.4255435	−4.8
9	4	5	9	3	6	A	13.7026778	−6.5
9	4	5	9	3	6	E	13.7235877	−0.2
5	5	1	5	4	2	A	24.1551978	5.6

Table S8: Observed frequencies (ν_{obs}) of the ^{34}S isotopologues of 2MTP. *J*, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	*J*	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.7924902	−0.7
3	0	3	2	0	2	A	13.9701075	−1.3
3	0	3	2	0	2	E	13.9638823	2.0
4	0	4	3	0	3	A	17.8299880	−1.4
4	0	4	3	0	3	E	17.8228123	4.0
5	0	5	4	0	4	A	21.6592420	−1.8
5	0	5	4	0	4	E	21.6532079	1.4
1	1	1	0	0	0	E	7.0749852	−0.1
2	1	2	1	0	1	A	11.0654144	−0.2
2	1	2	1	0	1	E	11.0356446	2.4
3	1	3	2	0	2	A	14.5844759	−0.6
3	1	3	2	0	2	E	14.5638346	2.2
4	1	4	3	0	3	A	18.0766208	−1.2
4	1	4	3	0	3	E	18.0627118	2.0
5	1	5	4	0	4	A	21.7476539	−0.9
5	1	5	4	0	4	E	21.7388521	2.4
1	1	0	1	0	1	E	3.2385089	2.0
2	1	1	2	0	2	E	4.7208033	1.0
3	1	2	3	0	3	A	7.4241107	0.7
3	1	2	3	0	3	E	7.4255676	0.6
4	1	3	4	0	4	A	11.2240290	1.2
4	1	3	4	0	4	E	11.2228121	−2.1
5	1	4	5	0	5	A	15.5533553	2.5
5	1	4	5	0	5	E	15.5423085	−4.3
6	1	5	6	0	6	A	19.8735277	5.5
6	1	5	6	0	6	E	19.8476466	−4.4
7	1	6	7	0	7	A	24.0027765	−0.4
2	0	2	1	1	1	A	7.7347798	−6.2
2	0	2	1	1	1	E	7.7926252	2.2
3	0	3	2	1	2	A	12.6971855	0.4
3	0	3	2	1	2	E	12.7182304	1.9
4	0	4	3	1	3	A	17.2156201	−1.6
4	0	4	3	1	3	E	17.2228569	1.5
5	0	5	4	1	4	A	21.4126086	−2.6
5	0	5	4	1	4	E	21.4133061	1.0
2	1	1	1	1	0	A	11.3030036	−6.2
2	1	1	1	1	0	E	11.2722871	0.5
3	1	2	2	1	1	A	16.6783421	−1.2
3	1	2	2	1	1	E	16.6686445	0.3
2	1	2	1	1	1	A	9.0077056	−4.1
2	1	2	1	1	1	E	9.0382753	1.3
3	1	3	2	1	2	A	13.3115518	−1.0
3	1	3	2	1	2	E	13.3181828	1.4

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
4	1	4	3	1	3	A	17.4622531	−1.2
4	1	4	3	1	3	E	17.4627590	2.1
5	1	5	4	1	4	A	21.5010200	−2.2
5	1	5	4	1	4	E	21.4989505	2.2
2	2	1	1	1	0	A	17.4760807	9.9
2	2	1	1	1	0	E	17.0728841	−3.3
2	2	1	2	1	2	A	9.6160246	11.8
2	2	1	2	1	2	E	9.2757492	−2.9
3	2	2	3	1	3	A	11.5374781	6.6
3	2	2	3	1	3	E	11.3957671	0.4
4	2	3	4	1	4	A	14.0965674	3.4
4	2	3	4	1	4	E	14.0239052	−0.6
5	2	4	5	1	5	A	17.1845277	−1.8
5	2	4	5	1	5	E	17.1316581	−1.4
6	2	5	6	1	6	A	20.6435157	1.1
6	2	5	6	1	6	E	20.5950092	−4.5
7	2	6	7	1	7	A	24.3208140	−0.1
4	2	2	4	1	3	A	7.2125207	0.5
4	2	2	4	1	3	E	7.2277703	3.9
5	2	3	5	1	4	A	9.4418207	−1.1
5	2	3	5	1	4	E	9.4511807	0.4
6	2	4	6	1	5	A	13.0415634	−2.9
6	2	4	6	1	5	E	13.0541242	−1.9
7	2	5	7	1	6	A	17.5156420	−0.8
7	2	5	7	1	6	E	17.5228281	−3.0
3	2	1	2	2	0	A	16.4959228	−12.0
3	2	1	2	2	0	E	16.2966934	−2.9
4	2	2	3	2	1	A	22.4889090	6.4
4	2	2	3	2	1	E	22.4228642	0.8
3	2	2	2	2	1	A	15.2330048	−6.6
3	2	2	2	2	1	E	15.4382020	6.0
4	2	3	3	2	2	A	20.0213479	1.1
4	2	3	3	2	2	E	20.0908977	1.7
5	2	4	4	2	3	A	24.5889866	−1.2
5	2	4	4	2	3	E	24.6067008	−1.2
4	1	3	3	2	2	A	16.9021807	2.6
4	1	3	3	2	2	E	17.0499022	−0.8
5	1	4	4	2	3	A	22.8693976	−2.4
5	1	4	4	2	3	E	22.9317101	−2.0
4	3	2	3	3	1	E	21.0544536	10.6
4	3	1	3	3	0	E	21.1047552	−7.2
3	3	0	3	2	1	A	11.8077325	−12.3
3	3	0	3	2	1	E	12.2842365	11.9
4	3	1	4	2	2	A	10.6055197	−4.6
4	3	1	4	2	2	E	10.9661274	3.8
5	3	2	5	2	3	A	9.6872973	0.2
5	3	2	5	2	3	E	9.8179171	−2.5
6	3	3	6	2	4	A	9.7884951	−2.0
6	3	3	6	2	4	E	9.8191275	0.0

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
7	3	4	7	2	5	A	11.3789027	−4.9
7	3	4	7	2	5	E	11.3947939	−0.2
8	3	5	8	2	6	A	14.5831301	−4.2
8	3	5	8	2	6	E	14.6083768	0.4
9	3	6	9	2	7	A	19.0357784	−5.5
9	3	6	9	2	7	E	19.0645361	−1.8
3	3	1	3	2	2	A	13.3573890	−0.3
3	3	1	3	2	2	E	12.7393343	−9.0
4	3	2	4	2	3	A	14.1998026	−1.8
4	3	2	4	2	3	E	13.7028899	−0.4
5	3	3	5	2	4	A	15.6618607	1.3
5	3	3	5	2	4	E	15.4124244	5.3
6	3	4	6	2	5	A	17.7957809	−1.1
6	3	4	6	2	5	E	17.6738582	5.0
7	3	5	7	2	6	A	20.5503073	−3.1
7	3	5	7	2	6	E	20.4743966	−1.9
8	3	6	8	2	7	A	23.7927846	0.3
4	4	1	4	3	2	A	17.9561466	−1.6
4	4	1	4	3	2	E	17.4097136	−15.5
5	4	2	5	3	3	A	18.0925880	4.1
5	4	2	5	3	3	E	17.3474352	−9.2
6	4	3	6	3	4	A	18.6011769	5.9
6	4	3	6	3	4	E	17.9288574	6.3
7	4	4	7	3	5	A	19.6686171	−1.8
7	4	4	7	3	5	E	19.2742285	17.9
8	4	5	8	3	6	E	21.2127848	15.2
9	4	6	9	3	7	E	23.7133065	7.0
5	4	1	5	3	2	A	16.4582484	2.3
5	4	1	5	3	2	E	17.0012636	14.4
6	4	2	6	3	3	A	14.8901597	0.8
6	4	2	6	3	3	E	15.3633110	−3.5
7	4	3	7	3	4	A	13.3261262	−2.9
7	4	3	7	3	4	E	13.5421232	−16.5
8	4	4	8	3	5	A	12.6154160	−8.1
8	4	4	8	3	5	E	12.6709940	−12.4

Table S9: Observed frequencies (ν_{obs}) of the ^{13}C(2) isotopologues of 2MTP. *J*, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	*J*	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.8315413	−0.3
2	0	2	1	0	1	E	9.8292631	−0.4
3	0	3	2	0	2	A	14.0732712	0.6
3	0	3	2	0	2	E	14.0673038	0.1
4	0	4	3	0	3	A	17.9822024	0.1
4	0	4	3	0	3	E	17.9748997	−1.0
5	0	5	4	0	4	A	21.8378091	1.1
5	0	5	4	0	4	E	21.8314656	0.9
2	1	2	1	0	1	A	11.2454725	−1.4
2	1	2	1	0	1	E	11.2137564	−0.6
3	1	3	2	0	2	A	14.7917708	−1.5
3	1	3	2	0	2	E	14.7696727	0.1
4	1	4	3	0	3	A	18.2873331	0.0
4	1	4	3	0	3	E	18.2720863	0.0
5	1	5	4	0	4	A	21.9534767	−0.4
5	1	5	4	0	4	E	21.9436790	0.3
3	1	2	3	0	3	A	7.3848872	0.9
3	1	2	3	0	3	E	7.3859754	0.8
4	1	3	4	0	4	A	11.0966084	0.2
4	1	3	4	0	4	E	11.0956536	−1.2
5	1	4	5	0	5	A	15.4200948	1.2
5	1	4	5	0	5	E	15.4105734	−1.7
2	0	2	1	1	1	E	7.6893596	2.7
3	0	3	2	1	2	A	12.6593414	3.0
3	0	3	2	1	2	E	12.6828107	0.5
4	0	4	3	1	3	A	17.2637018	1.2
4	0	4	3	1	3	E	17.2725305	−1.3
5	0	5	4	1	4	A	21.5326770	−0.2
5	0	5	4	1	4	E	21.5342786	−0.4
2	1	1	1	1	0	A	11.2847320	−13.4
2	1	1	1	1	0	E	11.2518822	3.7
3	1	2	2	1	1	A	16.6787892	3.6
3	1	2	2	1	1	E	16.6686899	0.8
4	1	3	3	1	2	A	21.6939249	0.8
4	1	3	3	1	2	E	21.6845801	−0.8
2	1	2	1	1	1	A	9.0411175	−2.9
2	1	2	1	1	1	E	9.0738513	0.8
3	1	3	2	1	2	A	13.3778425	2.5
3	1	3	2	1	2	E	13.3851806	1.5
4	1	4	3	1	3	A	17.5688320	0.6
4	1	4	3	1	3	E	17.5697177	0.3
5	1	5	4	1	4	A	21.6483465	0.1
5	1	5	4	1	4	E	21.6464900	−3.0

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	2	1	1	1	0	A	17.8977434	−1.6
2	2	1	1	1	0	E	17.4665764	0.4
2	2	1	2	1	2	A	9.9784422	3.5
2	2	1	2	1	2	E	9.6147926	−0.6
3	2	2	3	1	3	A	11.8449680	0.8
3	2	2	3	1	3	E	11.6861905	−0.6
4	2	3	4	1	4	A	14.3385539	−2.2
4	2	3	4	1	4	E	14.2580605	2.7

Table S10: Observed frequencies (ν_{obs}) of the ^{13}C(3) isotopologues of 2MTP. J, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.8122561	0.3
2	0	2	1	0	1	E	9.8098187	−0.1
3	0	3	2	0	2	A	14.0080462	0.3
3	0	3	2	0	2	E	14.0018887	−0.2
4	0	4	3	0	3	A	17.8822913	0.4
4	0	4	3	0	3	E	17.8751027	0.3
5	0	5	4	0	4	A	21.7213255	0.2
5	0	5	4	0	4	E	21.7152451	0.8
2	1	2	1	0	1	A	11.1147941	−2.4
2	1	2	1	0	1	E	11.0847477	1.1
3	1	3	2	0	2	A	14.6435233	−2.0
3	1	3	2	0	2	E	14.6226520	2.2
4	1	4	3	0	3	A	18.1403999	−1.3
4	1	4	3	0	3	E	18.1262598	−0.1
5	1	5	4	0	4	A	21.8149292	−1.5
5	1	5	4	0	4	E	21.8059560	−0.5
4	1	3	4	0	4	A	11.2109949	2.4
4	1	3	4	0	4	E	11.2098371	−5.7
5	1	4	5	0	5	A	15.5455005	−3.7
5	1	4	5	0	5	E	15.5348202	6.6
2	0	2	1	1	1	A	7.7226778	−3.1
3	0	3	2	1	2	A	12.7055082	3.1
3	0	3	2	1	2	E	12.7269630	1.9
4	0	4	3	1	3	A	17.2468119	0.4
4	0	4	3	1	3	E	17.2543400	−1.5
5	0	5	4	1	4	A	21.4632155	0.6
5	0	5	4	1	4	E	21.4640862	−0.5
2	1	1	1	1	0	A	11.3126021	−1.8
2	1	1	1	1	0	E	11.2816394	2.7
3	1	2	2	1	1	A	16.6983536	3.1

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
3	1	2	2	1	1	E	16.6886495	−0.4
4	1	3	3	1	2	A	21.6693625	−0.9
4	1	3	3	1	2	E	21.6596731	−4.6
2	1	2	1	1	1	A	9.0252191	−2.6
2	1	2	1	1	1	E	9.0560591	1.3
3	1	3	2	1	2	A	13.3409846	0.1
3	1	3	2	1	2	E	13.3477220	0.0
4	1	4	3	1	3	A	17.5049226	0.8
4	1	4	3	1	3	E	17.5054992	0.2
5	1	5	4	1	4	A	21.5568222	1.9
5	1	5	4	1	4	E	21.5547996	0.7
2	2	1	1	1	0	A	17.5812743	0.9
2	2	1	1	1	0	E	17.1738654	−0.2
3	2	2	3	1	3	A	11.6121018	−0.6
3	2	2	3	1	3	E	11.4676603	1.0
4	2	3	4	1	4	A	14.1607852	2.0
5	2	4	5	1	5	E	14.0868480	−2.3

Table S11: Observed frequencies (ν_{obs}) of the ^{13}C(4) isotopologues of 2MTP. J, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.7469532	0.1
2	0	2	1	0	1	E	9.7446943	−0.2
3	0	3	2	0	2	A	13.9443347	1.3
3	0	3	2	0	2	E	13.9383947	−0.5
4	0	4	3	0	3	A	17.8136786	0.1
4	0	4	3	0	3	E	17.8064743	−1.1
5	0	5	4	0	4	A	21.6339097	1.3
5	0	5	4	0	4	E	21.6276907	−1.8
2	1	2	1	0	1	A	11.1261308	2.4
2	1	2	1	0	1	E	11.0949708	−0.5
3	1	3	2	0	2	A	14.6393781	−0.8
3	1	3	2	0	2	E	14.6177017	1.3
4	1	4	3	0	3	A	18.1061635	−1.0
4	1	4	3	0	3	E	18.0912767	−1.7
5	1	5	4	0	4	A	21.7437810	0.1
5	1	5	4	0	4	E	21.7342550	0.1
3	1	2	3	0	3	A	7.3330960	0.3
3	1	2	3	0	3	E	7.3343825	1.4
4	1	3	4	0	4	A	11.0310070	4.6
4	1	3	4	0	4	E	11.0302429	−1.5
5	1	4	5	0	5	A	15.3228958	0.4
5	1	4	5	0	5	E	15.3134914	−3.1
6	1	5	6	0	6	A	19.6657831	0.3

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
6	1	5	6	0	6	E	19.6420202	−1.0
2	0	2	1	1	1	A	7.5842810	−5.1
2	0	2	1	1	1	E	7.6454374	1.6
3	0	3	2	1	2	A	12.5651575	−0.6
3	0	3	2	1	2	E	12.5881207	2.3
4	0	4	3	1	3	A	17.1186352	2.1
4	0	4	3	1	3	E	17.1271695	−0.7
5	0	5	4	1	4	A	21.3414232	0.8
5	0	5	4	1	4	E	21.3428892	−0.4
2	1	1	1	1	0	A	11.1980632	−7.7
2	1	1	1	1	0	E	11.1657523	3.4
3	1	2	2	1	1	A	16.5463404	2.1
3	1	2	2	1	1	E	16.5364562	1.2
4	1	3	3	1	2	A	21.5115868	1.6
4	1	3	3	1	2	E	21.5023373	−1.4
2	1	2	1	1	1	A	8.9634569	−4.5
2	1	2	1	1	1	E	8.9957119	−0.8
3	1	3	2	1	2	A	13.2602037	0.1
3	1	3	2	1	2	E	13.2674238	0.2
4	1	4	3	1	3	A	17.4111176	−1.5
4	1	4	3	1	3	E	17.4119741	0.9
5	1	5	4	1	4	A	21.4512947	−0.2
5	1	5	4	1	4	E	21.4494524	0.4
2	2	1	1	1	0	A	17.6860183	3.9
2	2	1	1	1	0	E	17.2619539	2.2
2	2	1	2	1	2	A	9.8398535	−5.7
2	2	1	2	1	2	E	9.4822455	−1.8
3	2	2	3	1	3	A	11.7007817	4.7
3	2	2	3	1	3	E	11.5459381	−3.1
4	2	3	4	1	4	A	14.1856884	−4.5
5	2	4	5	1	5	A	17.2001975	−2.2
5	2	4	5	1	5	E	17.1444186	6.1

Table S12: Observed frequencies (ν_{obs}) of the ^{13}C(5) isotopologues of 2MTP. *J*, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	*J*	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.7417230	−1.7
2	0	2	1	0	1	E	9.7395648	0.3
3	0	3	2	0	2	A	13.9638420	4.6
3	0	3	2	0	2	E	13.9580817	−0.9
4	0	4	3	0	3	A	17.8517619	−2.8
4	0	4	3	0	3	E	17.8445535	−0.4
5	0	5	4	0	4	A	21.6773603	−1.6
5	0	5	4	0	4	E	21.6710040	−3.2
2	1	2	1	0	1	A	11.2011232	−0.9
2	1	2	1	0	1	E	11.1690008	−0.7
3	1	3	2	0	2	A	14.7207413	−1.9
3	1	3	2	0	2	E	14.6983654	−1.7
4	1	4	3	0	3	A	18.1805445	−1.3
4	1	4	3	0	3	E	18.1649831	0.8
5	1	5	4	0	4	A	21.8048350	0.8
5	1	5	4	0	4	E	21.7947673	0.6
3	1	2	3	0	3	A	7.2940898	−3.5
3	1	2	3	0	3	E	7.2951255	−1.9
4	1	3	4	0	4	A	10.9280457	2.9
4	1	3	4	0	4	E	10.9272484	−1.0
5	1	4	5	0	5	A	15.1988599	2.6
5	1	4	5	0	5	E	15.1901541	−2.4
6	1	5	6	0	6	A	19.5652793	0.7
2	0	2	1	1	1	E	7.5619042	2.2
3	0	3	2	1	2	A	12.5044367	−1.4
3	0	3	2	1	2	E	12.5286458	0.2
4	0	4	3	1	3	A	17.0948592	0.3
4	0	4	3	1	3	E	17.1042683	−1.2
5	0	5	4	1	4	A	21.3485818	1.0
5	0	5	4	1	4	E	21.3505783	−0.6
2	1	1	1	1	0	A	11.1568628	−2.3
2	1	1	1	1	0	E	11.1233457	2.6
3	1	2	2	1	1	A	16.5001650	−0.6
3	1	2	2	1	1	E	16.4899716	0.6
4	1	3	3	1	2	A	21.4857135	−0.7
4	1	3	3	1	2	E	21.4766750	−0.9
2	1	2	1	1	1	A	8.9579517	−3.9
2	1	2	1	1	1	E	8.9913411	2.1
3	1	3	2	1	2	A	13.2613444	0.5
3	1	3	2	1	2	E	13.2689289	−1.2
4	1	4	3	1	3	A	17.4236462	6.2
4	1	4	3	1	3	E	17.4246986	0.8
5	1	5	4	1	4	A	21.4760541	0.9

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
5	1	5	4	1	4	E	21.4743403	2.0
2	2	1	1	1	0	A	17.8863113	0.7
2	2	1	1	1	0	E	17.4478081	2.9
2	2	1	2	1	2	A	10.0278116	0.4
2	2	1	2	1	2	E	9.6582602	−3.9
3	2	2	3	1	3	A	11.8525559	3.0
3	2	2	3	1	3	E	11.6880368	0.1
4	2	3	4	1	4	A	14.2930733	2.0
4	2	3	4	1	4	E	14.2102101	0.3
5	2	4	5	1	5	A	17.2639600	−6.5
5	2	4	5	1	5	E	17.2057869	3.7

Table S13: Observed frequencies (ν_{obs}) of the ^{13}C(9) isotopologues of 2MTP. J, K_a and K_c are the quantum numbers for an asymmetric top. *Sym* is for the respective torsional A or E species. Observed minus calculated ($\nu_o - \nu_c$) values (in kHz) as obtained after a fit with the program *XIAM*.

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	0	2	1	0	1	A	9.6247952	1.3
2	0	2	1	0	1	E	9.6227892	−0.2
3	0	3	2	0	2	A	13.8202740	0.6
3	0	3	2	0	2	E	13.8148066	−0.3
4	0	4	3	0	3	A	17.6810627	0.0
4	0	4	3	0	3	E	17.6740010	−0.1
5	0	5	4	0	4	A	21.4681599	−0.7
5	0	5	4	0	4	E	21.4618164	0.1
2	1	2	1	0	1	A	11.1427421	−1.1
2	1	2	1	0	1	E	11.1101997	−6.0
3	1	3	2	0	2	A	14.6278394	0.9
3	1	3	2	0	2	E	14.6051763	2.6
4	1	4	3	0	3	E	18.0260233	4.0
5	1	5	4	0	4	A	21.6121059	0.0
5	1	5	4	0	4	E	21.6017124	2.5
4	1	3	4	0	4	A	10.7129629	1.7
4	1	3	4	0	4	E	10.7123286	7.8
5	1	4	5	0	5	A	14.9119090	−1.1
5	1	4	5	0	5	E	14.9041995	−2.0
2	0	2	1	1	1	A	7.3322625	−2.1
3	0	3	2	1	2	A	12.3023249	0.9
3	0	3	2	1	2	E	12.3273959	5.3
4	0	4	3	1	3	A	16.8734983	0.7
4	0	4	3	1	3	E	16.8836324	−1.9
5	0	5	4	1	4	A	21.1072765	−0.7
5	0	5	4	1	4	E	21.1097938	−4.3

J'	K_a'	K_c'	J	K_a	K_c	*Sym*	ν_{obs} / GHz	$\nu_o - \nu_c$
2	1	1	1	1	0	A	10.9922329	−5.6
3	1	2	2	1	1	A	16.2692213	2.5
3	1	2	2	1	1	E	16.2589401	−9.2
4	1	3	3	1	2	A	21.2140914	0.3
2	1	2	1	1	1	A	8.8502080	−6.0
3	1	3	2	1	2	A	13.1098899	0.7
3	1	3	2	1	2	E	13.1177638	6.4
4	1	4	3	1	3	A	17.2343829	2.0
4	1	4	3	1	3	E	17.2356533	0.9
5	1	5	4	1	4	A	21.2512231	0.5
5	1	5	4	1	4	E	21.2496902	−1.5
2	2	1	1	1	0	A	17.8697656	1.5
2	2	1	1	1	0	E	17.4236401	1.4
3	2	2	3	1	3	A	11.8624793	−3.9
4	2	3	4	1	4	A	14.2355208	1.8
4	2	3	4	1	4	E	14.1497478	−1.5