Supplementary Materials

Surprising torsional barrier reduction in the coupled methyl internal rotations of 2,3-dimethylfuran observed by microwave spectroscopy

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Table S-1. Nuclear coordinates in the principal axis system of 23DMF calculated at the MP2/6-311++G(d,p) and B3LYP-D3BJ/6-311++G(d,p) levels of theory. The atoms are numbered according to Figure 1.

	MP2/6-311++G(d,p)			**B3LYP-D3BJ/6-311++G(d,p)**		
	a **/ Å**	***b*** **/ Å**	***c*** **/ Å**	***a*** **/ Å**	***b*** **/ Å**	***c*** **/ Å**
O1	1.243934	0.750359	0.000106	1.220931	0.782929	0.000076
C2	−0.121685	0.689216	−0.000012	−0.147486	0.685223	0.000024
C3	−0.539327	−0.622526	−0.000007	−0.520891	−0.627249	−0.000045
C4	0.658776	−1.411778	0.000061	0.703309	−1.385482	0.000292
C5	1.706756	−0.529673	−0.000129	1.719894	−0.486910	−0.000282
H6	2.779970	−0.643824	−0.000223	2.792797	−0.573266	−0.000496
H7	0.730906	−2.491107	0.000110	0.796951	−2.460453	0.000514
C8	−1.957944	−1.117866	−0.000004	−1.917855	−1.176639	−0.000101
H9	−1.978079	−2.210539	−0.000259	−1.900409	−2.268017	−0.000422
H10	−2.504087	−0.776109	0.885041	−2.480497	−0.858278	0.882512
H11	−2.504239	−0.775691	−0.884793	−2.480661	−0.857752	−0.882418
C12	−0.849596	1.987074	−0.000030	−0.909244	1.959274	0.000029
H13	−1.926305	1.800316	−0.000017	−1.980088	1.750800	−0.000007
H14	−0.603407	2.580598	0.886427	−0.678922	2.563273	0.883421
H15	−0.603424	2.580569	−0.886514	−0.678869	2.563302	−0.883329

Table S-2a. Rotational constants of 23DMF (in MHz) predicted at various levels of theory. The differences between the calculated and the experimental values (in MHz) are given as ΔA, ΔB and ΔC. Σ is the sum of the absolute values of ΔA, ΔB and ΔC.

Method/Basis set	***A***	ΔA	***B***	ΔB	***C***	ΔC	**Σ**
B3LYP-D3/6-31G(d,p)	3570.9	18.4	3245.5	–22.7	1737.0	–1.7	42.9
B3LYP-D3/6-31+G(d,p)	3564.2	11.7	3239.9	–28.2	1733.9	–4.8	44.8
B3LYP-D3/6-31++G(d,p)	3564.2	11.7	3240.0	–28.2	1733.9	–4.8	44.7
B3LYP-D3/6-311G(d,p)	3580.7	28.2	3252.8	–15.4	1741.3	2.6	46.2
B3LYP-D3/6-311+G(d,p)	3579.8	27.3	3250.0	–18.2	1740.4	1.7	47.2
B3LYP-D3/6-311++G(d,p)	3579.8	27.3	3250.0	–18.2	1740.4	1.7	47.1
B3LYP-D3/6-311G(2d,2p)	3592.3	39.8	3260.6	–7.6	1746.1	7.4	54.8
B3LYP-D3/6-311+G(2d,2p)	3591.4	38.9	3258.0	–10.2	1745.2	6.5	55.5
B3LYP-D3/6-311++G(2d,2p)	3591.5	39.0	3257.9	–10.3	1745.2	6.5	55.7
B3LYP-D3/6-311G(df,pd)	3591.9	39.4	3262.8	–5.4	1746.8	8.1	52.9
B3LYP-D3/6-311+G(df,pd)	3589.7	37.2	3260.7	–7.5	1745.7	7.0	51.6
B3LYP-D3/6-311++G(df,pd)	3589.8	37.3	3260.7	–7.5	1745.7	7.0	51.7
B3LYP-D3/6-311G(2df,2pd)	3596.8	44.3	3265.8	–2.4	1748.6	9.9	56.6
B3LYP-D3/6-311+G(2df,2pd)	3595.3	42.8	3263.4	–4.8	1747.6	8.9	56.5
B3LYP-D3/6-311++G(2df,2pd)	3595.4	42.9	3263.4	–4.8	1747.6	8.9	56.6
B3LYP-D3/6-311G(3df,3pd)	3596.0	43.5	3267.8	–0.4	1749.1	10.4	54.2
B3LYP-D3/6-311+G(3df,3pd)	3596.9	44.4	3264.3	–3.9	1748.3	9.6	57.8
B3LYP-D3/6-311++G(3df,3pd)	3596.8	44.3	3264.3	–3.8	1748.3	9.6	57.7
B3LYP-D3/cc-pVDZ	3565.0	12.5	3236.3	–31.9	1733.4	–5.3	49.7
B3LYP-D3/aug-cc-pVDZ	3565.9	13.4	3233.7	–34.5	1732.8	–5.9	53.8
B3LYP-D3/cc-pVTZ	3594.5	42.0	3264.0	–4.2	1747.6	8.9	55.1
B3LYP-D3/aug-cc-pVTZ	3594.3	41.8	3263.2	–5.0	1747.3	8.6	55.4
B3LYP-D3BJ/6-31G(d,p)	3569.1	16.6	3247.0	–21.2	1736.9	–1.8	39.6
B3LYP-D3BJ/6-31+G(d,p)	3562.5	10.0	3241.5	–26.7	1733.9	–4.8	41.5
B3LYP-D3BJ/6-31++G(d,p)	3562.4	9.9	3241.5	–26.7	1733.9	–4.8	41.4
B3LYP-D3BJ/6-311G(d,p)	3579.8	27.3	3253.7	–14.5	1741.4	2.7	44.4
B3LYP-D3BJ/6-311+G(d,p)	3576.8	24.3	3251.7	–16.4	1740.1	1.4	42.1
B3LYP-D3BJ/6-311++G(d,p)	3576.8	24.3	3251.7	–16.4	1740.1	1.4	42.1
B3LYP-D3BJ/6-311G(2d,2p)	3590.2	37.7	3261.8	–6.4	1745.9	7.2	51.3
B3LYP-D3BJ/6-311+G(2d,2p)	3589.4	36.9	3259.2	–8.9	1745.0	6.3	52.2
B3LYP-D3BJ/6-311++G(2d,2p)	3589.5	37.0	3259.2	–9.0	1745.0	6.3	52.4
B3LYP-D3BJ/6-311G(df,pd)	3589.9	37.4	3263.9	–4.3	1746.6	7.9	49.6
B3LYP-D3BJ/6-311+G(df,pd)	3587.6	35.1	3262.0	–6.2	1745.5	6.8	48.1
B3LYP-D3BJ/6-311++G(df,pd)	3587.8	35.3	3262.0	–6.2	1745.5	6.8	48.3
B3LYP-D3BJ/6-311G(2df,2pd)	3594.7	42.1	3267.0	–1.2	1748.5	9.8	53.1
B3LYP-D3BJ/6-311+G(2df,2pd)	3593.3	40.8	3264.6	–3.6	1747.5	8.8	53.1
B3LYP-D3BJ/6-311++G(2df,2pd)	3593.3	40.8	3264.6	–3.6	1747.5	8.8	53.2
B3LYP-D3BJ/6-311G(3df,3pd)	3593.8	41.3	3269.0	0.8	1748.9	10.2	52.3

B3LYP-D3BJ/6-311+G(3df,3pd)	3594.8	42.3	3265.5	–2.7	1748.1	9.4	54.3
B3LYP-D3BJ/6-311++G(3df,3pd)	3594.7	42.2	3265.5	–2.7	1748.1	9.4	54.3
B3LYP-D3BJ/cc-pVDZ	3563.3	10.8	3237.9	–30.3	1733.4	–5.3	46.4
B3LYP-D3BJ/aug-cc-pVDZ	3564.3	11.8	3235.3	–32.9	1732.8	–5.9	50.6
B3LYP-D3BJ/cc-pVTZ	3592.4	39.9	3265.2	–3.0	1747.4	8.7	51.6
B3LYP-D3BJ/aug-cc-pVTZ	3592.2	39.7	3264.4	–3.8	1747.2	8.5	51.9
CAM-B3LYP-D3BJ/6-311G(d,p)	3604.3	51.8	3276.8	8.7	1753.8	15.0	75.5
CAM-B3LYP-D3BJ/6-311+G(d,p)	3602.4	49.9	3274.5	6.3	1752.6	13.9	70.1
CAM-B3LYP-D3BJ/6-311++G(d,p)	3602.4	49.9	3274.5	6.3	1752.6	13.9	70.1
CAM-B3LYP-D3BJ/cc-pVDZ	3587.4	34.9	3260.6	–7.6	1745.6	6.9	49.4
CAM-B3LYP-D3BJ/aug-cc-pVDZ	3589.1	36.6	3257.8	–10.4	1745.1	6.4	53.3
CAM-B3LYP-D3BJ/cc-pVTZ	3618.8	66.3	3287.3	19.1	1760.0	21.3	106.7
CAM-B3LYP-D3BJ/aug-cc-pVTZ	3618.5	66.0	3286.4	18.2	1759.7	21.0	105.2
CCSD/cc-pVDZ	3540.1	–12.4	3212.7	–55.4	1721.1	–17.6	85.5
M06-2X/6-31G(d,p)	3600.6	48.1	3262.1	–6.1	1748.8	10.1	64.3
M06-2X/6-31+G(d,p)	3593.3	40.8	3258.5	–9.7	1746.1	7.4	57.8
M06-2X/6-31++G(d,p)	3593.2	40.7	3258.6	–9.6	1746.1	7.4	57.7
M06-2X/6-311G(d,p)	3611.5	59.0	3265.2	–3.0	1752.2	13.5	75.4
M06-2X/6-311+G(d,p)	3609.1	56.6	3263.8	–4.4	1751.3	12.6	73.5
M06-2X/6-311++G(d,p)	3609.1	56.6	3263.8	–4.4	1751.3	12.6	73.5
M06-2X/6-311G(df,pd)	3620.0	67.5	3273.2	5.1	1756.4	17.7	90.3
M06-2X/6-311+G(df,pd)	3618.4	65.8	3271.8	3.6	1755.6	16.9	86.4
M06-2X/6-311++G(df,pd)	3618.4	65.9	3271.8	3.6	1755.6	16.9	86.4
M06-2X/6-311G(3df,3pd)	3625.8	73.3	3277.2	9.0	1758.8	20.1	102.4
M06-2X/6-311+G(3df,3pd)	3626.6	74.1	3274.3	6.2	1758.2	19.5	99.7
M06-2X/6-311++G(3df,3pd)	3626.5	74.0	3274.3	6.1	1758.2	19.5	99.6
M06-2X/cc-pVDZ	3594.9	42.4	3255.4	–12.8	1745.9	7.2	62.4
M06-2X/aug-cc-pVDZ	3597.9	45.4	3251.7	–16.5	1745.5	6.8	68.7
M06-2X/cc-pVTZ	3625.0	72.5	3273.7	5.6	1757.6	18.9	97.0
M06-2X/aug-cc-pVTZ	3625.7	73.2	3273.3	5.1	1757.7	19.0	97.2
M06-2X-D3/6-31G(d,p)	3600.1	47.6	3262.1	–6.0	1748.7	10.0	63.6
M06-2X-D3/6-31+G(d,p)	3592.7	40.2	3258.5	–9.6	1746.0	7.3	57.1
M06-2X-D3/6-31++G(d,p)	3592.6	40.1	3258.6	–9.6	1746.0	7.3	57.0
M06-2X-D3/6-311G(d,p)	3610.9	58.4	3265.2	–2.9	1752.1	13.4	74.7
M06-2X-D3/6-311+G(d,p)	3608.5	56.0	3263.8	–4.3	1751.1	12.4	72.8
M06-2X-D3/6-311++G(d,p)	3608.5	56.0	3263.8	–4.3	1751.1	12.4	72.8
M06-2X-D3/6-311G(2d,2p)	3623.5	71.0	3270.6	2.4	1756.4	17.7	91.1
M06-2X-D3/6-311+G(2d,2p)	3622.2	69.7	3268.8	0.6	1755.6	16.9	87.2
M06-2X-D3/6-311++G(2d,2p)	3622.3	69.8	3268.7	0.5	1755.6	16.9	87.2
M06-2X-D3/6-311G(df,pd)	3619.4	66.9	3273.3	5.1	1756.3	17.6	89.6
M06-2X-D3/6-311+G(df,pd)	3617.8	65.3	3271.8	3.6	1755.5	16.8	85.7
M06-2X-D3/6-311G(2df,2pd)	3626.2	73.7	3275.3	7.1	1758.4	19.7	100.5

M06-2X-D3/6-311+G(2df,2pd)	3624.7	72.2	3273.7	5.5	1757.5	18.8	96.5
M06-2X-D3/6-311++G(2df,2pd)	3624.7	72.2	3273.6	5.5	1757.5	18.8	96.5
M06-2X-D3/6-311G(3df,3pd)	3625.2	72.6	3277.2	9.0	1758.7	20.0	101.7
M06-2X-D3/6-311+G(3df,3pd)	3626.0	73.5	3274.4	6.2	1758.0	19.3	99.0
M06-2X-D3/6-311++G(3df,3pd)	3625.9	73.4	3274.3	6.2	1758.0	19.3	98.9
M06-2X-D3/cc-pVDZ	3594.4	41.9	3255.4	–12.8	1745.8	7.1	61.7
M06-2X-D3/aug-cc-pVDZ	3597.4	44.9	3251.7	–16.5	1745.4	6.7	68.0
M06-2X-D3/cc-pVTZ	3624.4	71.9	3273.8	5.6	1757.5	18.8	96.2
M06-2X-D3/aug-cc-pVTZ	3625.1	72.6	3273.3	5.1	1757.5	18.8	96.5
MN15/6-31G(d,p)	3599.8	47.3	3250.4	–17.8	1745.2	6.5	71.6
MN15/6-31+G(d,p)	3590.1	37.6	3246.9	–21.3	1742.0	3.3	62.3
MN15/6-31++G(d,p)	3590.2	37.7	3246.8	–21.4	1742.0	3.3	62.4
MN15/6-311G(d,p)	3615.9	63.4	3259.2	–9.0	1751.5	12.8	85.2
MN15/6-311+G(d,p)	3613.9	61.4	3257.3	–10.9	1750.5	11.7	84.1
MN15/6-311++G(d,p)	3614.2	61.7	3257.2	–11.0	1750.5	11.8	84.5
MN15/6-311G(2d,2p)	3626.1	73.6	3264.3	–3.9	1755.1	16.4	93.9
MN15/6-311+G(2d,2p)	3624.3	71.8	3262.6	–5.6	1754.2	15.5	92.9
MN15/6-311++G(2d,2p)	3624.6	72.1	3262.5	–5.7	1754.3	15.6	93.3
MN15/6-311G(df,pd)	3628.4	75.9	3269.9	1.7	1757.4	18.7	96.3
MN15/6-311+G(df,pd)	3627.1	74.6	3267.4	–0.8	1756.3	17.6	93.0
MN15/6-311G(2df,2pd)	3632.0	79.4	3268.9	0.8	1757.8	19.1	99.3
MN15/6-311+G(2df,2pd)	3629.9	77.4	3267.4	–0.8	1756.9	18.2	96.4
MN15/6-311++G(2df,2pd)	3630.2	77.7	3267.3	–0.9	1756.9	18.2	96.8
MN15/6-311G(3df,3pd)	3634.3	81.8	3271.6	3.4	1759.1	20.4	105.6
MN15/6-311+G(3df,3pd)	3634.6	82.1	3268.5	0.3	1758.3	19.6	102.0
MN15/6-311++G(3df,3pd)	3634.7	82.1	3268.5	0.3	1758.3	19.6	102.1
MN15/cc-pVDZ	3596.6	44.1	3245.0	–23.2	1743.2	4.5	71.8
MN15/aug-cc-pVDZ	3600.7	48.2	3242.3	–25.9	1743.4	4.7	78.8
MN15/cc-pVTZ	3631.8	79.3	3267.7	–0.5	1757.4	18.7	98.5
MN15/aug-cc-pVTZ	3633.0	80.5	3269.0	0.8	1758.1	19.4	100.8
MP2/6-31G(d,p)	3565.9	13.4	3257.3	–10.9	1739.0	0.3	24.6
MP2/6-31+G(d,p)	3557.7	5.2	3248.0	–20.2	1734.5	–4.2	29.7
MP2/6-31++G(d,p)	3558.4	5.9	3247.4	–20.8	1734.5	–4.2	30.8
MP2/6-311G(d,p)	3573.0	20.5	3248.0	–20.2	1738.4	–0.4	41.1
MP2/6-311+G(d,p)	3567.1	14.5	3243.9	–24.3	1735.8	–2.9	41.7
MP2/6-311++G(d,p)	3567.1	14.5	3243.9	–24.3	1735.8	–2.9	41.7
MP2/6-311G(2d,2p)	3589.4	36.9	3255.4	–12.8	1743.8	5.1	54.8
MP2/6-311+G(2d,2p)	3585.4	32.9	3252.4	–15.8	1742.1	3.4	52.0
MP2/6-311++G(2d,2p)	3585.6	33.1	3252.2	–15.9	1742.1	3.4	52.5
MP2/6-311G(df,pd)	3599.2	46.7	3268.8	0.6	1750.3	11.6	58.9
MP2/6-311+G(df,pd)	3592.9	40.4	3265.1	–3.1	1747.8	9.1	52.7
MP2/6-311++G(df,pd)	3593.4	40.9	3264.9	–3.3	1747.9	9.2	53.4
MP2/6-311G(2df,2pd)	3604.7	52.2	3272.7	4.5	1752.5	13.8	70.5

MP2/6-311+G(2df,2pd)	3600.4	47.9	3269.5	1.3	1750.6	11.9	61.1
MP2/6-311++G(2df,2pd)	3600.6	48.0	3269.4	1.2	1750.6	11.9	61.2
MP2/6-311G(3df,3pd)	3598.0	45.5	3272.0	3.8	1750.8	12.1	61.3
MP2/6-311+G(3df,3pd)	3596.9	44.4	3268.1	–0.1	1749.4	10.7	55.2
MP2/6-311++G(3df,3pd)	3596.9	44.3	3268.1	–0.1	1749.4	10.7	55.1
MP2/cc-pVDZ	3542.8	–9.7	3222.4	–45.8	1724.4	–14.3	69.8
MP2/aug-cc-pVDZ	3528.8	–23.8	3210.5	–57.7	1717.7	–21.0	102.5
MP2/cc-pVTZ	3596.3	43.8	3265.6	–2.6	1748.5	9.8	56.2
MP2/aug-cc-pVTZ	3592.9	40.4	3263.4	–4.8	1747.2	8.4	53.6
PBE0/6-31G(d,p)	3531.6	–20.9	3225.8	–42.3	1722.5	–16.2	79.5
PBE0/6-31+G(d,p)	3524.2	–28.3	3221.0	–47.2	1719.5	–19.2	94.7
PBE0/6-31++G(d,p)	3524.3	–28.2	3221.0	–47.2	1719.5	–19.2	94.6
PBE0/6-311G(d,p)	3542.7	–9.8	3234.1	–34.0	1727.5	–11.2	55.1
PBE0/6-311+G(d,p)	3540.4	–12.1	3231.8	–36.4	1726.3	–12.4	61.0
PBE0/6-311++G(d,p)	3540.5	–12.0	3231.8	–36.4	1726.3	–12.4	60.9
PBE0/6-311G(2d,2p)	3550.5	–2.0	3240.5	–27.7	1730.9	–7.8	37.5
PBE0/6-311+G(2d,2p)	3549.4	–3.1	3238.1	–30.1	1730.0	–8.7	41.8
PBE0/6-311++G(2d,2p)	3549.5	–3.0	3238.0	–30.2	1730.0	–8.7	41.8
PBE0/6-311G(df,pd)	3552.6	0.1	3243.4	–24.8	1732.4	–6.3	31.2
PBE0/6-311+G(df,pd)	3550.9	–1.6	3240.9	–27.3	1731.3	–7.4	36.3
PBE0/6-311G(2df,2pd)	3555.8	3.3	3245.1	–23.1	1733.5	–5.2	31.6
PBE0/6-311+G(2df,2pd)	3554.3	1.7	3242.8	–25.4	1732.5	–6.2	33.4
PBE0/6-311++G(2df,2pd)	3553.6	1.1	3243.2	–25.0	1732.5	–6.2	32.3
PBE0/6-311G(3df,3pd)	3555.5	3.0	3247.5	–20.7	1734.2	–4.6	28.3
PBE0/6-311+G(3df,3pd)	3556.7	4.2	3243.9	–24.3	1733.4	–5.3	33.8
PBE0/6-311++G(3df,3pd)	3556.7	4.2	3243.9	–24.3	1733.4	–5.3	33.8
PBE0/cc-pVDZ	3528.0	–24.5	3219.2	–49.0	1720.1	–18.6	92.1
PBE0/aug-cc-pVDZ	3527.7	–24.8	3216.1	–52.0	1719.1	–19.6	96.4
PBE0/cc-pVTZ	3552.6	0.1	3243.6	–24.6	1732.4	–6.3	31.1
PBE0/aug-cc-pVTZ	3552.2	–0.4	3242.9	–25.3	1732.1	–6.7	32.3
PBE0-D3/6-31G(d,p)	3537.7	–14.8	3224.1	–44.1	1723.4	–15.3	74.2
PBE0-D3/6-31+G(d,p)	3530.4	–22.1	3219.2	–48.9	1720.4	–18.3	89.4
PBE0-D3/6-31++G(d,p)	3530.4	–22.1	3219.2	–49.0	1720.4	–18.3	89.3
PBE0-D3/6-311G(d,p)	3548.8	–3.7	3232.4	–35.8	1728.4	–10.3	49.8
PBE0-D3/6-311+G(d,p)	3546.5	–6.0	3230.0	–38.2	1727.2	–11.5	55.7
PBE0-D3/6-311++G(d,p)	3546.6	–5.9	3229.9	–38.2	1727.2	–11.5	55.6
PBE0-D3/6-311G(2d,2p)	3556.6	4.1	3238.7	–29.5	1731.9	–6.8	40.4
PBE0-D3/6-311+G(2d,2p)	3555.5	3.0	3236.3	–31.9	1731.0	–7.7	42.7
PBE0-D3/6-311++G(2d,2p)	3555.6	3.1	3236.2	–32.0	1731.0	–7.7	42.8
PBE0-D3/6-311G(df,pd)	3558.7	6.1	3241.6	–26.6	1733.3	–5.4	38.1
PBE0-D3/6-311+G(df,pd)	3557.0	4.5	3239.1	–29.1	1732.2	–6.5	40.0
PBE0-D3/6-311G(2df,2pd)	3561.9	9.4	3243.3	–24.9	1734.5	–4.2	38.5
PBE0-D3/6-311+G(2df,2pd)	3560.4	7.9	3241.0	–27.2	1733.5	–5.3	40.4

PBE0-D3/6-311++G(2df,2pd)	3560.4	7.9	3240.9	–27.3	1733.5	–5.2	40.4
PBE0-D3/6-311G(3df,3pd)	3561.6	9.1	3245.7	–22.5	1735.1	–3.6	35.2
PBE0-D3/6-311+G(3df,3pd)	3562.8	10.3	3242.0	–26.1	1734.4	–4.4	40.8
PBE0-D3/6-311++G(3df,3pd)	3562.8	10.3	3242.0	–26.1	1734.3	–4.4	40.8
PBE0-D3/cc-pVDZ	3533.8	–18.7	3217.5	–50.7	1721.0	–17.7	87.0
PBE0-D3/aug-cc-pVDZ	3533.8	–18.7	3214.3	–53.8	1720.1	–18.6	91.2
PBE0-D3/cc-pVTZ	3559.4	6.9	3241.3	–26.9	1733.3	–5.4	39.1
PBE0-D3/aug-cc-pVTZ	3558.3	5.8	3241.0	–27.2	1733.0	–5.7	38.7
ωB97X-D /6-31G(d,p)	3597.1	44.6	3264.4	–3.8	1748.6	9.9	58.3
ωB97X-D /6-31+G(d,p)	3591.2	38.7	3260.6	–7.6	1746.2	7.5	53.8
ωB97X-D /6-31++G(d,p)	3591.1	38.6	3260.7	–7.5	1746.2	7.5	53.6
ωB97X-D /6-311G(d,p)	3607.1	54.6	3269.2	1.0	1752.4	13.7	69.2
ωB97X-D /6-311+G(d,p)	3607.1	54.5	3269.2	1.0	1752.3	13.6	69.2
ωB97X-D /6-311++G(d,p)	3609.4	56.9	3270.8	2.6	1753.4	14.7	74.2
ωB97X-D /6-311G(2d,2p)	3620.3	67.8	3277.4	9.3	1757.6	18.9	96.0
ωB97X-D /6-311+G(2d,2p)	3619.0	66.5	3275.5	7.3	1756.8	18.1	91.9
ωB97X-D /6-311++G(2d,2p)	3619.1	66.6	3275.4	7.3	1756.8	18.1	91.9
ωB97X-D /6-311G(df,pd)	3618.8	66.3	3280.1	11.9	1758.1	19.4	97.6
ωB97X-D /6-311+G(df,pd)	3616.9	64.4	3278.3	10.1	1757.2	18.5	93.0
ωB97X-D /6-311G(2df,2pd)	3624.1	71.6	3282.3	14.1	1759.9	21.2	106.8
ωB97X-D /6-311+G(2df,2pd)	3622.4	69.9	3280.5	12.3	1759.0	20.3	102.5
ωB97X-D /6-311++G(2df,2pd)	3622.4	69.9	3280.5	12.3	1759.0	20.3	102.5
ωB97X-D /6-311G(3df,3pd)	3623.7	71.2	3284.1	15.9	1760.3	21.6	108.7
ωB97X-D /6-311+G(3df,3pd)	3624.2	71.7	3281.4	13.2	1759.7	21.0	105.9
ωB97X-D /6-311++G(3df,3pd)	3624.1	71.6	3281.4	13.2	1759.7	21.0	105.8
ωB97X-D /cc-pVDZ	3589.2	36.7	3256.3	–11.8	1744.9	6.2	54.7
ωB97X-D /aug-cc-pVDZ	3591.5	39.0	3253.0	–15.2	1744.4	5.7	59.9
ωB97X-D /cc-pVTZ	3622.4	69.9	3281.8	13.6	1759.4	20.6	104.2
ωB97X-D /aug-cc-pVTZ	3622.9	70.4	3281.2	13.0	1759.3	20.6	104.0
Experimental	**3552.5**		**3268.2**		**1738.7**		

Table S-2b. Rotational constants of 25DMF (in MHz) predicted at various levels of theory. The differences between the calculated and the experimental values (in MHz) are given as ΔA, ΔB and ΔC. Σ is the sum of the absolute values of ΔA, ΔB and ΔC.

Method/Basis set	***A***	**Δ*A***	***B***	**Δ*B***	***C***	**Δ*C***	**Σ**
B3LYP-D3/6-31G(d,p)	6159.6	–1.1	2124.5	–6.3	1611.4	–3.6	11.0
B3LYP-D3/6-31+G(d,p)	6143.3	–17.4	2121.0	–9.8	1608.3	–6.7	33.8
B3LYP-D3/6-31++G(d,p)	6143.9	–16.8	2121.0	–9.8	1608.3	–6.7	33.3
B3LYP-D3/6-311G(d,p)	6179.8	19.1	2129.6	–1.2	1615.6	0.6	20.9
B3LYP-D3/6-311+G(d,p)	6179.8	19.1	2126.6	–4.2	1613.9	–1.1	24.4
B3LYP-D3/6-311++G(d,p)	6179.8	19.1	2126.6	–4.2	1613.9	–1.1	24.3
B3LYP-D3/6-311G(2d,2p)	6211.0	50.3	2132.7	1.9	1619.4	4.4	56.6
B3LYP-D3/6-311+G(2d,2p)	6211.9	51.2	2130.1	–0.7	1618.0	3.0	54.8
B3LYP-D3/6-311++G(2d,2p)	6212.1	51.4	2130.0	–0.8	1617.9	2.9	55.1
B3LYP-D3/6-311G(df,pd)	6202.6	41.9	2134.9	4.1	1620.1	5.1	51.1
B3LYP-D3/6-311+G(df,pd)	6202.5	41.8	2132.6	1.8	1618.8	3.8	47.4
B3LYP-D3/6-311++G(df,pd)	6202.2	41.5	2132.6	1.8	1618.9	3.9	47.2
B3LYP-D3/6-311G(2df,2pd)	6217.6	56.9	2136.2	5.4	1621.9	6.9	69.2
B3LYP-D3/6-311+G(2df,2pd)	6216.0	55.3	2134.1	3.3	1620.5	5.5	64.1
B3LYP-D3/6-311++G(2df,2pd)	6216.1	55.4	2134.0	3.2	1620.5	5.5	64.2
B3LYP-D3/6-311G(3df,3pd)	6212.8	52.1	2137.8	7.0	1622.4	7.4	66.5
B3LYP-D3/6-311+G(3df,3pd)	6216.0	55.3	2134.9	4.1	1621.0	6.0	65.4
B3LYP-D3/6-311++G(3df,3pd)	6216.0	55.3	2134.9	4.1	1621.0	6.0	65.4
B3LYP-D3/cc-pVDZ	6136.2	–24.5	2121.3	–9.5	1608.3	–6.7	40.8
B3LYP-D3/aug-cc-pVDZ	6142.1	–18.6	2117.6	–13.2	1606.5	–8.5	40.3
B3LYP-D3/cc-pVTZ	6217.1	56.4	2133.4	2.6	1620.2	5.2	64.2
B3LYP-D3/aug-cc-pVTZ	6214.8	54.1	2133.3	2.5	1620.0	5.0	61.6
B3LYP-D3BJ/6-31G(d,p)	6162.0	1.3	2124.2	–6.6	1611.3	–3.7	11.7
B3LYP-D3BJ/6-31+G(d,p)	6148.6	–12.1	2119.7	–11.1	1607.9	–7.1	30.2
B3LYP-D3BJ/6-31++G(d,p)	6149.2	–11.5	2119.7	–11.1	1608.0	–7.0	29.6
B3LYP-D3BJ/6-311G(d,p)	6184.9	24.2	2128.1	–2.7	1615.1	0.1	27.0
B3LYP-D3BJ/6-311+G(d,p)	6185.0	24.3	2125.2	–5.6	1613.5	–1.5	31.5
B3LYP-D3BJ/6-311++G(d,p)	6184.9	24.2	2125.2	–5.6	1613.5	–1.5	31.4
B3LYP-D3BJ/6-311G(2d,2p)	6213.4	52.7	2132.0	1.2	1619.1	4.1	58.1
B3LYP-D3BJ/6-311+G(2d,2p)	6216.9	56.2	2128.6	–2.2	1617.4	2.4	60.8
B3LYP-D3BJ/6-311++G(2d,2p)	6217.2	56.5	2128.5	–2.3	1617.4	2.4	61.1
B3LYP-D3BJ/6-311G(df,pd)	6207.5	46.8	2133.2	2.4	1619.5	4.5	53.7
B3LYP-D3BJ/6-311+G(df,pd)	6207.5	46.8	2131.0	0.2	1618.3	3.3	50.3
B3LYP-D3BJ/6-311++G(df,pd)	6207.3	46.6	2131.1	0.3	1618.3	3.3	50.2
B3LYP-D3BJ/6-311G(2df,2pd)	6222.4	61.7	2134.6	3.8	1621.2	6.2	71.7
B3LYP-D3BJ/6-311+G(2df,2pd)	6221.0	60.3	2132.5	1.7	1619.9	4.9	66.9
B3LYP-D3BJ/6-311++G(2df,2pd)	6221.1	60.4	2132.4	1.6	1619.9	4.9	67.0
B3LYP-D3BJ/6-311G(3df,3pd)	6217.5	56.8	2136.1	5.3	1621.8	6.8	68.9

B3LYP-D3BJ/6-311+G(3df,3pd)	6221.0	60.3	2133.3	2.5	1620.4	5.4	68.1
B3LYP-D3BJ/6-311++G(3df,3pd)	6221.0	60.3	2133.3	2.5	1620.4	5.4	68.2
B3LYP-D3BJ/cc-pVDZ	6141.2	–19.5	2120.0	–10.8	1607.9	–7.1	37.4
B3LYP-D3BJ/aug-cc-pVDZ	6147.6	–13.1	2116.3	–14.5	1606.2	–8.8	36.4
B3LYP-D3BJ/cc-pVTZ	6219.5	58.8	2132.8	2.0	1620.0	5.0	65.7
B3LYP-D3BJ/aug-cc-pVTZ	6219.8	59.1	2131.7	0.9	1619.4	4.4	64.5
CAM-B3LYP-D3BJ/6-31G(d,p)	6203.4	42.7	2140.2	9.4	1623.3	8.3	60.4
CAM-B3LYP-D3BJ/6-31+G(d,p)	6186.5	25.8	2137.1	6.3	1620.5	5.5	37.6
CAM-B3LYP-D3BJ/6-31++G(d,p)	6187.0	26.3	2137.1	6.3	1620.5	5.5	38.1
CAM-B3LYP-D3BJ/6-311G(d,p)	6226.3	65.6	2144.5	13.7	1627.3	12.3	91.6
CAM-B3LYP-D3BJ/6-311+G(d,p)	6223.7	63.0	2142.7	11.9	1626.2	11.2	86.1
CAM-B3LYP-D3BJ/6-311++G(d,p)	6223.7	63.0	2142.7	11.9	1626.2	11.2	86.1
CAM-B3LYP-D3BJ/6-311G(2d,2p)	6257.4	96.7	2148.2	17.4	1631.4	16.4	130.5
CAM-B3LYP-D3BJ/6-311+G(2d,2p)	6257.5	96.8	2145.9	15.1	1630.1	15.1	127.0
CAM-B3LYP-D3BJ/6-311++G(2d,2p)	6258.4	97.7	2145.8	15.0	1630.1	15.1	127.8
CAM-B3LYP-D3BJ/6-311G(df,pd)	6246.5	85.8	2150.3	19.5	1632.0	17.0	122.3
CAM-B3LYP-D3BJ/6-311+G(df,pd)	6248.8	88.1	2147.2	16.4	1630.4	15.4	119.9
CAM-B3LYP-D3BJ/6-311++G(df,pd)	6248.6	87.9	2147.3	16.5	1630.4	15.4	119.8
CAM-B3LYP-D3BJ/6-311G(2df,2pd)	6263.7	103.0	2151.3	20.5	1633.7	18.7	142.2
CAM-B3LYP-D3BJ/6-311+G(2df,2pd)	6264.1	103.4	2148.4	17.6	1632.0	17.0	138.0
CAM-B3LYP-D3BJ/6-311++G(2df,2pd)	6264.4	103.7	2148.3	17.5	1632.0	17.0	138.2
CAM- B3LYP-D3BJ/6-311G(3df,3pd)	6258.6	97.9	2152.9	22.1	1634.2	19.2	139.2
CAM- B3LYP-D3BJ/6-311+G(3df,3pd)	6263.6	102.9	2149.2	18.4	1632.5	17.5	138.8
CAM- B3LYP-D3BJ/6-311++G(3df,3pd)	6263.6	102.9	2149.2	18.4	1632.5	17.5	138.8
CAM-B3LYP-D3BJ/cc-pVDZ	6180.3	19.6	2137.0	6.2	1620.3	5.3	31.1
CAM-B3LYP-D3BJ/aug-cc-pVDZ	6186.7	26.0	2133.6	2.8	1618.7	3.7	32.5
CAM-B3LYP-D3BJ/cc-pVTZ	6263.0	102.3	2148.6	17.8	1632.1	17.1	137.2
CAM-B3LYP-D3BJ/aug-cc-pVTZ	6263.3	102.6	2147.6	16.8	1631.5	16.5	135.9
CCSD/cc-pVDZ	6076.8	–83.9	2112.8	–18.0	1599.6	–15.4	117.2
M06-2X/6-31G(d,p)	6186.6	25.9	2141.4	10.6	1622.9	7.9	44.4
M06-2X/6-31+G(d,p)	6171.5	10.8	2138.6	7.8	1620.4	5.4	24.0
M06-2X/6-31++G(d,p)	6171.8	11.1	2138.6	7.8	1620.4	5.4	24.4
M06-2X/6-311G(d,p)	6205.9	45.2	2144.2	13.4	1625.8	10.8	69.4
M06-2X/6-311+G(d,p)	6203.3	42.6	2142.4	11.6	1624.7	9.7	63.8
M06-2X/6-311++G(d,p)	6203.4	42.7	2142.4	11.6	1624.6	9.6	63.9
M06-2X/6-311G(2d,2p)	6237.4	76.7	2146.8	16.0	1629.3	14.3	106.9
M06-2X/6-311+G(2d,2p)	6238.1	77.4	2144.3	13.5	1628.0	13.0	103.9
M06-2X/6-311++G(2d,2p)	6235.8	75.1	2145.3	14.5	1628.4	13.4	102.9
M06-2X/6-311G(df,pd)	6222.2	61.5	2149.0	18.2	1629.6	14.6	94.3
M06-2X/6-311+G(df,pd)	6222.4	61.7	2146.9	16.1	1628.5	13.5	91.4
M06-2X/6-311++G(df,pd)	6222.2	61.5	2147.0	16.2	1628.5	13.5	91.2
M06-2X/6-311G(2df,2pd)	6240.8	80.1	2149.8	19.0	1631.3	16.3	115.4
M06-2X/6-311+G(2df,2pd)	6240.3	79.6	2147.6	16.8	1630.0	15.0	111.4

M06-2X/6-311++G(2df,2pd)	6240.5	79.8	2147.6	16.8	1630.0	15.0	111.5
M06-2X/6-311G(3df,3pd)	6235.8	75.1	2151.3	20.5	1631.8	16.8	112.4
M06-2X/6-311+G(3df,3pd)	6239.6	78.9	2148.4	17.6	1630.4	15.4	111.8
M06-2X/6-311++G(3df,3pd)	6239.5	78.8	2148.4	17.6	1630.4	15.4	111.7
M06-2X/cc-pVDZ	6166.8	6.1	2139.5	8.7	1620.8	5.8	20.7
M06-2X/aug-cc-pVDZ	6175.0	14.3	2134.9	4.1	1618.7	3.7	22.0
M06-2X/cc-pVTZ	6239.2	78.5	2147.3	16.5	1629.8	14.8	109.8
M06-2X/aug-cc-pVTZ	6242.0	81.3	2146.5	15.7	1629.5	14.5	111.5
MN15/6-31G(d,p)	6187.1	26.4	2132.5	1.7	1617.8	2.8	30.9
MN15/6-31+G(d,p)	6169.4	8.7	2129.6	–1.2	1615.1	0.1	10.0
MN15/6-31++G(d,p)	6170.0	9.3	2129.5	–1.3	1615.1	0.1	10.7
MN15/6-311G(d,p)	6213.9	53.2	2139.4	8.6	1623.6	8.6	70.4
MN15/6-311+G(d,p)	6210.9	50.2	2137.6	6.8	1622.4	7.4	64.3
MN15/6-311++G(d,p)	6211.2	50.5	2137.6	6.8	1622.4	7.4	64.6
MN15/6-311G(2d,2p)	6235.5	74.8	2142.7	11.9	1626.8	11.8	98.6
MN15/6-311+G(2d,2p)	6235.0	74.3	2140.3	9.5	1625.4	10.4	94.3
MN15/6-311++G(2d,2p)	6235.5	74.8	2140.2	9.4	1625.4	10.4	94.6
MN15/6-311G(df,pd)	6237.5	76.8	2145.6	14.8	1628.7	13.7	105.3
MN15/6-311+G(df,pd)	6237.4	76.7	2143.2	12.4	1627.3	12.3	101.3
MN15/6-311++G(df,pd)	6237.2	76.5	2143.2	12.4	1627.3	12.3	101.2
MN15/6-311G(2df,2pd)	6242.9	82.2	2146.0	15.2	1629.2	14.2	111.5
MN15/6-311+G(2df,2pd)	6241.6	80.9	2143.7	12.9	1627.8	12.8	106.6
MN15/6-311++G(2df,2pd)	6241.9	81.2	2143.7	12.9	1627.8	12.8	106.9
MN15/6-311G(3df,3pd)	6246.1	85.4	2147.5	16.7	1630.2	15.2	117.3
MN15/6-311+G(3df,3pd)	6249.9	89.2	2144.1	13.3	1628.6	13.6	116.1
MN15/6-311++G(3df,3pd)	6249.8	89.1	2144.2	13.4	1628.6	13.6	116.1
MN15/cc-pVDZ	6168.1	7.4	2132.5	1.7	1616.8	1.8	10.9
MN15/aug-cc-pVDZ	6176.7	16.0	2128.9	–1.9	1615.4	0.4	18.3
MN15/cc-pVTZ	6246.1	85.4	2143.3	12.5	1627.9	12.9	110.7
MN15/aug-cc-pVTZ	6246.8	86.1	2144.4	13.6	1628.6	13.6	113.3
MP2/6-31G(d,p)	6128.8	–31.9	2132.4	1.6	1613.6	–1.4	34.9
MP2/6-31+G(d,p)	6113.4	–47.3	2125.8	–5.0	1608.9	–6.1	58.4
MP2/6-31++G(d,p)	6114.4	–46.3	2125.6	–5.2	1608.9	–6.1	57.6
MP2/6-311G(d,p)	6118.5	–42.2	2133.2	2.4	1613.7	–1.3	46.0
MP2/6-311+G(d,p)	6112.5	–48.2	2129.3	–1.5	1611.1	–3.9	53.6
MP2/6-311++G(d,p)	6112.5	–48.2	2129.2	–1.6	1611.0	–4.0	53.7
MP2/6-311G(2d,2p)	6162.4	1.7	2134.7	3.9	1617.1	2.1	7.8
MP2/6-311+G(2d,2p)	6162.0	1.3	2131.1	0.3	1615.0	0.0	1.6
MP2/6-311++G(2d,2p)	6162.4	1.7	2131.0	0.2	1615.1	0.1	2.0
MP2/6-311G(df,pd)	6163.2	2.5	2147.8	17.0	1625.0	10.0	29.6
MP2/6-311+G(df,pd)	6157.1	–3.6	2143.5	12.7	1622.2	7.2	23.5
MP2/6-311++G(df,pd)	6156.8	–3.9	2143.5	12.7	1622.1	7.1	23.8
MP2/6-311G(2df,2pd)	6181.2	20.5	2148.2	17.4	1626.2	11.2	49.1

MP2/6-311+G(2df,2pd)	6178.4	17.7	2144.0	13.2	1623.7	8.7	39.6
MP2/6-311++G(2df,2pd)	6178.2	17.5	2144.0	13.2	1623.7	8.7	39.5
MP2/6-311G(3df,3pd)	6159.2	–1.5	2149.3	18.5	1625.4	10.4	30.4
MP2/6-311+G(3df,3pd)	6162.9	2.2	2144.6	13.8	1623.0	8.0	24.0
MP2/6-311++G(3df,3pd)	6162.7	2.0	2144.7	13.9	1623.0	8.0	23.9
MP2/cc-pVDZ	6057.3	–103.4	2118.6	–12.2	1601.5	–13.5	129.2
MP2/aug-cc-pVDZ	6041.5	–119.2	2105.6	–25.2	1593.0	–22.0	166.5
MP2/cc-pVTZ	6171.0	10.3	2141.6	10.8	1621.8	6.8	27.8
MP2/aug-cc-pVTZ	6159.5	–1.2	2140.1	9.3	1620.2	5.2	15.8
PBE0/6-31G(d,p)	6189.6	28.9	2143.9	13.1	1624.5	9.5	51.5
PBE0/6-31+G(d,p)	6178.0	17.3	2140.6	9.8	1622.0	7.0	34.1
PBE0/6-31++G(d,p)	6178.2	17.5	2140.7	9.9	1622.0	7.0	34.3
PBE0/6-311G(d,p)	6211.8	51.1	2148.7	17.9	1628.8	13.8	82.7
PBE0/6-311+G(d,p)	6210.9	50.2	2146.3	15.5	1627.4	12.4	78.0
PBE0/6-311++G(d,p)	6210.6	49.9	2146.3	15.5	1627.4	12.4	77.7
PBE0/6-311G(2d,2p)	6237.5	76.8	2151.9	21.1	1632.3	17.3	115.1
PBE0/6-311+G(2d,2p)	6240.1	79.4	2148.8	18.0	1630.7	15.7	113.1
PBE0/6-311++G(2d,2p)	6237.3	76.6	2149.6	18.8	1631.0	16.0	111.4
PBE0/6-311G(df,pd)	6227.3	66.6	2154.2	23.4	1633.0	18.0	107.9
PBE0/6-311+G(df,pd)	6229.0	68.3	2151.3	20.5	1631.5	16.5	105.2
PBE0/6-311++G(df,pd)	6228.6	67.9	2151.3	20.5	1631.5	16.5	104.9
PBE0/6-311G(2df,2pd)	6243.1	82.4	2154.7	23.9	1634.3	19.3	125.7
PBE0/6-311+G(2df,2pd)	6243.7	83.0	2151.9	21.1	1632.7	17.7	121.9
PBE0/6-311++G(2df,2pd)	6243.9	83.2	2151.9	21.1	1632.7	17.7	122.0
PBE0/6-311G(3df,3pd)	6236.9	76.2	2156.4	25.6	1634.8	19.8	121.6
PBE0/6-311+G(3df,3pd)	6242.6	81.9	2152.9	22.1	1633.2	18.2	122.1
PBE0/6-311++G(3df,3pd)	6242.6	81.9	2152.8	22.0	1633.2	18.2	122.2
PBE0/cc-pVDZ	6172.2	11.5	2142.1	11.3	1622.7	7.7	30.5
PBE0/aug-cc-pVDZ	6177.7	17.0	2136.6	5.8	1619.9	4.9	27.7
PBE0/cc-pVTZ	6240.6	79.9	2151.6	20.8	1632.4	17.4	118.1
PBE0/aug-cc-pVTZ	6241.0	80.3	2150.7	19.9	1631.9	16.9	117.1
ωB97X-D/6-31G(d,p)	6196.6	35.9	2139.5	8.7	1622.5	7.5	52.1
ωB97X-D/6-31+G(d,p)	6181.1	20.4	2137.7	6.9	1620.5	5.5	32.8
ωB97X-D/6-31++G(d,p)	6181.4	20.7	2137.7	6.9	1620.6	5.6	33.1
ωB97X-D/6-311G(d,p)	6219.3	58.6	2144.1	13.3	1626.8	11.8	83.7
ωB97X-D/6-311+G(d,p)	6216.9	56.2	2142.2	11.4	1625.5	10.5	78.1
ωB97X-D/6-311++G(d,p)	6216.8	56.1	2142.2	11.4	1625.5	10.5	78.0
ωB97X-D/6-311G(2d,2p)	6247.8	87.1	2147.4	16.6	1630.4	15.4	119.2
ωB97X-D/6-311+G(2d,2p)	6248.6	87.9	2144.9	14.1	1629.1	14.1	116.1
ωB97X-D/6-311++G(2d,2p)	6246.4	85.7	2145.9	15.1	1629.5	14.5	115.2
ωB97X-D/6-311G(df,pd)	6237.5	76.8	2149.6	18.8	1631.1	16.1	111.7
ωB97X-D/6-311+G(df,pd)	6237.6	76.9	2147.3	16.5	1629.8	14.8	108.2
ωB97X-D/6-311++G(df,pd)	6237.3	76.6	2147.4	16.6	1629.8	14.8	108.0

ωB97X-D/6-311G(2df,2pd)	6254.4	93.7	2150.4	19.6	1632.6	17.6	130.9
ωB97X-D/6-311+G(2df,2pd)	6253.4	92.7	2148.2	17.4	1631.3	16.3	126.3
ωB97X-D/6-311++G(2df,2pd)	6253.6	92.9	2148.2	17.4	1631.2	16.2	126.5
ωB97X-D/6-311G(3df,3pd)	6249.2	88.5	2152.1	21.3	1633.2	18.2	128.1
ωB97X-D/6-311+G(3df,3pd)	6252.7	92.0	2149.3	18.5	1631.9	16.9	127.4
ωB97X-D/6-311++G(3df,3pd)	6252.8	92.1	2149.3	18.5	1631.8	16.8	127.4
ωB97X-D/cc-pVDZ	6174.9	14.2	2136.4	5.6	1619.6	4.6	24.5
ωB97X-D/aug-cc-pVDZ	6180.5	19.8	2132.4	1.6	1617.7	2.7	24.1
ωB97X-D/cc-pVTZ	6253.7	93.0	2148.8	18.0	1631.6	16.6	127.6
ωB97X-D/aug-cc-pVTZ	6254.4	93.7	2148.1	17.3	1631.3	16.3	127.4
Experimental	**6160.7**		**2130.8**		**1615.0**		

Table S-3. Coefficients of Fourier expansion for the one-dimensional potential energy curves of 23DMF given in Figure 2 calculated at the B3LYP-D3BJ/6-311++G(d,p) and MP2/6-311++G(d,p) levels of theory. The potential is expanded as $V(\alpha) = \sum_{i=0}^{n} a_i f_i$.

	B3LYP-D3BJ/6-311++G(d,p)			
	2-Me		**3-Me**	
f_i	a_i / Hartree	a_i / cm^{-1}	ai / Hartree	a_i / cm^{-1}
1	–308.7687900		–308.7689020	
cos(3α)	–0.000634845	–139.3	0.000511936	112.4
cos(6α)	0.000040516	8.9	0.000028873	6.3
cos(9α)	–0.000004116	–0.9	0.000003487	0.8

	MP2/6-311++G(d,p)			
	2-Me		**3-Me**	
f_i	a_i / Hartree	a_i / cm^{-1}	a_i / Hartree	a_i / cm^{-1}
1	–307.8391596		–307.8392166	
cos(3α)	–0.000538787	–118.3	0.000400957	88.0
cos(6α)	0.000165559	36.3	0.000096843	21.3
cos(9α)			0.000035251	7.7
cos(12α)	0.000012299	2.7	–0.000013924	3.1
cos(15α)	–0.000026088	–5.7	–0.000016006	3.5
sin(3α)	–0.000011470	–2.5	0.000056708	12.4
sin(6α)	0.000021587	4.7	0.000027179	6.0
sin(9α)	–0.000022940	5.0	–0.000029066	–6.5
sin(12α)	0.000021587	4.7	–0.000025735	–5.6
sin(15α)	–0.000011470	2.5		

Table S-4. Coefficients of Fourier expansion for the two-dimensional potential energy curves of 23DMF given in Figure 3 calculated at the B3LYP-D3BJ/6-311++G(d,p) and MP2/6-311++G(d,p) levels of theory. The potential is expanded as $V(\alpha) = \sum_{i=0}^{n} a_i f_i$.

		B3LYP-D3BJ		**MP2**	
i	f_i	a_i / Hartree	a_i / cm^{-1}	a_i / Hartree	a_i / cm^{-1}
0	1	–308.7472860		–307.8388284	
1	cos(3α_1)	–0.000455361	–99.9	–0.000360726	–79.2
2	cos(3α_2)	–0.000575129	–126.2	–0.000496203	–108.9
3	cos(6α_1)	0.000021623	4.7	0.000057630	12.6
4	cos(6α_2)	0.000031669	7.0	0.000119520	26.2
5	cos(3α_1)cos(3α_2)	–0.000066875	–14.7	–0.000043560	–9.6
6	sin(3α_1)sin(3α_2)	0.000112630	24.7		

Table S-5. Observed frequencies (ν_{obs}) of 23DMF. The $\nu_{obs} - \nu_{calc}$ residuals are obtained with the *XIAM* program.

J''	K_a''	K_c''	J'	K_a'	K_c'	Species	$\nu_{obs.}$	$\nu_{obs.} - \nu_{calc.}$
Upper level			Lower level				MHz	*XIAM* / kHz
1	0	1	0	0	0	(00)	5007.7056	0.1
1	0	1	0	0	0	(01)	5007.0709	3.8
1	0	1	0	0	0	(10)	5006.3497	–5.7
1	0	1	0	0	0	(11)	5004.9383	0.6
1	0	1	0	0	0	(12)	5006.5130	2.1
2	0	2	1	0	1	(00)	8734.6061	0.3
2	0	2	1	0	1	(01)	8731.5693	–2.3
2	0	2	1	0	1	(10)	8734.3046	–3.8
2	0	2	1	0	1	(11)	8732.0179	–2.7
2	0	2	1	0	1	(12)	8730.5238	0.3
2	0	2	1	1	1	(00)	8448.8540	1.2
2	0	2	1	1	1	(01)	8452.2120	7.4
2	0	2	1	1	1	(10)	8447.6841	–4.8
2	0	2	1	1	1	(11)	8449.3678	0.7
2	0	2	1	1	1	(12)	8452.7408	2.1
2	1	2	1	0	1	(00)	8771.0139	0.4
2	1	2	1	0	1	(01)	8766.8892	–4.3
2	1	2	1	0	1	(10)	8770.9331	0.5
2	1	2	1	0	1	(11)	8767.8768	–3.6
2	1	2	1	0	1	(12)	8765.7244	–4.0
2	1	1	1	1	0	(00)	11545.5514	3.1
2	1	1	1	1	0	(01)	11541.0427	8.8
2	1	1	1	1	0	(10)	11541.4622	–2.2
2	1	1	1	1	0	(11)	11535.8461	3.0
2	1	1	1	1	0	(12)	11538.0994	6.2
2	1	2	1	1	1	(00)	8485.2612	0.6
2	1	2	1	1	1	(01)	8487.5318	5.4
2	1	2	1	1	1	(10)	8484.3075	–5.5
2	1	2	1	1	1	(11)	8485.2268	–0.2
2	1	2	1	1	1	(12)	8487.9443	0.6
2	2	0	1	1	1	(00)	15213.7471	7.2
2	2	0	1	1	1	(01)	15226.3413	–7.0
2	2	0	1	1	1	(10)	15212.3393	6.5
2	2	0	1	1	1	(11)	15218.8536	–4.8
2	2	0	1	1	1	(12)	15230.9914	–6.2
2	2	1	1	1	0	(00)	12402.7955	1.5
2	2	1	1	1	0	(01)	12375.0302	–14.7
2	2	1	1	1	0	(10)	12400.7607	–17.1
2	2	1	1	1	0	(11)	12380.0449	–1.3

2	2	1	1	1	0	(12)	12366.0049	–3.7
2	1	1	2	0	2	(00)	4626.8373	–4.2
2	1	1	2	0	2	(01)	4627.0705	8.1
2	1	1	2	0	2	(10)	4623.7699	0.4
2	1	1	2	0	2	(11)	4622.0581	2.1
2	1	1	2	0	2	(12)	4625.9565	4.7
2	1	1	2	1	2	(00)	4590.4422	8.5
2	1	1	2	1	2	(10)	4587.1451	–0.2
2	1	1	2	1	2	(11)	4586.1999	3.8
2	1	1	2	1	2	(12)	4590.7526	5.7
2	2	1	2	0	2	(00)	5484.0897	2.4
2	2	1	2	0	2	(01)	5461.0591	–14.2
2	2	1	2	0	2	(10)	5483.0793	–3.5
2	2	1	2	0	2	(11)	5466.2567	–2.6
2	2	1	2	0	2	(12)	5453.8621	–5.1
2	2	1	2	1	2	(00)	5447.6672	–12.3
2	2	1	2	1	2	(10)	5446.4526	–6.1
2	2	1	2	1	2	(11)	5430.3971	–2.2
2	2	1	2	1	2	(12)	5418.6587	–3.5
3	0	3	2	0	2	(00)	12117.7028	4.1
3	0	3	2	0	2	(01)	12115.7690	3.8
3	0	3	2	0	2	(10)	12117.1817	–3.9
3	0	3	2	0	2	(11)	12115.3963	–2.7
3	0	3	2	0	2	(12)	12115.0982	–2.7
3	0	3	2	1	2	(00)	12081.2954	4.5
3	0	3	2	1	2	(01)	12080.4489	5.5
3	0	3	2	1	2	(10)	12080.5571	–4.3
3	0	3	2	1	2	(11)	12079.5373	–1.8
3	0	3	2	1	2	(12)	12079.8946	–1.4
3	1	3	2	0	2	(00)	12120.6303	3.7
3	1	3	2	0	2	(01)	12118.5841	3.9
3	1	3	2	0	2	(10)	12120.1341	–4.5
3	1	3	2	0	2	(11)	12118.2628	–2.4
3	1	3	2	0	2	(12)	12117.9100	–3.0
3	1	2	2	1	1	(00)	15702.0590	–1.2
3	1	2	2	1	1	(01)	15694.5858	–3.2
3	1	2	2	1	1	(10)	15700.5406	–6.3
3	1	2	2	1	1	(11)	15694.3881	–3.3
3	1	2	2	1	1	(12)	15691.7631	–4.4
3	1	3	2	1	2	(00)	12084.2237	4.8
3	1	3	2	1	2	(01)	12083.2634	5.1
3	1	3	2	1	2	(10)	12083.5112	–3.2
3	1	3	2	1	2	(11)	12082.4034	–1.9
3	1	3	2	1	2	(12)	12082.7063	–1.8
3	2	2	2	1	1	(00)	15880.3260	–7.4

3	2	2	2	1	1	(01)	15867.5387	–8.4
3	2	2	2	1	1	(10)	15879.8328	–8.6
3	2	2	2	1	1	(11)	15869.9290	–5.5
3	2	2	2	1	1	(12)	15864.1213	–7.6
3	2	1	2	2	0	(00)	17928.4892	5.5
3	2	1	2	2	0	(01)	17915.8294	5.4
3	2	1	2	2	0	(10)	17921.3404	2.4
3	2	1	2	2	0	(11)	17910.2164	6.3
3	2	1	2	2	0	(12)	17907.2531	12.1
3	2	2	2	2	1	(00)	15023.0937	6.1
3	2	2	2	2	1	(01)	15033.5503	14.3
3	2	2	2	2	1	(10)	15020.5274	–0.5
3	2	2	2	2	1	(11)	15025.7309	–0.4
3	2	2	2	2	1	(12)	15036.2154	1.9
3	3	0	2	2	1	(00)	21893.3969	9.8
3	3	0	2	2	1	(10)	21892.6824	11.5
3	3	1	2	2	0	(00)	19640.0102	2.1
3	3	1	2	2	0	(01)	19566.5849	–27.8
3	3	1	2	2	0	(10)	19635.4850	–26.4
3	3	1	2	2	0	(11)	19583.7755	11.2
3	3	1	2	2	0	(12)	19541.0555	9.7
3	1	2	3	0	3	(01)	8205.8771	–9.0
3	1	2	3	0	3	(10)	8207.1260	–4.8
3	1	2	3	0	3	(11)	8201.0500	1.7
3	1	2	3	0	3	(12)	8202.6217	3.4
3	1	2	3	1	3	(00)	8208.2769	1.8
3	1	2	3	1	3	(01)	8203.0739	2.8
3	1	2	3	1	3	(10)	8204.1768	–1.1
3	1	2	3	1	3	(11)	8198.1838	1.7
3	1	2	3	1	3	(12)	8199.8096	3.3
3	2	2	3	0	3	(00)	8389.4743	–1.8
3	2	2	3	0	3	(01)	8378.8421	–2.1
3	2	2	3	0	3	(10)	8386.4237	–1.5
3	2	2	3	0	3	(11)	8376.5913	–0.2
3	2	2	3	0	3	(12)	8374.9796	–0.1
3	2	2	3	1	3	(00)	8386.5473	–0.9
3	2	2	3	1	3	(01)	8376.0256	–3.6
3	2	2	3	1	3	(10)	8383.4695	–2.7
3	2	2	3	1	3	(11)	8373.7246	–0.7
3	2	2	3	1	3	(12)	8372.1685	0.8
3	2	1	3	2	2	(00)	4186.1912	–4.8
3	2	1	3	2	2	(01)	4195.3545	–3.9
3	2	1	3	2	2	(10)	4182.3771	5.9
3	2	1	3	2	2	(11)	4187.7137	2.7
3	2	1	3	2	2	(12)	4195.4261	7.0

4	0	4	3	0	3	(00)	15579.0114	5.7
4	0	4	3	0	3	(01)	15577.4576	6.2
4	0	4	3	0	3	(10)	15578.3870	–4.9
4	0	4	3	0	3	(11)	15576.8461	–2.9
4	0	4	3	0	3	(12)	15576.8237	–2.7
4	0	4	3	1	3	(00)	15576.0880	10.3
4	0	4	3	1	3	(01)	15574.6352	–1.2
4	0	4	3	1	3	(10)	15575.4348	–4.1
4	0	4	3	1	3	(11)	15573.9881	5.4
4	0	4	3	1	3	(12)	15574.0171	2.8
4	1	4	3	0	3	(00)	15579.2017	1.0
4	1	4	3	0	3	(01)	15577.6448	7.6
4	1	4	3	0	3	(10)	15578.5824	–6.7
4	1	4	3	0	3	(11)	15577.0342	–4.5
4	1	4	3	0	3	(12)	15577.0086	–3.9
4	1	3	3	1	2	(00)	19000.8980	5.5
4	1	3	3	1	2	(01)	18994.3387	3.3
4	1	3	3	1	2	(10)	18999.5276	–6.5
4	1	3	3	1	2	(11)	18993.6658	–3.3
4	1	3	3	1	2	(12)	18992.2620	–4.0
4	1	4	3	1	3	(00)	15576.2785	5.7
4	1	4	3	1	3	(01)	15574.8284	6.2
4	1	4	3	1	3	(10)	15575.6311	–5.0
4	1	4	3	1	3	(11)	15574.1695	–2.9
4	1	4	3	1	3	(12)	15574.1969	–3.5
4	1	3	3	2	2	(00)	18822.6267	7.3
4	1	3	3	2	2	(01)	18821.3851	7.9
4	1	3	3	2	2	(10)	18820.2357	–3.9
4	1	3	3	2	2	(11)	18818.1247	–1.2
4	1	3	3	2	2	(12)	18819.9039	–0.7
4	2	3	3	1	2	(00)	19021.2014	4.9
4	2	3	3	1	2	(01)	19013.8612	1.9
4	2	3	3	1	2	(10)	19020.0036	–6.5
4	2	3	3	1	2	(11)	19013.5438	–2.1
4	2	3	3	1	2	(12)	19011.7646	–4.2
4	2	2	3	2	1	(00)	22625.1514	1.6
4	2	2	3	2	1	(01)	22614.0141	–1.5
4	2	2	3	2	1	(10)	22621.3457	–13.0
4	2	2	3	2	1	(11)	22611.1627	–4.6
4	2	2	3	2	1	(12)	22609.3290	–5.0
4	2	3	3	2	2	(00)	18842.9315	8.1
4	2	3	3	2	2	(01)	18840.9077	6.5
4	2	3	3	2	2	(10)	18840.7127	–3.1
4	2	3	3	2	2	(11)	18838.0010	–1.6
4	2	3	3	2	2	(12)	18839.4065	–1.0

4	3	1	3	3	0	(00)	24120.9007	11.7
4	3	1	3	3	0	(01)	24088.7909	–16.9
4	3	1	3	3	0	(10)	24110.3379	–6.6
4	3	1	3	3	0	(11)	24089.3759	9.2
4	3	1	3	3	0	(12)	24067.8721	20.9
4	3	2	3	3	1	(00)	21424.9761	7.6
4	3	2	3	3	1	(01)	21459.2873	14.1
4	3	2	3	3	1	(10)	21421.2473	3.3
4	3	2	3	3	1	(11)	21440.8154	–5.3
4	3	2	3	3	1	(12)	21469.7021	–2.3
4	1	3	4	1	4	(00)	11632.8992	4.3
4	1	3	4	1	4	(01)	11622.5745	–9.8
4	1	3	4	1	4	(10)	11628.0716	–4.1
4	1	3	4	1	4	(11)	11617.6802	1.5
4	1	3	4	1	4	(12)	11617.8742	2.3
4	2	3	4	0	4	(00)	11653.3982	4.4
4	2	3	4	0	4	(01)	11642.2843	–9.7
4	2	3	4	0	4	(10)	11648.7447	–4.4
4	2	3	4	0	4	(11)	11637.7464	1.1
4	2	3	4	0	4	(12)	11637.5630	2.2
4	2	2	4	1	3	(00)	7988.7320	5.6
4	2	2	4	1	3	(01)	7987.9883	–8.4
4	2	2	4	1	3	(10)	7983.4855	–4.9
4	2	2	4	1	3	(11)	7980.7511	–1.2
4	2	2	4	1	3	(12)	7984.8495	1.0
4	2	3	4	1	4	(00)	11653.2040	5.2
4	2	3	4	1	4	(01)	11642.1068	–1.3
4	2	3	4	1	4	(10)	11648.5496	–2.3
4	2	3	4	1	4	(11)	11637.5569	1.4
4	2	3	4	1	4	(12)	11637.3752	0.4
4	2	2	4	2	3	(00)	7968.4271	4.7
4	2	2	4	2	3	(01)	7968.4736	0.8
4	2	2	4	2	3	(10)	7963.0102	–4.1
4	2	2	4	2	3	(11)	7960.8748	–0.7
4	2	2	4	2	3	(12)	7965.3485	2.9
4	3	2	4	1	3	(00)	8500.0670	–2.4
4	3	2	4	1	3	(01)	8484.0370	–6.1
4	3	2	4	1	3	(10)	8497.5407	–8.2
4	3	2	4	1	3	(12)	8479.0263	2.5
5	0	5	4	0	4	(00)	19055.0201	7.6
5	0	5	4	0	4	(01)	19053.4954	7.3
5	0	5	4	0	4	(10)	19054.3789	–5.5
5	0	5	4	0	4	(11)	19052.8560	–4.1
5	0	5	4	0	4	(12)	19052.8560	–4.9
5	0	5	4	1	4	(00)	19054.8341	16.6

5	0	5	4	1	4	(01)	19053.3212	19.0
5	0	5	4	1	4	(10)	19054.1920	4.8
5	0	5	4	1	4	(11)	19052.6820	11.6
5	0	5	4	1	4	(12)	19052.6820	7.2
5	1	5	4	0	4	(00)	19055.0201	–4.1
5	1	5	4	0	4	(01)	19053.4954	–3.8
5	1	5	4	0	4	(10)	19054.3790	–17.4
5	1	5	4	0	4	(11)	19052.8560	–15.5
5	1	5	4	0	4	(12)	19052.8560	–16.0
5	1	4	4	1	3	(00)	22402.4259	8.8
5	1	4	4	1	3	(01)	22397.5450	7.6
5	1	4	4	1	3	(10)	22400.6252	–6.2
5	1	4	4	1	3	(11)	22395.8391	–3.5
5	1	4	4	1	3	(12)	22395.6551	–2.4
5	1	5	4	1	4	(00)	19054.8339	4.7
5	1	5	4	1	4	(01)	19053.3214	8.1
5	1	5	4	1	4	(10)	19054.1920	–7.1
5	1	5	4	1	4	(11)	19052.6789	–2.9
5	1	5	4	1	4	(12)	19052.6820	–4.0
5	2	4	4	1	3	(10)	22402.3953	0.5
5	2	4	4	1	3	(11)	22397.5378	–1.7
5	2	4	4	2	3	(00)	22383.8656	8.4
5	2	4	4	2	3	(01)	22379.6825	6.8
5	2	4	4	2	3	(10)	22381.9130	–5.6
5	2	4	4	2	3	(11)	22377.6614	–1.3
5	2	4	4	2	3	(12)	22377.8168	–2.2
5	1	4	5	1	5	(00)	14980.4873	4.6
5	1	4	5	1	5	(01)	14966.7994	–9.0
5	1	4	5	1	5	(10)	14974.5059	–2.0
5	1	4	5	1	5	(11)	14960.8416	2.0
5	1	4	5	1	5	(12)	14960.8460	2.5
5	2	4	5	0	5	(00)	14982.2443	5.8
5	2	4	5	0	5	(01)	14968.4776	–4.0
5	2	4	5	0	5	(10)	14976.2805	–2.8
5	2	4	5	0	5	(11)	14962.5497	1.9
5	2	4	5	0	5	(12)	14962.5241	5.1
5	2	3	5	1	4	(00)	11558.5238	0.7
5	2	3	5	1	4	(01)	11549.9626	–7.9
5	2	3	5	1	4	(10)	11553.1976	–4.0
5	2	3	5	1	4	(11)	11544.2579	–0.4
5	2	4	5	1	5	(00)	14982.2223	–4.5
5	2	4	5	1	5	(01)	14968.4733	2.8
5	2	4	5	1	5	(10)	14976.2771	5.6
5	2	4	5	1	5	(11)	14962.5322	–4.3
5	2	4	5	1	5	(12)	14962.5079	0.1

5	2	3	5	2	4	(00)	11556.7784	–0.6
5	2	3	5	2	4	(01)	11548.3042	–4.2
5	2	3	5	2	4	(10)	11551.4338	–4.3
5	2	3	5	2	4	(11)	11542.5638	2.5
5	2	3	5	2	4	(12)	11543.4249	2.7
5	3	3	5	1	4	(00)	11638.2343	5.0
5	3	3	5	1	4	(01)	11626.6344	–4.4
5	3	3	5	1	4	(10)	11633.5693	–2.0
5	3	3	5	1	4	(11)	11622.2942	0.2
5	3	3	5	1	4	(12)	11621.6704	3.8
5	3	2	5	3	3	(00)	7549.5896	–20.8
5	3	2	5	3	3	(01)	7558.2846	–23.5
5	3	2	5	3	3	(10)	7542.3639	–15.7
5	3	2	5	3	3	(11)	7546.8626	–17.8
5	3	2	5	3	3	(12)	7555.4144	–11.1
5	4	2	5	2	3	(00)	8737.5919	12.8
5	4	2	5	2	3	(01)	8709.1625	1.6
5	4	2	5	2	3	(10)	8736.1727	4.6
5	4	2	5	2	3	(11)	8713.9808	14.6
5	4	2	5	2	3	(12)	8701.3945	16.3
6	0	6	5	0	5	(00)	22532.3670	8.7
6	0	6	5	0	5	(01)	22530.8385	9.7
6	0	6	5	0	5	(10)	22531.7221	–6.7
6	0	6	5	0	5	(11)	22530.1958	–3.1
6	0	6	5	0	5	(12)	22530.1958	–4.9
6	0	6	5	1	5	(00)	22532.3534	6.9
6	0	6	5	1	5	(01)	22530.8253	7.6
6	0	6	5	1	5	(10)	22531.7074	–9.5
6	0	6	5	1	5	(11)	22530.1829	–4.7
6	0	6	5	1	5	(12)	22530.1829	–6.7
6	1	6	5	0	5	(00)	22532.3670	8.1
6	1	6	5	0	5	(01)	22530.8385	9.1
6	1	6	5	0	5	(10)	22531.7221	–7.4
6	1	6	5	0	5	(11)	22530.1958	–3.8
6	1	6	5	0	5	(12)	22530.1958	–5.6
6	1	6	5	1	5	(00)	22532.3534	6.2
6	1	6	5	1	5	(01)	22530.8253	6.9
6	1	6	5	1	5	(10)	22531.7074	–10.2
6	1	6	5	1	5	(11)	22530.1829	–5.3
6	1	6	5	1	5	(12)	22530.1829	–7.4
6	1	5	6	1	6	(00)	18317.2160	5.5
6	1	5	6	1	6	(10)	18309.9881	3.4
6	1	5	6	1	6	(11)	18293.2707	9.5
6	1	5	6	1	6	(12)	18293.2512	3.8
6	2	5	6	0	6	(00)	18317.3453	5.7

6	2	5	6	0	6	(10)	18310.1194	3.8
6	2	5	6	0	6	(11)	18293.3947	8.7
6	2	5	6	0	6	(12)	18293.3745	4.7
6	2	4	6	1	5	(00)	14943.6044	6.5
6	2	4	6	1	5	(01)	14930.6350	–1.5
6	2	4	6	1	5	(10)	14937.4175	–1.1
6	2	4	6	1	5	(11)	14924.4261	10.8
6	2	4	6	1	5	(12)	14924.5315	6.6
6	2	4	6	2	5	(00)	14943.4697	0.2
6	2	4	6	2	5	(01)	14930.5116	–3.6
6	2	4	6	2	5	(10)	14937.2874	–1.0
6	2	4	6	2	5	(11)	14924.2955	4.3
6	2	4	6	2	5	(12)	14924.4077	4.6
6	3	4	6	1	5	(00)	14952.2294	5.2
6	3	4	6	1	5	(01)	14938.8542	–5.5
6	3	4	6	1	5	(10)	14946.1364	–3.4
6	3	4	6	1	5	(11)	14932.8121	3.1
6	3	4	6	1	5	(12)	14932.7655	6.5
6	3	3	6	3	4	(00)	11397.7347	–8.7
6	3	3	6	3	4	(01)	11393.4213	–17.6
6	3	3	6	3	4	(10)	11391.2911	–13.6
6	3	3	6	3	4	(11)	11385.8074	–10.7
6	3	3	6	3	4	(12)	11388.2822	–8.4
6	4	3	6	2	4	(00)	11637.5803	1.2
6	4	3	6	2	4	(01)	11624.1764	–3.0
6	4	3	6	2	4	(10)	11633.0977	0.8
6	4	3	6	2	4	(11)	11620.6150	5.2
6	4	3	6	2	4	(12)	11618.7615	7.2