Supplementary Materials

Revealing internal rotation and ^{14}N nuclear quadrupole coupling in the atmospheric pollutant 4-methyl-2-nitrophenol: interplay of microwave spectroscopy and quantum chemical calculations

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Table S1. Nuclear coordinates in the inertial principal axis system for conformer 4MNP-1 calculated using the MP2, B3LYP-D3BJ and B3PW91 methods with the 6-311++G(d,p) basis set. The atom numbers correspond to Figure 1.

	MP2			B3LYP-D3BJ			B3PW91		
	a **/ Å**	***b*** **/ Å**	***c*** **/ Å**	***a*** **/ Å**	***b*** **/ Å**	***c*** **/ Å**	***a*** **/ Å**	***b*** **/ Å**	***c*** **/ Å**
C1	0.300712	1.231849	–0.026556	0.298163	1.230874	0.000002	0.302240	1.229639	0.000002
C2	0.381686	–0.174675	0.038264	0.382630	–0.177752	0.000050	0.382488	–0.178122	0.000006
C3	–0.766623	–0.981366	0.016070	–0.770294	–0.977537	0.000086	–0.769920	–0.974955	0.000006
C4	–2.035602	–0.407149	0.019758	–2.029266	–0.408915	0.000028	–2.028288	–0.406630	0.000004
C5	–2.124004	0.998978	–0.032945	–2.111135	0.998758	–0.000088	–2.105697	0.999838	–0.000002
C6	–0.986917	1.797329	–0.027739	–0.985977	1.797353	–0.000126	–0.980463	1.796080	–0.000005
O7	1.349566	2.077662	–0.035666	1.348043	2.058792	0.000105	1.351759	2.049029	0.000001
N8	1.680139	–0.844664	0.001435	1.670324	–0.842283	–0.000015	1.665805	–0.842371	0.000000
C9	–3.279737	–1.258803	0.046078	–3.278570	–1.251263	0.000058	–3.275339	–1.245967	0.000000
O10	2.697743	–0.140663	0.140485	2.695836	–0.130642	0.000011	2.685683	–0.132570	0.000008
O11	1.714719	–2.063899	–0.137112	1.714357	–2.061423	–0.000108	1.709205	–2.055780	–0.000012
H12	2.149477	1.521524	0.008605	2.156146	1.501313	0.000085	2.152525	1.479089	0.000001
H13	–0.639153	–2.058722	0.039934	–0.639830	–2.051025	0.000130	–0.638254	–2.050239	0.000010
H14	–3.039484	–2.310310	–0.129992	–3.037589	–2.315178	0.000676	–3.036506	–2.311062	0.000020
H15	–3.781521	–1.182899	1.016517	–3.893104	–1.044612	0.881182	–3.890672	–1.040287	0.881620
H16	–3.987479	–0.934995	–0.722808	–3.892533	–1.045529	–0.881687	–3.890643	–1.040315	–0.881647
H17	–3.103135	1.473432	–0.043698	–3.088298	1.470359	–0.000203	–3.082437	1.475595	–0.000002
H18	–1.057834	2.880448	–0.068070	–1.058297	2.877468	–0.000227	–1.052648	2.877583	–0.000011

Table S2. Coefficients of the one-dimensional Fourier expansion for the potential energy curves of 4MNP-1 corresponding to Figure S1 calculated at the MP2/6-311++G(d,p) and B3LYP-D3BJ/6-311++G(d,p) levels of theory. The potential is expanded as $V(\alpha) = \sum_{i=0}^{n} a_i \; f_i$.

		MP2		B3LYP-D3BJ	
i	**f_i**	**a_i / Hartree**	**a_i / cm^{-1}**	**a_i / Hartree**	**a_i / cm^{-1}**
0	1	−549.977643082		−551.489572611	
1	cos(3α)	−0.000197646	43.4	−0.000268241	58.9
2	cos(6α)	0.000047188	10.4	0.000009863	2.2
3	sin(3α)	0.000032343	7.1	/	/

Figure S1. Potential energy curve of 4MNP-1 obtained at the B3LYP-D3BJ/6-311++G(d,p) (black) and MP2/6-311++G(d,p) (blue) levels of theory by varying the dihedral angle α = ∠(C3,C4,C9,H14), corresponding to a rotation of the methyl group about the C4-C9 bond.

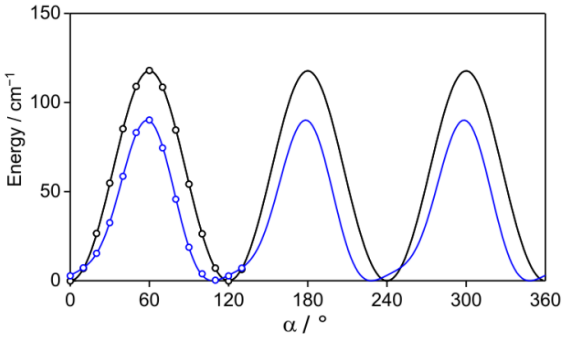

Table S3. First eigenvalues (in cm^{-1}) after diagonalization of the one-dimensional (E_{1D}) and two-dimensional (E_{2D}) potentials of Figure 2. All listed E_{2D} levels correspond to excitations of the methyl group torsion.

Level	E_{1D}	E_{2D}	Level	E_{1D}	E_{2D}
0	33.24	304.66	10	195.51	465.21
1	34.05	305.55	11	253.79	523.63
2	34.05	305.55	12	254.08	523.88
3	89.14	358.89	13	323.72	593.62
4	89.14	358.89	14	323.72	593.62
5	100.09	370.77	15	404.58	674.54
6	123.26	392.19	16	404.58	674.54
7	148.99	418.51	17	496.40	766.42
8	148.99	418.51	18	496.40	766.42
9	195.51	465.21			

The one-dimensional levels were obtained by the diagonalization of the V_3 potential whereas the two-dimensional levels involved the diagonalization of the Schrödinger equation with a potential of the type:

$$V(\phi_1,\phi_2) = a_0 + a_3(\phi_1) + \sum_{k=1}^{6} b_k \cos(k\phi_2) + \sum_{k=1}^{6} c_{3,k} \cos(3\phi_1)\cos(k\phi_2) + \sum_{k=1}^{6} d_{3,k} \sin(3\phi_1)\sin(k\phi_2) \quad \text{(S1)}$$

Table S4. Coefficients of the Fourier series of equation S1.

a_0	3159.0
a_3	19.19
b_1	1776.1
b_2	–1197.1
b_3	120.08
b_4	–20.38
b_5	–8.88
b_6	1.25
$c_{3,1}$	–19.44
$c_{3,2}$	13.67
$c_{3,3}$	–3.79
$c_{3,4}$	1.75
$c_{3,5}$	0.23
$c_{3,6}$	–2.06
$d_{3,1}$	1.36
$d_{3,2}$	–8.37
$d_{3,3}$	–0.081
$d_{3,4}$	–1.32
$d_{3,5}$	–0.89
$d_{3,6}$	–1.59

Table S5. Observed frequencies (ν_{obs}) of the A and E species of 4MNP-1. The $\nu_{obs} - \nu_{calc}$ residuals are obtained with the *XIAM* and *BELGI-C_s-hyperfine* programs.

J	K_a	K_c	F	J	K_a	K_c	F	*Species*	νobs	νobs − νcalc	νobs − νcalc
Upper level				Lower level					/ MHz	*XIAM*/ kHz	*BELGI*/ kHz
2	0	2	2	1	0	1	2	A	3040.9781	1.7	–1
2	0	2	1	1	0	1	0	A	3041.0739	1.6	–1
2	0	2	2	1	0	1	1	A	3041.2236	3.0	2
2	0	2	3	1	0	1	2	A	3041.2749	1.4	0
2	0	2	2	1	0	1	2	E	3027.1453	–9.9	–1
2	0	2	2	1	0	1	1	E	3027.3654	–28.2	1
2	0	2	3	1	0	1	2	E	3027.4484	1.5	1
2	1	1	2	1	1	0	1	A	3418.7926	16.4	12
2	1	1	3	1	1	0	2	A	3419.0219	3.0	0
2	1	1	1	1	1	0	0	A	3419.4051	0.7	–1
2	1	1	2	1	1	0	1	E	3316.6403	17.3	2
2	1	1	3	1	1	0	2	E	3316.8156	1.8	2
2	1	1	1	1	1	0	0	E	3317.0695	–22.5	0
2	1	2	2	1	1	1	2	A	2796.9410	1.2	2
2	1	2	2	1	1	1	1	A	2796.9598	–1.4	–2
2	1	2	3	1	1	1	2	A	2797.2258	1.5	2
2	1	2	1	1	1	1	0	A	2797.3462	–4.1	–1
2	1	2	1	1	1	1	1	A	2797.4047	0.9	0
2	1	2	2	1	1	1	1	E	2896.5013	–21.2	–2
2	1	2	3	1	1	1	2	E	2896.8367	0.0	–4
2	1	2	1	1	1	1	1	E	2896.8913	–32.8	–5
2	1	2	1	1	1	1	0	E	2897.1141	49.8	5
3	0	3	3	2	0	2	3	A	4412.6220	1.2	–1
3	0	3	3	2	0	2	2	A	4412.9153	–2.5	–3
3	0	3	2	2	0	2	1	A	4412.9384	3.6	2
3	0	3	4	2	0	2	3	A	4412.9756	0.0	–1
3	0	3	2	2	0	2	2	A	4413.3951	–1.8	–1
3	0	3	3	2	0	2	3	E	4404.1628	–6.6	–1
3	0	3	3	2	0	2	2	E	4404.4676	6.5	2
3	0	3	2	2	0	2	1	E	4404.4782	–3.0	1
3	0	3	4	2	0	2	3	E	4404.5172	–3.2	–3
3	0	3	2	2	0	2	2	E	4404.9464	11.5	0
3	1	2	3	2	1	1	2	A	5081.0913	4.6	0
3	1	2	4	2	1	1	3	A	5081.1113	–56.1	–2
3	1	2	2	2	1	1	1	A	5081.2045	4.2	0
3	1	2	3	2	1	1	2	E	5018.7405	3.7	1
3	1	2	4	2	1	1	3	E	5018.8011	2.6	–1
3	1	2	2	2	1	1	1	E	5018.8331	14.7	10
3	1	3	3	2	1	2	3	A	4157.3121	–0.4	0
3	1	3	3	2	1	2	2	A	4157.5965	–0.6	0
3	1	3	4	2	1	2	3	A	4157.6860	0.4	2
3	1	3	2	2	1	2	2	A	4158.0992	–1.5	0

3	1	3	3	2	1	2	3	E	4197.9070	1.5	0
3	1	3	3	2	1	2	2	E	4198.1602	–3.5	1
3	1	3	4	2	1	2	3	E	4198.2708	1.2	0
3	1	3	2	2	1	2	2	E	4198.6504	–4.8	0
3	2	1	3	2	2	0	2	A	4911.1013	7.6	4
3	2	1	4	2	2	0	3	A	4911.3156	8.4	7
3	2	1	2	2	2	0	1	A	4911.4477	4.8	4
3	2	1	4	2	2	0	2	E	4792.2381	3.7	–12
3	2	1	3	2	2	0	2	E	4792.2959	13.2	4
3	2	1	2	2	2	0	1	E	4792.6468	–3.3	4
3	2	2	3	2	2	1	2	A	4661.9065	3.0	0
3	2	2	4	2	2	1	3	A	4662.1713	6.3	5
3	2	2	2	2	2	1	1	A	4662.3088	–1.6	–2
3	2	2	3	2	2	1	2	E	4791.2494	–4.5	–1
3	2	2	4	2	2	1	3	E	4791.5085	9.6	4
3	2	2	2	2	2	1	1	E	4791.6417	–0.6	–13
4	0	4	4	3	0	3	4	A	5677.0971	0.1	–1
4	0	4	4	3	0	3	3	A	5677.4441	–7.8	–8
4	0	4	3	3	0	3	2	A	5677.4957	10.1	9
4	0	4	5	3	0	3	4	A	5677.5114	6.5	6
4	0	4	3	3	0	3	3	A	5677.9632	–1.5	–1
4	0	4	4	3	0	3	4	E	5672.1561	–3.3	–1
4	0	4	4	3	0	3	3	E	5672.5121	1.7	–1
4	0	4	3	3	0	3	2	E	5672.5442	–2.1	–1
4	0	4	5	3	0	3	4	E	5672.5643	–0.6	0
4	0	4	3	3	0	3	3	E	5673.0254	5.3	0
4	1	3	4	3	1	2	3	A	6673.8627	2.7	–1
4	1	3	5	3	1	2	4	A	6673.9164	3.1	–1
4	1	3	3	3	1	2	2	A	6673.9266	5.0	1
4	1	3	4	3	1	2	3	E	6624.8384	6.2	4
4	1	3	5	3	1	2	4	E	6624.8816	4.0	0
4	1	3	3	3	1	2	2	E	6624.8879	5.1	1
4	1	4	4	3	1	3	4	A	5483.4649	0.4	2
4	1	4	4	3	1	3	3	A	5483.8380	0.5	2
4	1	4	5	3	1	3	4	A	5483.8859	–1.1	0
4	1	4	3	3	1	3	3	A	5484.3673	–1.4	1
4	1	4	4	3	1	3	4	E	5498.2813	–1.2	0
4	1	4	4	3	1	3	3	E	5498.6457	–0.8	1
4	1	4	3	3	1	3	2	E	5498.6802	–1.0	0
4	1	4	5	3	1	3	4	E	5498.6997	–1.3	0
4	1	4	3	3	1	3	3	E	5499.1721	–0.6	1
4	2	2	4	3	2	1	3	A	6701.1152	–5.4	–9
4	2	2	5	3	2	1	4	A	6701.2006	6.7	4
4	2	2	3	3	2	1	2	A	6701.2263	5.7	3
4	2	2	4	3	2	1	3	E	6527.4763	–2.8	–9
4	2	2	5	3	2	1	4	E	6527.5547	6.0	5
4	2	2	3	3	2	1	2	E	6527.5863	15.2	16
4	2	3	4	3	2	2	3	A	6163.4830	0.8	–1

4	2	3	5	3	2	2	4	A	6163.6044	2.3	1
4	2	3	3	3	2	2	2	A	6163.6332	0.2	0
4	2	3	5	3	2	2	4	E	6346.8323	2.7	–2
4	3	1	4	3	3	0	3	A	6380.0359	1.9	–1
4	3	1	5	3	3	0	4	A	6380.2628	11.3	10
4	3	1	3	3	3	0	2	A	6380.3368	–3.4	–4
5	0	5	5	4	0	4	5	A	6893.7557	–0.2	–1
5	0	5	5	4	0	4	4	A	6894.1645	0.7	1
5	0	5	4	4	0	4	3	A	6894.1894	–2.4	–2
5	0	5	6	4	0	4	5	A	6894.2049	–0.2	0
5	0	5	4	4	0	4	4	A	6894.7019	–2.7	–2
5	0	5	5	4	0	4	5	E	6890.1574	–2.6	–1
5	0	5	5	4	0	4	4	E	6890.5655	0.0	–1
5	0	5	4	4	0	4	3	E	6890.5898	–4.8	–4
5	0	5	6	4	0	4	5	E	6890.6064	–1.3	–1
5	0	5	4	4	0	4	4	E	6891.1060	1.6	–1
5	1	4	5	4	1	3	4	A	8158.9412	2.5	–1
5	1	4	6	4	1	3	5	A	8158.9911	1.6	–2
5	1	4	4	4	1	3	3	A	8158.9959	2.0	–2
5	1	4	5	4	1	3	4	E	8123.4494	2.0	0
5	1	4	6	4	1	3	5	E	8123.4961	1.9	–1
5	1	4	4	4	1	3	3	E	8123.4961	–1.4	–4
5	1	5	5	4	1	4	5	A	6778.5709	–4.2	–3
5	1	5	6	4	1	4	5	A	6779.0149	–17.0	–15
5	1	5	4	4	1	4	4	A	6779.5413	–6.2	–4
5	1	5	5	4	1	4	4	E	6784.1612	–1.6	0
5	1	5	6	4	1	4	5	E	6784.1973	–1.6	0
5	1	5	4	4	1	4	4	E	6784.7101	0.0	1
5	2	3	5	4	2	2	4	A	8489.9893	2.9	0
5	2	3	6	4	2	2	5	A	8490.0247	1.8	–1
5	2	3	4	4	2	2	3	A	8490.0346	3.7	1
5	2	3	5	4	2	2	4	E	8346.9344	10.6	6
5	2	3	6	4	2	2	5	E	8346.9490	1.8	–1
5	2	3	4	4	2	2	3	E	8346.9490	–1.8	–4
5	2	4	5	4	2	3	4	A	7622.2239	–0.3	0
5	2	4	6	4	2	3	5	A	7622.2969	0.7	1
5	2	4	4	4	2	3	3	A	7622.3108	6.3	6
5	2	4	5	4	2	3	4	E	7755.6592	–2.1	–1
5	2	4	6	4	2	3	5	E	7755.7498	1.4	–1
5	2	4	4	4	2	3	3	E	7755.7674	6.1	3
5	3	2	5	4	3	1	4	A	8094.5379	3.0	1
5	3	2	6	4	3	1	5	A	8094.6333	1.2	1
5	3	2	4	4	3	1	3	A	8094.6527	–6.4	–7
5	3	2	5	4	3	1	4	E	7993.8461	0.3	–2
5	3	2	6	4	3	1	5	E	7993.9530	0.2	2
5	3	2	4	4	3	1	3	E	7993.9714	–9.9	–8
5	3	3	5	4	3	2	4	A	7920.0503	3.2	2
5	3	3	6	4	3	2	5	A	7920.1670	1.3	0

5	3	3	4	4	3	2	3	A	7920.1956	–0.7	–1
5	3	3	5	4	3	2	4	E	8028.4663	6.7	5
5	3	3	6	4	3	2	5	E	8028.5750	7.1	2
5	3	3	4	4	3	2	3	E	8028.6038	6.9	1
5	4	1	5	4	4	0	4	A	7926.1737	4.4	1
5	4	1	6	4	4	0	5	A	7926.3785	5.3	4
5	4	1	4	4	4	0	3	A	7926.4507	14.7	14
5	4	1	5	4	4	0	4	E	7912.3163	0.5	–2
5	4	1	6	4	4	0	5	E	7912.5143	–6.7	–5
5	4	1	4	4	4	0	3	E	7912.5784	–5.6	–2
5	4	2	5	4	4	1	4	A	7917.9245	6.7	4
5	4	2	6	4	4	1	5	A	7918.1280	4.8	3
5	4	2	4	4	4	1	3	A	7918.1985	12.2	11
5	4	2	5	4	4	1	4	E	7929.4577	5.5	2
6	0	6	6	5	0	5	5	A	8109.4255	–1.3	0
6	0	6	5	5	0	5	4	A	8109.4438	–2.8	–2
6	0	6	7	5	0	5	6	A	8109.4584	1.3	2
6	0	6	6	5	0	5	5	E	8106.6738	–0.6	0
6	0	6	5	5	0	5	4	E	8106.6933	–1.5	–1
6	0	6	7	5	0	5	6	E	8106.7061	0.9	2
6	1	5	6	5	1	4	5	A	9509.9805	2.8	0
6	1	5	7	5	1	4	6	A	9510.0340	3.5	0
6	1	5	5	5	1	4	4	A	9510.0340	0.2	–3
6	1	5	6	5	1	4	5	E	9489.4463	1.5	–1
6	1	5	7	5	1	4	6	E	9489.4993	3.1	1
6	1	5	5	5	1	4	4	E	9489.4993	0.1	–1
6	1	6	6	5	1	5	5	A	8051.0889	–2.0	0
6	1	6	5	5	1	5	4	A	8051.1030	–2.5	–1
6	1	6	7	5	1	5	6	A	8051.1168	–0.2	2
6	1	6	6	5	1	5	5	E	8052.3795	–1.3	1
6	1	6	5	5	1	5	4	E	8052.3932	–3.2	–1
6	1	6	7	5	1	5	6	E	8052.4072	–0.5	1
6	2	4	6	5	2	3	5	A	10211.7823	0.6	–2
6	2	4	7	5	2	3	6	A	10211.8121	1.5	–1
6	2	4	5	5	2	3	4	A	10211.8121	–2.5	–5
6	2	4	6	5	2	3	5	E	10109.9390	3.1	1
6	2	4	7	5	2	3	6	E	10109.9600	3.3	1
6	2	4	5	5	2	3	4	E	10109.9600	1.4	–1
6	2	5	6	5	2	4	5	A	9032.7385	0.0	2
6	2	5	7	5	2	4	6	A	9032.7911	1.1	3
6	2	5	5	5	2	4	4	A	9032.7911	–1.0	1
6	2	5	6	5	2	4	5	E	9096.7785	–1.2	1
6	2	5	7	5	2	4	6	E	9096.8404	0.7	2
6	2	5	5	5	2	4	4	E	9096.8404	–3.3	–3
6	3	3	6	5	3	2	5	A	9899.7747	0.6	2
6	3	3	7	5	3	2	6	A	9899.8145	–1.8	0
6	3	3	5	5	3	2	4	A	9899.8244	–0.3	1
6	3	3	6	5	3	2	5	E	9712.9566	0.1	0

6	3	3	7	5	3	2	6	E	9713.0015	–4.3	–1
6	3	3	5	5	3	2	4	E	9713.0108	–4.0	–1
6	3	4	6	5	3	3	5	A	9494.2856	2.1	2
6	3	4	7	5	3	3	6	A	9494.3579	2.0	3
6	3	4	5	5	3	3	4	A	9494.3743	6.1	7
6	3	4	6	5	3	3	5	E	9694.9451	3.9	3
6	3	4	7	5	3	3	6	E	9695.0117	4.9	2
6	3	4	5	5	3	3	4	E	9695.0270	8.4	5
6	4	2	6	5	4	1	5	A	9576.2218	1.4	1
6	4	2	7	5	4	1	6	A	9576.3330	–0.2	0
6	4	2	5	5	4	1	4	A	9576.3587	–0.4	0
6	4	2	6	5	4	1	5	E	9542.7489	–4.4	–3
6	4	2	7	5	4	1	6	E	9542.8636	–5.5	–2
6	4	2	5	5	4	1	4	E	9542.8860	–9.3	–5
6	4	3	6	5	4	2	5	A	9540.4916	1.6	1
6	4	3	7	5	4	2	6	A	9540.6046	–2.8	–3
6	4	3	5	5	4	2	4	A	9540.6309	–3.1	–3
6	4	3	6	5	4	2	5	E	9573.1121	10.3	7
6	4	3	7	5	4	2	6	E	9573.2125	–3.7	–9
6	4	3	5	5	4	2	4	E	9573.2356	–6.7	–13
6	5	1	6	5	5	0	5	A	9495.3807	0.9	–2
6	5	1	7	5	5	0	6	A	9495.5674	1.2	0
6	5	1	5	5	5	0	4	A	9495.6094	–3.2	–4
6	5	2	6	5	5	1	5	E	9499.6290	9.7	4
6	5	2	7	5	5	1	6	E	9499.8208	15.4	7
6	5	2	5	5	5	1	4	E	9499.8623	10.5	2
7	0	7	7	6	0	6	6	A	9335.4858	–2.3	–2
7	0	7	6	6	0	6	5	A	9335.5012	–1.0	0
7	0	7	8	6	0	6	7	A	9335.5114	0.7	1
7	0	7	7	6	0	6	6	E	9333.2957	–2.1	–2
7	0	7	6	6	0	6	5	E	9333.3113	–0.9	0
7	0	7	8	6	0	6	7	E	9333.3217	1.0	2
7	1	6	7	6	1	5	6	A	10747.1221	0.0	–1
7	1	6	8	6	1	5	7	A	10747.1731	0.4	–1
7	1	6	6	6	1	5	5	A	10747.1731	–1.6	–3
7	1	6	7	6	1	5	6	E	10735.1906	–0.7	–3
7	1	6	8	6	1	5	7	E	10735.2423	0.4	0
7	1	6	6	6	1	5	5	E	10735.2423	–1.6	–2
7	1	7	7	6	1	6	6	A	9308.7110	–2.3	–1
7	1	7	6	6	1	6	5	A	9308.7238	–1.2	0
7	1	7	8	6	1	6	7	A	9308.7342	0.3	2
7	1	7	7	6	1	6	6	E	9308.3353	–2.5	–1
7	1	7	6	6	1	6	5	E	9308.3493	–0.7	1
7	1	7	8	6	1	6	7	E	9308.3600	1.2	3
7	2	5	7	6	2	4	6	A	11826.4375	–3.0	–4
7	2	5	8	6	2	4	7	A	11826.4680	–3.6	–5
7	2	5	6	6	2	4	5	A	11826.4680	–6.7	–8
7	2	5	7	6	2	4	6	E	11747.4375	–2.8	–1

7	2	5	8	6	2	4	7	E	11747.4649	–1.3	–1
7	2	5	6	6	2	4	5	E	11747.4649	–3.5	–3
7	2	6	7	6	2	5	6	A	10395.1520	0.2	4
7	2	6	8	6	2	5	7	A	10395.1924	–0.5	3
7	2	6	6	6	2	5	5	A	10395.1924	–0.4	3
7	2	6	7	6	2	5	6	E	10421.1487	–1.6	3
7	2	6	8	6	2	5	7	E	10421.1939	–0.9	3
7	2	6	6	6	2	5	5	E	10421.1939	–1.5	2
7	3	4	7	6	3	3	6	A	11765.1705	–6.1	–2
7	3	4	8	6	3	3	7	A	11765.1915	–4.0	1
7	3	4	6	6	3	3	5	A	11765.1915	–6.6	–2
7	3	4	7	6	3	3	6	E	11541.8692	–4.4	–2
7	3	4	8	6	3	3	7	E	11541.8870	–2.0	2
7	3	4	6	6	3	3	5	E	11541.8870	–3.4	1
7	3	5	7	6	3	4	6	A	11032.9521	–1.1	2
7	3	5	8	6	3	4	7	A	11033.0006	–3.5	0
7	3	5	6	6	3	4	5	A	11033.0085	–1.2	2
7	3	5	7	6	3	4	6	E	11264.5671	–2.2	1
7	3	5	8	6	3	4	7	E	11264.6246	–0.7	0
7	3	5	6	6	3	4	5	E	11264.6335	1.2	2
7	4	3	7	6	4	2	6	A	11281.4615	–3.5	0
7	4	3	8	6	4	2	7	A	11281.5229	–5.4	–2
7	4	3	6	6	4	2	5	A	11281.5396	0.2	4
7	4	3	7	6	4	2	6	E	11203.3777	–9.6	–4
7	4	3	8	6	4	2	7	E	11203.4433	–12.7	–6
7	4	3	6	6	4	2	5	E	11203.4623	–5.4	2
7	4	4	8	6	4	3	7	A	11170.1914	–4.9	–2
7	4	4	6	6	4	3	5	A	11170.2094	0.7	3
7	4	4	7	6	4	3	6	E	11251.1448	7.6	7
7	4	4	8	6	4	3	7	E	11251.2112	6.3	4
7	4	4	6	6	4	3	5	E	11251.2246	8.0	6
7	5	2	7	6	5	1	6	A	11124.2054	–0.4	0
7	5	2	8	6	5	1	7	A	11124.3122	–8.9	–8
7	5	2	6	6	5	1	5	A	11124.3403	–3.5	–2
7	5	2	7	6	5	1	6	E	11107.3588	–9.8	–5
7	5	2	8	6	5	1	7	E	11107.4729	–11.7	–5
7	5	2	6	6	5	1	5	E	11107.4982	–9.1	–2
7	5	3	7	6	5	2	6	A	11118.4883	1.1	1
7	5	3	8	6	5	2	7	A	11118.5965	–6.8	–6
7	5	3	6	6	5	2	5	A	11118.6229	–3.1	–2
7	5	3	7	6	5	2	6	E	11130.4885	14.7	10
7	5	3	8	6	5	2	7	E	11130.5429	–46.1	5
7	5	3	6	6	5	2	5	E	11130.5996	–12.0	–18
7	6	1	7	6	6	0	6	A	11069.3415	3.6	2
7	6	1	8	6	6	0	7	A	11069.5148	6.6	6
7	6	1	6	6	6	0	5	A	11069.5392	–4.7	–5
7	6	2	7	6	6	1	6	A	11069.2089	–4.9	–7
7	6	2	8	6	6	1	7	A	11069.3824	–1.7	–3

7	6	2	6	6	6	1	5	A	11069.4263	6.5	6
7	6	2	7	6	6	1	6	E	11072.4218	13.7	6
7	6	2	8	6	6	1	7	E	11072.5936	15.5	6
7	6	2	6	6	6	1	5	E	11072.6212	7.4	–3
8	0	8	8	7	0	7	7	A	10569.9750	–5.6	–6
8	0	8	7	7	0	7	6	A	10569.9981	7.1	7
8	0	8	8	7	0	7	7	E	10568.0703	–3.3	–4
8	0	8	7	7	0	7	6	E	10568.0848	0.5	0
8	0	8	9	7	0	7	8	E	10568.0922	1.0	1
8	1	7	8	7	1	6	7	A	11933.5782	–0.4	1
8	1	7	9	7	1	6	8	A	11933.6211	–0.8	0
8	1	7	7	7	1	6	6	A	11933.6211	–1.4	0
8	1	7	8	7	1	6	7	E	11924.8234	–0.9	0
8	1	7	9	7	1	6	8	E	11924.8682	0.3	2
8	1	7	7	7	1	6	6	E	11924.8682	–0.3	1
8	1	8	8	7	1	7	7	A	10558.4278	–4.6	–4
8	1	8	7	7	1	7	6	A	10558.4399	–2.0	–2
8	1	8	9	7	1	7	8	A	10558.4492	0.2	0
8	1	8	8	7	1	7	7	E	10557.3054	–2.9	–3
8	1	8	7	7	1	7	6	E	10557.3166	–1.4	–1
8	1	8	9	7	1	7	8	E	10557.3260	0.9	1
9	0	9	9	8	0	8	8	A	11809.0607	–3.7	–6
9	0	9	10	8	0	8	9	A	11809.0794	1.1	–1
9	0	9	8	8	0	8	7	A	11809.0794	6.9	5
9	0	9	9	8	0	8	8	E	11807.2632	–1.4	–4
9	0	9	8	8	0	8	7	E	11807.2632	–9.6	–12
9	0	9	10	8	0	8	9	E	11807.2798	1.2	–1
9	1	8	9	8	1	7	8	A	13121.9479	1.1	6
9	1	8	10	8	1	7	9	A	13121.9816	–0.3	4
9	1	8	8	8	1	7	7	A	13121.9816	0.2	5
9	1	8	9	8	1	7	8	E	13114.6922	–0.6	4
9	1	8	10	8	1	7	9	E	13114.7257	–2.4	2
9	1	8	8	8	1	7	7	E	13114.7257	–1.9	3
9	1	9	9	8	1	8	8	A	11804.2883	–0.4	–2
9	1	9	8	8	1	8	7	A	11804.2970	0.5	–2
9	1	9	10	8	1	8	9	A	11804.3053	3.0	1
9	1	9	9	8	1	8	8	E	11802.8157	0.5	–1
9	1	9	8	8	1	8	7	E	11802.8240	0.9	–1
9	1	9	10	8	1	8	9	E	11802.8324	3.4	2
10	0	10	10	9	0	9	9	A	13050.3358	1.1	–4
10	0	10	9	9	0	9	8	A	13050.3445	3.2	–2
10	0	10	11	9	0	9	10	A	13050.3504	4.2	–1
10	0	10	10	9	0	9	9	E	13048.5670	9.1	4
10	0	10	9	9	0	9	8	E	13048.5755	11.0	6
10	0	10	11	9	0	9	10	E	13048.5806	11.2	6

Table S6. Rotational constants of 4MNP-1 calculated at different levels of theory. The difference between the calculated and the experimental (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)	1843.5	1.8	928.1	–4.0	619.7	–1.9	7.6
B3LYP-D3/6-31+G(d,p)	1837.8	–4.0	926.7	–5.4	618.4	–3.1	12.5
B3LYP-D3/6-31++G(d,p)	1837.8	–4.0	926.7	–5.4	618.4	–3.2	12.5
B3LYP-D3/6-311G(d,p)	1844.2	2.5	930.0	–2.1	620.6	–0.9	5.5
B3LYP-D3/6-311+G(d,p)	1841.9	0.1	929.7	–2.3	620.2	–1.3	3.8
B3LYP-D3/6-311++G(d,p)	1841.9	0.2	929.7	–2.3	620.2	–1.3	3.8
B3LYP-D3/6-311G(2d,2p)	1852.8	11.1	932.4	0.4	622.7	1.1	12.6
B3LYP-D3/6-311+G(2d,2p)	1850.3	8.5	932.4	0.3	622.4	0.8	9.7
B3LYP-D3/6-311++G(2d,2p)	1850.3	8.6	932.4	0.3	622.4	0.8	9.7
B3LYP-D3/6-311G(df,pd)	1851.5	9.7	932.2	0.2	622.4	0.9	10.8
B3LYP-D3/6-311+G(df,pd)	1849.0	7.3	932.1	0.0	622.1	0.5	7.8
B3LYP-D3/6-311++G(df,pd)	1849.1	7.4	932.1	0.0	622.1	0.5	7.9
B3LYP-D3/6-311G(2df,2pd)	1856.8	15.1	933.6	1.5	623.6	2.1	18.7
B3LYP-D3/6-311+G(2df,2pd)	1854.6	12.9	933.4	1.3	623.3	1.7	15.9
B3LYP-D3/6-311++G(2df,2pd)	1854.7	12.9	933.4	1.3	623.3	1.7	15.9
B3LYP-D3/6-311G(3df,3pd)	1857.3	15.5	933.6	1.6	623.7	2.1	19.2
B3LYP-D3/6-311+G(3df,3pd)	1855.5	13.7	933.7	1.7	623.5	2.0	17.4
B3LYP-D3/6-311++G(3df,3pd)	1855.5	13.8	933.8	1.7	623.6	2.0	17.5
B3LYP-D3/cc-pVDZ	1844.4	2.6	925.2	–6.8	618.5	–3.0	12.5
B3LYP-D3/aug-cc-pVDZ	1840.0	1.8	925.5	–6.6	618.1	–3.5	11.9
B3LYP-D3/cc-pVTZ	1855.4	13.6	933.0	0.9	623.2	1.6	16.2
B3LYP-D3/aug-cc-pVTZ	1854.5	12.7	933.3	1.2	623.2	1.6	15.5
B3LYP-D3BJ/6-31G(d,p)	1847.8	6.0	930.4	–1.6	621.2	–0.4	8.0
B3LYP-D3BJ/6-31+G(d,p)	1842.3	0.6	929.1	–3.0	620.0	–1.6	5.1
B3LYP-D3BJ/6-31++G(d,p)	1842.3	0.5	929.1	–3.0	620.0	–1.6	5.1
B3LYP-D3BJ/6-311G(d,p)	1848.5	6.7	932.4	0.4	622.2	0.6	7.7
B3LYP-D3BJ/6-311+G(d,p)	1846.2	4.5	932.2	0.2	621.8	0.3	4.9
B3LYP-D3BJ/6-311++G(d,p)	1846.2	4.5	932.2	0.1	621.8	0.3	4.9
B3LYP-D3BJ/6-311G(2d,2p)	1857.0	15.3	934.9	2.9	624.2	2.7	20.8
B3LYP-D3BJ/6-311+G(2d,2p)	1854.7	12.9	934.8	2.8	623.9	2.4	18.0
B3LYP-D3BJ/6-311++G(2d,2p)	1854.7	12.9	934.8	2.8	623.9	2.4	18.1
B3LYP-D3BJ/6-311G(df,pd)	1855.8	14.0	934.7	2.6	624.0	2.4	19.1
B3LYP-D3BJ/6-311+G(df,pd)	1853.5	11.8	934.5	2.5	623.7	2.1	16.3
B3LYP-D3BJ/6-311++G(df,pd)	1853.6	11.8	934.5	2.4	623.7	2.1	16.4
B3LYP-D3BJ/6-311G(2df,2pd)	1857.0	15.3	934.9	2.9	624.2	2.7	20.8
B3LYP-D3BJ/6-311+G(2df,2pd)	1854.7	12.9	934.8	2.8	623.9	2.4	18.0
B3LYP-D3BJ/6-311++G(2df,2pd)	1854.7	12.9	934.8	2.8	623.9	2.4	18.1
B3LYP-D3BJ/6-311G(3df,3pd)	1861.5	19.7	936.1	4.1	625.3	3.7	27.5
B3LYP-D3BJ/6-311+G(3df,3pd)	1859.8	18.1	936.2	4.2	625.2	3.6	25.8
B3LYP-D3BJ/6-311++G(3df,3pd)	1859.8	18.0	936.2	4.2	625.1	3.6	25.8
B3LYP-D3BJ/cc-pVDZ	1848.4	6.6	927.7	–4.4	620.1	–1.5	12.5
B3LYP-D3BJ/aug-cc-pVDZ	1844.3	2.5	927.9	–4.1	619.7	–1.8	8.5
B3LYP-D3BJ/cc-pVTZ	1859.5	17.8	935.5	3.4	624.8	3.2	24.4

B3LYP-D3BJ/aug-cc-pVTZ	1858.7	17.0	935.8	3.7	624.8	3.3	24.0
CAM-B3LYP-D3BJ/6-311G(d,p)	1862.3	20.5	939.5	7.5	626.9	5.3	33.3
CAM-B3LYP-D3BJ/6-311+G(d,p)	1859.8	18.0	939.3	7.2	626.5	4.9	30.2
CAM-B3LYP-D3BJ/6-311++G(d,p)	1859.8	18.0	939.3	7.2	626.5	5.0	30.2
CAM-B3LYP-D3BJ/cc-pVDZ	1861.9	20.1	934.9	2.9	624.8	3.3	26.3
CAM-B3LYP-D3BJ/aug-cc-pVDZ	1857.5	15.7	935.0	2.9	624.4	2.8	21.5
CAM-B3LYP-D3BJ/cc-pVTZ	1873.1	31.3	942.6	10.6	629.5	7.9	49.8
CAM-B3LYP-D3BJ/aug-cc-pVTZ	1872.1	30.3	942.9	10.8	629.5	7.9	49.1
CCSD/cc-pVDZ	1823.7	–18.0	921.9	–10.1	614.8	–6.8	35.0
M06-2X/6-31G(d,p)	1849.1	7.3	936.8	4.7	624.2	2.6	14.7
M06-2X/6-31+G(d,p)	1843.6	1.9	935.6	3.6	623.1	1.5	7.0
M06-2X/6-31++G(d,p)	1843.6	1.9	935.6	3.5	623.0	1.5	6.9
M06-2X/6-311G(d,p)	1850.2	8.5	938.0	5.9	624.8	3.3	17.6
M06-2X/6-311+G(d,p)	1848.2	6.4	937.7	5.6	624.5	2.9	14.9
M06-2X/6-311++G(d,p)	1848.1	6.4	937.7	5.6	624.5	2.9	15.0
M06-2X/6-311G(2d,2p)	1858.3	16.6	940.1	8.1	626.7	5.1	29.8
M06-2X/6-311+G(2d,2p)	1855.9	14.2	940.0	7.9	626.4	4.8	26.9
M06-2X/6-311++G(2d,2p)	1856.0	14.2	940.0	7.9	626.4	4.8	27.0
M06-2X/6-311G(df,pd)	1857.5	15.7	939.4	7.3	626.3	4.7	27.8
M06-2X/6-311+G(df,pd)	1854.9	13.1	939.2	7.2	625.9	4.4	24.7
M06-2X/6-311++G(df,pd)	1854.9	13.1	939.3	7.2	625.9	4.4	24.7
M06-2X/6-311G(2df,2pd)	1863.6	21.8	940.6	8.6	627.5	6.0	36.4
M06-2X/6-311+G(2df,2pd)	1861.2	19.4	940.4	8.4	627.2	5.6	33.4
M06-2X/6-311++G(2df,2pd)	1861.2	19.4	940.4	8.4	627.2	5.6	33.4
M06-2X/6-311G(3df,3pd)	1863.4	21.6	940.5	8.4	627.4	5.9	35.9
M06-2X/6-311+G(3df,3pd)	1861.6	19.8	940.6	8.6	627.3	5.7	34.1
M06-2X/6-311++G(3df,3pd)	1861.6	19.8	940.6	8.6	627.3	5.7	34.1
M06-2X/cc-pVDZ	1851.7	9.9	934.6	2.5	623.5	2.0	14.4
M06-2X/aug-cc-pVDZ	1847.8	6.0	934.2	2.1	622.9	1.3	9.4
M06-2X/cc-pVTZ	1862.3	20.5	940.3	8.2	627.2	5.7	34.4
M06-2X/aug-cc-pVTZ	1861.0	19.2	940.6	8.5	627.2	5.7	33.4
MN15/6-31G(d,p)	1845.2	3.5	934.2	2.1	622.6	1.0	6.6
MN15/6-31+G(d,p)	1839.5	–2.2	932.7	0.6	621.3	–0.3	3.1
MN15/6-31++G(d,p)	1839.5	–2.2	932.7	0.6	621.3	–0.3	3.1
MN15/6-311G(d,p)	1849.0	7.2	937.0	5.0	624.3	2.7	14.9
MN15/6-311+G(d,p)	1846.8	5.1	936.7	4.7	623.9	2.3	12.0
MN15/6-311++G(d,p)	1846.8	5.0	936.8	4.7	623.9	2.4	12.1
MN15/6-311G(2d,2p)	1857.4	15.6	939.5	7.4	626.3	4.8	27.8
MN15/6-311+G(2d,2p)	1855.1	13.4	939.3	7.2	626.0	4.4	25.0
MN15/6-311++G(2d,2p)	1855.2	13.4	939.3	7.2	626.0	4.4	25.0
MN15/6-311G(df,pd)	1855.6	13.8	939.8	7.7	626.2	4.7	26.2
MN15/6-311+G(df,pd)	1853.2	11.5	939.4	7.4	625.8	4.3	23.1
MN15/6-311++G(df,pd)	1853.2	11.4	939.5	7.4	625.8	4.3	23.1
MN15/6-311G(2df,2pd)	1860.8	19.0	940.6	8.6	627.2	5.6	33.2
MN15/6-311+G(2df,2pd)	1858.8	17.1	940.3	8.2	626.8	5.3	30.6
MN15/6-311++G(2df,2pd)	1858.8	17.1	940.3	8.2	626.8	5.3	30.6

MN15/6-311G(3df,3pd)	1861.8	20.1	941.0	8.9	627.5	5.9	34.9
MN15/6-311+G(3df,3pd)	1860.4	18.7	941.0	8.9	627.3	5.8	33.4
MN15/6-311++G(3df,3pd)	1860.5	18.7	941.0	8.9	627.3	5.8	33.4
MN15/cc-pVDZ	1849.3	7.6	932.3	0.2	622.2	0.7	8.4
MN15/aug-cc-pVDZ	1845.2	3.4	932.7	0.7	622.0	0.4	4.5
MN15/cc-pVTZ	1860.5	18.7	940.4	8.4	627.1	5.5	32.6
MN15/aug-cc-pVTZ	1860.5	18.7	941.1	9.0	627.4	5.8	33.5
PBE0/6-31G(d,p)	1837.9	–3.8	920.3	–11.8	615.6	–6.0	21.6
PBE0/6-31+G(d,p)	1833.0	–8.7	918.8	–13.2	614.4	–7.2	29.1
PBE0/6-31++G(d,p)	1833.0	–8.8	918.8	–13.2	614.4	–7.2	29.1
PBE0/6-311G(d,p)	1838.3	–3.4	922.6	–9.4	616.7	–4.9	17.7
PBE0/6-311+G(d,p)	1836.1	–5.6	922.3	–9.7	616.3	–5.2	20.6
PBE0/6-311++G(d,p)	1836.2	–5.6	922.4	–9.7	616.3	–5.2	20.5
PBE0/6-311G(2d,2p)	1846.9	5.1	924.6	–7.5	618.5	–3.0	15.6
PBE0/6-311+G(2d,2p)	1844.6	2.8	924.6	–7.5	618.2	–3.3	13.6
PBE0/6-311++G(2d,2p)	1844.6	2.9	924.5	–7.5	618.2	–3.3	13.7
PBE0/6-311G(df,pd)	1845.5	3.8	924.7	–7.4	618.4	–3.1	14.3
PBE0/6-311+G(df,pd)	1843.5	1.7	924.4	–7.7	618.1	–3.5	12.9
PBE0/6-311++G(df,pd)	1843.5	1.8	924.4	–7.7	618.1	–3.5	12.9
PBE0/6-311G(2df,2pd)	1850.5	8.7	925.8	–6.3	619.4	–2.1	17.1
PBE0/6-311+G(2df,2pd)	1848.7	6.9	925.5	–6.5	619.1	–2.4	15.9
PBE0/6-311++G(2df,2pd)	1848.7	6.9	925.5	–6.5	619.1	–2.4	15.9
PBE0/6-311G(3df,3pd)	1851.2	9.5	925.9	–6.2	619.6	–2.0	17.6
PBE0/6-311+G(3df,3pd)	1849.6	7.8	926.0	–6.1	619.4	–2.1	16.0
PBE0/6-311++G(3df,3pd)	1849.6	7.8	926.0	–6.1	619.4	–2.1	16.0
PBE0/cc-pVDZ	1839.3	–2.4	918.1	–14.0	614.8	–6.8	23.2
PBE0/aug-cc-pVDZ	1834.5	–7.3	918.3	–13.7	614.4	–7.2	28.2
PBE0/cc-pVTZ	1849.2	7.4	925.1	–6.9	619.0	–2.5	16.9
PBE0/aug-cc-pVTZ	1848.3	6.5	925.4	–6.7	619.0	–2.5	15.7
PBE0-D3/6-31G(d,p)	1837.4	–4.3	920.1	–12.0	615.5	–6.1	22.4
PBE0-D3/6-31+G(d,p)	1832.4	–9.4	918.7	–13.3	614.3	–7.3	30.0
PBE0-D3/6-31++G(d,p)	1832.4	–9.4	918.7	–13.3	614.3	–7.3	30.0
PBE0-D3/6-311G(d,p)	1837.8	–4.0	922.5	–9.6	616.6	–5.0	18.6
PBE0-D3/6-311+G(d,p)	1835.6	–6.2	922.2	–9.9	616.2	–5.4	21.4
PBE0-D3/6-311++G(d,p)	1835.6	–6.2	922.2	–9.9	616.2	–5.4	21.4
PBE0-D3/6-311G(2d,2p)	1846.2	4.5	924.5	–7.6	618.4	–3.2	15.2
PBE0-D3/6-311+G(2d,2p)	1844.0	2.3	924.4	–7.7	618.1	–3.5	13.4
PBE0-D3/6-311++G(2d,2p)	1844.1	2.3	924.4	–7.7	618.1	–3.4	13.4
PBE0-D3/6-311G(df,pd)	1845.0	3.2	924.5	–7.5	618.3	–3.3	14.1
PBE0-D3/6-311+G(df,pd)	1842.9	1.2	924.2	–7.9	617.9	–3.6	12.7
PBE0-D3/6-311++G(df,pd)	1842.9	1.2	924.2	–7.8	617.9	–3.6	12.7
PBE0-D3/6-311G(2df,2pd)	1850.0	8.2	925.6	–6.5	619.3	–2.2	17.0
PBE0-D3/6-311+G(2df,2pd)	1848.2	6.4	925.4	–6.7	619.0	–2.6	15.7
PBE0-D3/6-311++G(2df,2pd)	1848.2	6.4	925.4	–6.7	619.0	–2.5	15.7
PBE0-D3/6-311G(3df,3pd)	1850.8	9.0	925.7	–6.4	619.4	–2.1	17.5
PBE0-D3/6-311+G(3df,3pd)	1849.1	7.3	925.8	–6.3	619.3	–2.3	15.9
PBE0-D3/6-311++G(3df,3pd)	1849.1	7.3	925.8	–6.3	619.3	–2.3	15.9
PBE0-D3/cc-pVDZ	1838.9	–2.8	917.9	–14.2	614.7	–6.9	23.9

PBE0-D3/aug-cc-pVDZ	1834.0	–7.8	918.2	–13.9	614.2	–7.3	29.0
PBE0-D3/cc-pVTZ	1848.8	7.0	925.0	–7.1	618.9	–2.7	16.8
PBE0-D3/aug-cc-pVTZ	1847.8	6.0	925.2	–6.9	618.9	–2.7	15.5
ωB97X-D/6-31G(d,p)	1852.7	11.0	935.7	3.6	624.1	2.5	17.1
ωB97X-D/6-31+G(d,p)	1848.1	6.3	934.7	2.6	623.1	1.6	10.6
ωB97X-D/6-31++G(d,p)	1848.1	6.3	934.7	2.6	623.1	1.6	10.5
ωB97X-D-6-311G(d,p)	1854.5	12.7	937.6	5.6	625.2	3.6	21.9
ωB97X-D-6-311+G(d,p)	1852.5	10.7	937.5	5.5	624.9	3.4	19.6
ωB97X-D-6-311++G(d,p)	1852.5	10.8	937.5	5.5	624.9	3.3	19.6
ωB97X-D/6-311G(2d,2p)	1862.7	21.0	939.9	7.8	627.1	5.5	34.3
ωB97X-D/6-311+G(2d,2p)	1860.7	18.9	939.9	7.8	626.9	5.3	32.0
ωB97X-D/6-311++G(2d,2p)	1860.7	18.9	939.8	7.8	626.9	5.3	32.0
ωB97X-D/6-311G(df,pd)	1860.7	18.9	939.5	7.5	626.7	5.2	31.6
ωB97X-D/6-311+G(df,pd)	1858.7	16.9	939.4	7.4	626.5	4.9	29.2
ωB97X-D/6-311++G(df,pd)	1858.7	16.9	939.5	7.4	626.5	4.9	29.2
ωB97X-D/6-311G(2df,2pd)	1866.0	24.3	940.8	8.8	627.9	6.3	39.4
ωB97X-D/6-311+G(2df,2pd)	1864.3	22.5	940.7	8.6	627.6	6.1	37.2
ωB97X-D/6-311++G(2df,2pd)	1864.4	22.6	940.6	8.6	627.6	6.1	37.2
ωB97X-D/6-311G(3df,3pd)	1866.3	24.5	940.8	8.8	627.9	6.4	39.7
ωB97X-D/6-311+G(3df,3pd)	1864.9	23.1	941.0	8.9	627.8	6.3	38.3
ωB97X-D/6-311++G(3df,3pd)	1864.9	23.2	940.9	8.9	627.8	6.3	38.3
ωB97X-D/cc-pVDZ	1853.1	11.4	933.2	1.2	623.1	1.5	14.0
ωB97X-D/aug-cc-pVDZ	1849.8	8.0	933.1	1.1	622.7	1.1	10.2
ωB97X-D/cc-pVTZ	1864.8	23.0	940.7	8.6	627.7	6.1	37.8
ωB97X-D/aug-cc-pVTZ	1865.5	23.7	940.4	8.3	627.6	6.1	38.1
MP2/6-31G(d,p)	1826.4	–15.4	931.4	–0.7	619.2	–2.4	18.4
MP2/6-31+G(d,p)	1819.1	–22.7	929.9	–2.1	617.8	–3.8	28.6
MP2/6-31++G(d,p)	1818.8	–23.0	930.0	–2.0	617.8	–3.8	28.8
MP2/6-311G(d,p)	1830.9	–10.9	929.2	–2.8	618.8	–2.8	16.5
MP2/6-311+G(d,p)	1827.9	–13.9	927.8	–4.3	619.3	–2.3	20.5
MP2/6-311++G(d,p)	1827.8	–14.0	928.0	–4.0	619.0	–2.6	20.6
MP2/6-311G(2d,2p)	1837.4	–4.4	934.0	2.0	621.6	0.0	6.4
MP2/6-311+G(2d,2p)	1834.8	–6.9	933.5	1.5	621.1	–0.5	8.9
MP2/6-311++G(2d,2p)	1834.8	–7.0	933.5	1.4	621.1	–0.5	8.9
MP2/6-311G(df,pd)	1853.6	11.8	934.5	2.4	623.7	2.1	16.4
MP2/6-311+G(df,pd)	1850.5	8.7	933.0	0.9	624.1	2.5	12.1
MP2/6-311++G(df,pd)	1850.5	8.7	933.1	1.0	623.8	2.3	12.0
MP2/6-311G(2df,2pd)	1852.5	10.7	938.7	6.6	625.4	3.9	21.2
MP2/6-311+G(2df,2pd)	1849.7	7.9	937.8	5.7	624.7	3.1	16.7
MP2/6-311++G(2df,2pd)	1849.7	7.9	937.8	5.7	624.7	3.1	16.7
MP2/6-311G(3df,3pd)	1849.6	7.8	937.1	5.0	624.4	2.8	15.6
MP2/6-311+G(3df,3pd)	1847.3	5.6	936.9	4.8	624.0	2.4	12.8
MP2/6-311++G(3df,3pd)	1847.3	5.6	936.9	4.8	624.0	2.4	12.8
MP2/cc-pVDZ	1821.4	–20.3	922.3	–9.8	614.6	–6.9	37.0
MP2/aug-cc-pVDZ	1814.1	–27.7	920.8	–11.3	613.1	–8.4	47.4
MP2/cc-pVTZ	1847.9	6.2	936.3	4.2	623.8	2.3	12.7
MP2/aug-cc-pVTZ	1844.0	2.2	936.4	4.3	623.4	1.8	8.3
Experimental	**1841.8**		**932.1**		**621.6**		