Electronic Supplementary Information for:

***Ab initio* conformational analysis of 1,2,3,4-tetrahydroquinoline and high-resolution rotational spectrum of its lowest energy conformer**

Kateřina Luková,[a] Radim Nesvadba,[a] Tereza Uhlíková,[*a] Daniel A. Obenchain,[b] Dennis Wachsmuth,[b] Jens-Uwe Grabow[b] and Štěpán Urban[a]

[a] *Department of Analytical Chemistry, University of Chemistry and Technology, Technická 5, 166 28, Prague 6, Czech Republic. E-mail: Tereza.Uhlikova@vscht.cz*

[b] *Institut für Physikalische Chemie und Elektrochemie, Wilhelm-Gottfried-Leibniz-Universität Hannover. Callinstraße 3A, 30167 Hannover, Germany*

Rotational Hamiltonian

The transition frequencies of all the measured lines (Table T5) assigned to rotational and hyperfine quantum numbers $J_{k_a k_c}$ and F were analyzed using an effective rotational Hamiltonian H_{rot} extended with a ^{14}N quadrupole coupling term H_Q:

$$H = H_{rot} + H_Q, \tag{E1}$$

where H_{rot} is the A-reduced Watson's rotational effective Hamiltonian in I^r axis representation (a=z, b=x, c=y), which provides both the diagonal and off-diagonal matrix elements in the $|J,K\rangle$ symmetric top rotational basis[1, 2]:

$$\begin{aligned}\langle J,K|\hat{H}_{rot}|J,K\rangle = \frac{1}{2}(B+C)J(J+1) + \left(A - \frac{1}{2}(B+C)\right)K^2 - \Delta_J J^2(J+1)^2 \\ - \Delta_{JK}J(J+1)K^2 - \Delta_K K^4 + \ higher\ terms\end{aligned} \tag{E2}$$

and

$$\begin{aligned}\langle J,K|\hat{H}_{rot}|J,K = \pm 2\rangle \\ = \left(\frac{1}{2}(B-C) - 2\delta_J J(J+1) \right.\\ \left. - \delta_K(K^2 \pm 2K + 2)\right)\left(J(J+1) - K(K\pm 1)\right)^{\frac{1}{2}}(J(J+1) \\ - (K\pm 1)(K\pm 2))^{\frac{1}{2}} + \ higher\ terms\end{aligned} \tag{E3}$$

respectively; and where A, B and C are the rotational constants; Δ_J, Δ_{JK}, Δ_K and δ_J, δ_K are the diagonal and off-diagonal centrifugal distortion parameters, respectively. The matrix elements of the ^{14}N quadrupole hyperfine-structure Hamiltonian H_Q can be written as[2]:

$$\langle J,I,F|\hat{H}_Q|J,I,F\rangle = eQq_j\frac{2J+3}{J}Y(J,I,F), \tag{E4}$$

where I is the nuclear spin quantum number, and eQq_j is the nuclear coupling constant that is often designated as χ:

$$\chi_{aa} = eQq_{aa}, \qquad \chi_{bb} = eQq_{bb}, \qquad \chi_{cc} = eQq_{cc}, \tag{E5}$$

and

$$Y(J,I,F) = \frac{\frac{3}{4}C(C+1) - I(I+1)J(J+1)}{2(2J-1)(2J+3)I(2I-1)}, \tag{E6}$$

where C can be written as[2]:

$$C = F(F+1) - J(J+1) - I(I+1). \tag{E7}$$

Table T1: The values of the bonds (B, Ångström), angles and dihedral angles (A and D, degree) for the optimized geometry of the half-chair conformer **1+** (Fig. F1). The calculations were performed at the MP2/cc-pVDZ level of theory.

Parameter	Value	Parameter	Value	Parameter	Value
B(1N-2C)	1.46019	A(5C-10C-9C)	118.82694	D(5C-10C-9C-8C)	-0.04817
B(2C-3C)	1.52761	A(10C-9C-8C)	119.25371	D(10C-9C-8C-7C)	-0.36918
B(3C-4C)	1.53245	A(9C-8C-7C)	121.03353	D(9C-10C-5C-6C)	0.38288
B(4C-10C)	1.51862	A(18H-5C-6C)	119.77912	D(18H-5C-6C-7C)	179.87539
B(9C-10C)	1.41869	A(6C-5C-10C)	121.82275	D(21H-8C-9C-10C)	179.29510
B(5C-10C)	1.40808	A(21H-8C-9C)	118.89892	D(20H-7C-8C-9C)	-179.75970
B(5C-6C)	1.40296	A(20H-7C-8C)	119.57863	D(19H-6C-5C-10C)	179.89778
B(6C-7C)	1.40634	A(19H-6C-5C)	120.35760	D(6C-5C-10C-4C)	-178.86082
B(7C-8C)	1.40077	A(5C-10C-4C)	120.57809	D(5C-10C-4C-3C)	-163.65440
B(8C-9C)	1.41322	A(10C-4C-3C)	111.58833	D(10C-4C-3C-2C)	-46.40266
B(9C-1N)	1.40725	A(4C-3C-2C)	109.37585	D(1N-9C-10C-5C)	176.46378
B(1N-11H)	1.01920	A(1N-9C-10C)	120.88537	D(17H-4C-10C-5C)	-40.81055
B(2C-12H)	1.11285	A(17H-4C-10C)	109.59521	D(16H-4C-10C-5C)	75.47568
B(2C-13H)	1.10254	A(16H-4C-10C)	109.21018	D(15H-3C-4C-10C)	72.39477
B(3C-14H)	1.10331	A(15H-3C-4C)	110.18491	D(14H-3C-4C-10C)	-168.22790
B(3C-15H)	1.10434	A(14H-3C-4C)	110.63381	D(13H-2C-3C-4C)	-176.96001
B(4C-16H)	1.10697	A(13H-2C-3C)	110.90322	D(12H-2C-3C-4C)	-58.34816
B(4C-17H)	1.10440	A(12H-2C-3C)	109.13042	D(11H-1N-9C-10C)	154.48959
B(5C-18H)	1.09722	A(11H-1N-2C)	112.77840		
B(6C-19H)	1.09454				
B(7C-20H)	1.09525				
B(8C-21H)	1.09709				

Fig. F1: The optimized geometry of the half-chair conformer **1+** of 1,2,3,4-tetrahydroquinoline.

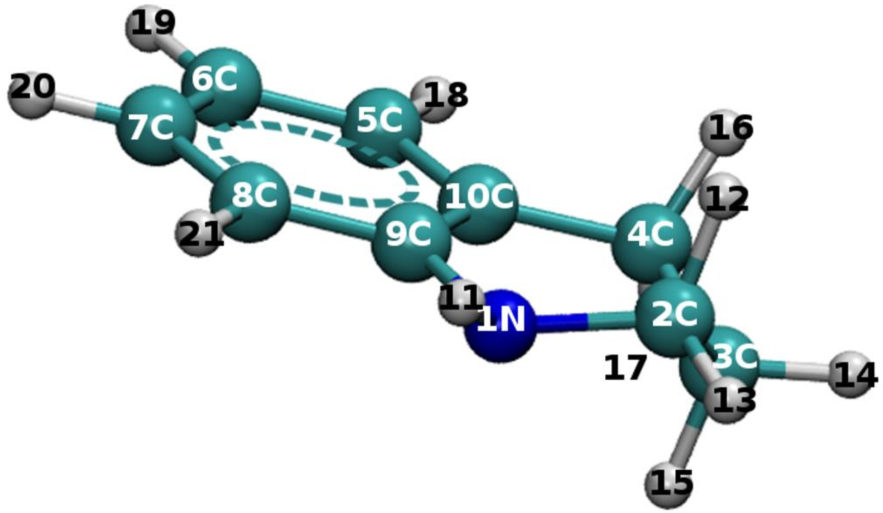

Table T2: The values of the bonds (B, Ångström), angles and dihedral angles (A and D, degree) for the optimized geometry of the stable conformer **2-** (Fig. F2). The calculations were performed at the MP2/cc-pVDZ level of theory.

Parameter	Value	Parameter	Value	Parameter	Value
B(1N-2C)	1.46394	A(5C-10C-9C)	118.95221	D(5C-10C-9C-8C)	-1.22685
B(2C-3C)	1.53051	A(10C-9C-8C)	119.21629	D(10C-9C-8C-7C)	0.64124
B(3C-4C)	1.53179	A(9C-8C-7C)	120.97475	D(9C-10C-5C-6C)	0.67897
B(4C-10C)	1.51539	A(18H-5C-6C)	119.83950	D(18H-5C-6C-7C)	-178.38627
B(9C-10C)	1.41794	A(6C-5C-10C)	121.69875	D(21H-8C-9C-10C)	179.74626
B(5C-10C)	1.40880	A(21H-8C-9C)	118.75856	D(20H-7C-8C-9C)	179.97066
B(5C-6C)	1.40238	A(20H-7C-8C)	119.58768	D(19H-6C-5C-10C)	179.83103
B(6C-7C)	1.40728	A(19H-6C-5C)	120.35073	D(6C-5C-10C-4C)	-176.76395
B(7C-8C)	1.40001	A(5C-10C-4C)	121.22862	D(5C-10C-4C-3C)	151.89478
B(8C-9C)	1.41425	A(10C-4C-3C)	109.94628	D(10C-4C-3C-2C)	55.22526
B(9C-1N)	1.40709	A(4C-3C-2C)	108.37813	D(1N-9C-10C-5C)	176.94227
B(1N-11H)	1.01752	A(1N-9C-10C)	121.83765	D(17H-4C-10C-5C)	-87.75500
B(2C-12H)	1.10233	A(17H-4C-10C)	110.43477	D(16H-4C-10C-5C)	29.59329
B(2C-13H)	1.10770	A(16H-4C-10C)	109.47661	D(15H-3C-4C-10C)	176.11059
B(3C-14H)	1.10557	A(15H-3C-4C)	111.01518	D(14H-3C-4C-10C)	-64.55996
B(3C-15H)	1.10384	A(14H-3C-4C)	109.79577	D(13H-2C-3C-4C)	62.89686
B(4C-16H)	1.10384	A(13H-2C-3C)	108.38969	D(12H-2C-3C-4C)	-179.82739
B(4C-17H)	1.10711	A(12H-2C-3C)	111.42339	D(11H-1N-9C-10C)	139.79608
B(5C-18H)	1.09714	A(11H-1N-2C)	113.43615		
B(6C-19H)	1.09458				
B(7C-20H)	1.09531				
B(8C-21H)	1.09670				

Fig. F2: The optimized geometry of the conformer **2-** of 1,2,3,4-tetrahydroquinoline.

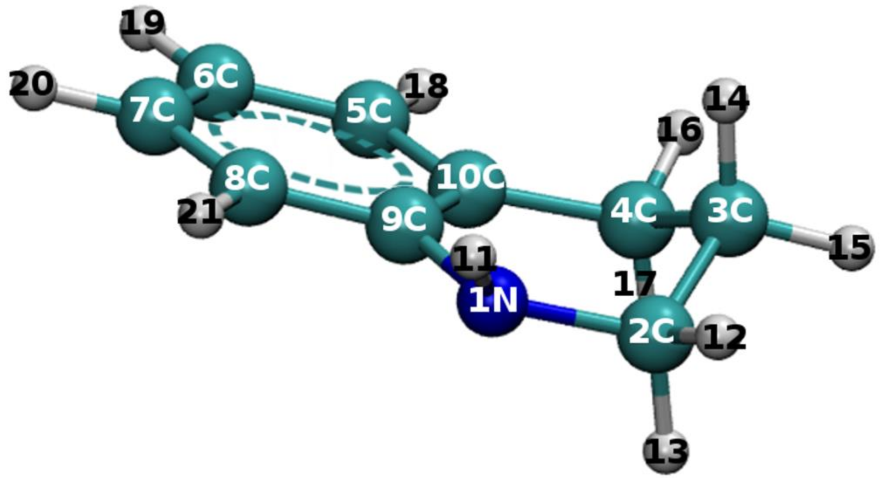

Table T3: Molecular parameters of the half-chair conformer **1** calculated by various computational methods. The Gibbs free energy (GFE_{298}) was calculated at the lowest initial temperature 298.15 K.

Parameters	DFT/B3LYP				DFT/B3PW91			
	6-311++G(d,p)	6-311++G(2d,3p)	cc-pVDZ	aug-cc-pVDZ	6-311++G(d,p)	6-311++G(2d,3p)	cc-pVDZ	aug-cc-pVDZ
E [a.u.]	-404.44740	-404.46237	-404.36144	-404.38667	-404.29157	-404.30609	-404.21868	-404.23897
GFE_{298} [a.u.]	-404.29855	-404.31317	-404.21251	-404.23794	-404.14226	-404.15658	-404.06907	-404.08977
μ_a[D]	1.71657	1.71200	1.62481	1.71012	1.76328	1.74908	1.69992	1.74845
μ_b[D]	0.49320	0.47636	0.62762	0.49579	0.51955	0.50100	0.63275	0.51464
μ_c[D]	-0.60035	-0.60649	-0.57037	-0.58428	-0.58450	-0.59443	-0.57093	-0.57703
A [MHz]	2847.39190	2855.94528	2833.62375	2833.79293	2860.61341	2868.40272	2846.98752	2846.87374
B [MHz]	1148.63951	1152.60441	1145.36112	1144.74359	1155.15380	1158.99775	1151.40576	1151.18336
C [MHz]	841.76680	844.53839	839.09315	838.58899	846.50618	849.14443	843.47216	843.23399
Δ_J [kHz]	0.01570	0.01585	0.01507	0.01551	0.01589	0.01604	0.01525	0.01569
Δ_{JK} [kHz]	0.10370	0.10626	0.10766	0.21812	0.10392	0.22457	0.10823	0.22039
Δ_K [kHz]	0.23382	0.22206	0.22440	0.10385	0.23763	0.10671	0.22715	0.10404
δ_J [kHz]	0.00327	0.00328	0.00303	0.00323	0.00334	0.00335	0.00309	0.00329
δ_K [kHz]	0.04688	0.04829	0.04863	0.04717	0.04706	0.04870	0.04913	0.04763
Φ_J[Hz]	1.11E-07	7.55E-08	5.41E-08	8.50E-08	1.81E-07	1.14E-07	1.10E-07	1.36E-07
Φ_K[Hz]	2.26E-05	2.77E-05	2.75E-05	2.65E-05	1.70E-05	2.64E-05	2.92E-05	2.61E-05
Φ_{JK} [Hz]	8.42E-06	9.17E-06	1.02E-05	9.84E-06	8.51E-06	1.01E-05	1.07E-05	1.03E-05
Φ_{KJ} [Hz]	-1.42E-05	-1.69E-05	-1.85E-05	-2.30E-05	-1.18E-05	-2.38E-05	-2.07E-05	-2.47E-05
φ_J [Hz]	9.34E-08	8.31E-08	5.83E-08	7.44E-08	1.18E-07	9.05E-08	7.28E-08	8.95E-08
φ_K [Hz]	7.24E-05	6.88E-05	6.42E-05	6.51E-05	7.87E-05	6.99E-05	6.61E-05	6.77E-05
φ_{JK} [Hz]	1.02E-06	1.21E-06	2.00E-06	1.45E-06	8.40E-07	1.36E-06	2.10E-06	1.53E-06
χ_{aa} [MHz]	2.7925	2.7638	2.5731	2.4730	2.7554	2.7209	2.5687	2.4728
χ_{bb} [MHz]	2.5918	2.4736	2.6197	2.4530	2.5289	2.4139	2.5589	2.4023
χ_{cc}[MHz]	-5.3843	-5.2375	-5.1928	-4.9261	-5.2843	-5.1348	-5.1276	-4.8751
$\chi_{bb} - \chi_{cc}$ [MHz]	7.9761	7.7111	7.8125	7.3791	7.8132	7.5487	7.6865	7.2774
χ_{ac} [MHz]	-1.1548	-1.1679	-1.1326	-1.0785	-1.1201	-1.1378	-1.0974	-1.0635
χ_{bc} [MHz]	-0.5357	-0.5709	-0.6171	-0.5090	-0.5283	-0.5742	-0.6159	-0.5285
χ_{ab} [MHz]	-0.0423	-0.0525	-0.0368	-0.0361	-0.0495	-0.0632	-0.0447	-0.0475

Table T3*: (Continued)*

Parameters	DFT/BP86				DFT/B3P86			
	6-311++G(d,p)	6-311++G(2d,3p)	cc-pVDZ	aug-cc-pVDZ	6-311++G(d,p)	6-311++G(2d,3p)	cc-pVDZ	aug-cc-pVDZ
E [a.u.]	-404.43685	-404.45031	-404.35511	-404.37977	-405.74856	-405.76330	-405.67356	-404.37977
GFE_{298} [a.u.]	-404.29352	-404.30674	-404.21167	-404.23658	-405.59900	-405.61349	-405.52383	-405.54495
μ_a[D]	1.86579	1.85603	1.81135	1.85854	1.75798	1.74535	1.69051	1.74690
μ_b[D]	0.55973	0.53747	0.69361	0.55679	0.51964	0.50001	0.63421	0.51537
μ_c[D]	-0.56626	-0.57425	-0.54377	-0.55049	-0.58492	-0.59563	-0.57373	-0.57704
A [MHz]	2819.32770	2826.62779	2805.78764	2806.10710	2866.41516	2874.42269	2852.32144	2852.62245
B [MHz]	1138.73064	1142.29870	1135.18720	1134.91049	1158.06597	1162.02412	1154.24091	1154.09508
C [MHz]	834.38342	836.83942	831.50882	831.25911	848.61319	851.33134	845.50762	845.34207
Δ_J [kHz]	0.01613	0.01628	0.01547	0.01595	0.01595	0.01609	0.01531	0.01912
Δ_{JK} [kHz]	0.10615	0.22862	0.11054	0.22519	0.10403	0.22452	0.10858	0.12248
Δ_K [kHz]	0.24171	0.10905	0.23109	0.10663	0.23814	0.10682	0.22660	0.05246
δ_J [kHz]	0.00339	0.00340	0.00313	0.00334	0.00336	0.00337	0.00311	0.00495
δ_K [kHz]	0.04769	0.04938	0.04983	0.04824	0.04707	0.04878	0.04914	0.04567
Φ_J[Hz]	1.49E-06	8.10E-08	8.16E-08	1.24E-07	1.63E-07	1.02E-07	9.16E-08	6.06E-07
Φ_K[Hz]	1.77E-05	2.72E-05	3.39E-05	2.10E-05	1.77E-05	2.70E-05	2.98E-05	1.06E-05
Φ_{JK} [Hz]	9.11E-06	1.01E-05	1.11E-05	1.03E-05	8.68E-06	1.02E-05	1.08E-05	7.09E-06
Φ_{KJ} [Hz]	-1.66E-05	-2.54E-05	-2.31E-05	-2.68E-05	-1.24E-05	-2.42E-05	-2.15E-05	-9.80E-05
φ_J [Hz]	1.15E-07	8.63E-08	7.05E-08	9.59E-08	1.14E-07	8.63E-08	6.64E-08	3.22E-07
φ_K [Hz]	8.15E-05	7.27E-05	6.76E-05	7.26E-05	7.93E-05	7.03E-05	6.60E-05	4.97E-05
φ_{JK} [Hz]	8.53E-07	1.28E-06	2.21E-06	1.51E-06	8.46E-07	1.44E-06	2.12E-06	2.10E-06
χ_{aa} [MHz]	2.6703	2.6338	2.4635	2.3647	2.7391	2.7038	2.5454	2.4529
χ_{bb} [MHz]	2.4660	2.3536	2.4799	2.3382	2.5277	2.4103	2.5483	2.3980
χ_{cc}[MHz]	-5.1362	-4.9874	-4.9434	-4.7029	-5.2668	-5.1141	-5.0937	-4.8509
χ_{bb} - χ_{cc} [MHz]	7.6022	7.3410	7.4233	7.0411	7.7945	7.5244	7.642	7.2489
χ_{ac}[MHz]	-1.0878	-1.1065	-1.0605	-1.0240	-1.1215	-1.1387	-1.1016	-1.0623
χ_{bc}[MHz]	-0.5153	-0.5543	-0.5873	-0.4874	-0.5305	-0.5771	-0.6169	-0.5270
χ_{ab} [MHz]	-0.0711	-0.0818	-0.0572	-0.0612	-0.0503	-0.0635	-0.0447	-0.0474

Table T3: *(Continued)*

Parameters	MP2	
	6-311++G(d,p)	cc-pVDZ
E [a.u.]	-403.21717	-404.07333
GFE_{298}[a.u.]	-403.06801	-403.92263
μ_a[D]	1.40367	1.30624
μ_b[D]	0.32341	0.46636
μ_c[D]	-0.79786	0.76788
A [MHz]	2831.57466	2811.40171
B [MHz]	1153.56979	1147.24125
C [MHz]	844.59468	839.66671
Δ_J [kHz]	0.01615	0.01575
Δ_{JK} [kHz]	0.10501	0.10033
Δ_K [kHz]	0.21267	0.20384
δ_J [kHz]	0.00337	0.00335
δ_K [kHz]	0.04977	0.04717
Φ_J[Hz]	2.93E-08	4.03E-08
Φ_K[Hz]	4.89E-05	3.96E-05
Φ_{JK} [Hz]	1.15E-05	1.09E-05
Φ_{KJ} [Hz]	-2.70E-05	-2.44E-05
φ_J [Hz]	6.15E-08	6.53E-08
φ_K [Hz]	7.20E-05	6.82E-05
φ_{JK} [Hz]	1.85E-06	1.48E-06
χ_{aa} [MHz]	2.5562	2.3546
χ_{bb} [MHz]	2.2512	2.2708
χ_{cc}[MHz]	-4.8075	-4.6254
χ_{bb} - χ_{cc} [MHz]	7.0587	6.8962
χ_{ac}[MHz]	-1.2230	1.2219
χ_{bc}[MHz]	-0.7604	0.7783
χ_{ab} [MHz]	-0.0410	-0.0599

Table T4: Molecular parameters of the stable conformer **2** calculated by MP2. The Gibbs free energy (GFE_{298}) was calculated at the lowest initial temperature 298.15 K.

Method	MP2	
Parameters	6-311++G(d,p)	cc-pVDZ
E [a.u.]	-404.44375	-404.07086
GFE_{298}[a.u.]	-404.29531	-403.92123
μ_a [D]	1.69724	1.53333
μ_b[D]	0.12551	-0.28211
μ_c [D]	0.85542	0.83796
A [MHz]	2794.90376	2795.09201
B [MHz]	1147.95485	1147.91554
C [MHz]	842.89225	842.86114
Δ_J [kHz]	0.01550	0.02062
Δ_{JK} [kHz]	0.10892	0.08302
Δ_K [kHz]	0.18833	0.10063
δ_J[kHz]	0.00286	0.00471
δ_K[kHz]	0.05095	0.04397
Φ_J[Hz]	6.42E-08	1.63E-06
Φ_K [Hz]	6.95E-05	2.61E-04
Φ_{JK} [Hz]	1.18E-05	2.61E-04
Φ_{KJ} [Hz]	-2.12E-05	-3.03E-04
φ_J[Hz]	-1.82E-08	2.95E-08
φ_K [Hz]	3.67E-05	-7.57E-06
φ_{JK} [Hz]	4.37E-06	3.50E-06
χ_{aa} [MHz]	2.9007	2.6590
χ_{bb} [MHz]	0.9719	1.0000
χ_{cc}[MHz]	-3.8726	-3.6590
χ_{bb}- χ_{cc}[MHz]	4.8445	4.6590
χ_{ab}[MHz]	0.2341	-0.2149
χ_{ac}[MHz]	-0.5215	-0.4723
χ_{bc}[MHz]	3.1513	-2.8910

Fig. F3: The potential energy curve along the dihedral angle 1N-2C-3C-4C calculated by the combination of DFT/B3LYP/6-311++G(2d,3p). Differently from Chakraborty *et al.*,[3] no minimum for the half-boat conformation was found around the dihedral angle 0° even though the same computational method was used in both cases.

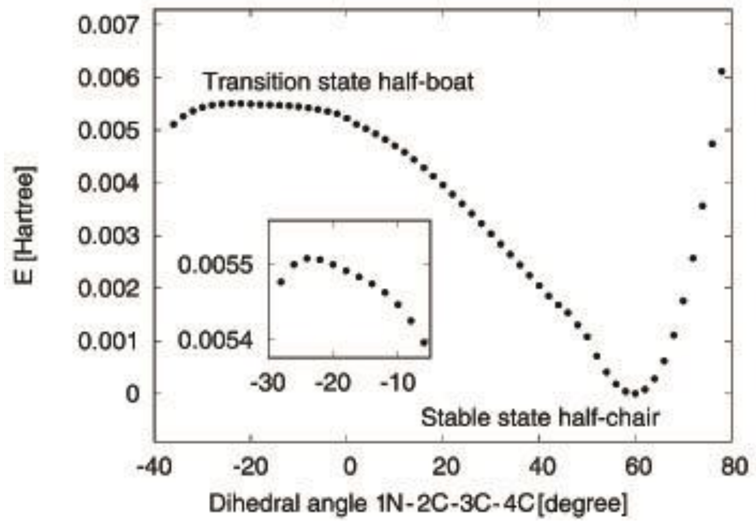

Fig. F4: The potential energy surface (PES) along the dihedral angles 1N-2C-3C-4C and 11H-1N-9C-8C calculated by DFT/B3LYP/6-311++G(2d,3p).

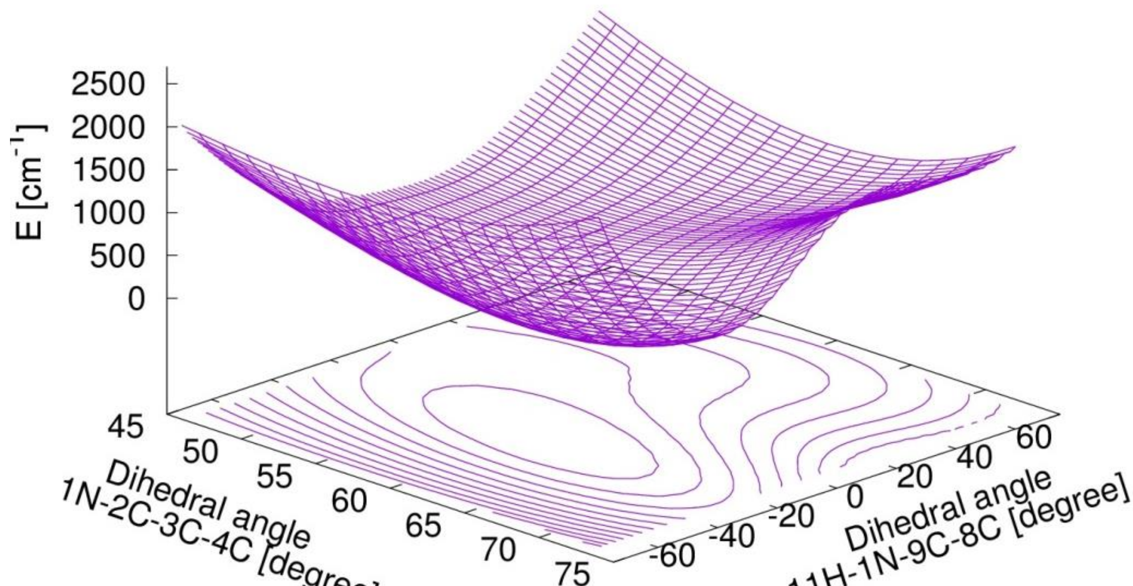

Fig. F5: The potential energy curve along the dihedral angles 1N-2C-3C-4C and 11H-1N-9C-8C calculated by DFT/B3LYP/6-311++G(2d,3p) displayed as the contour diagram.

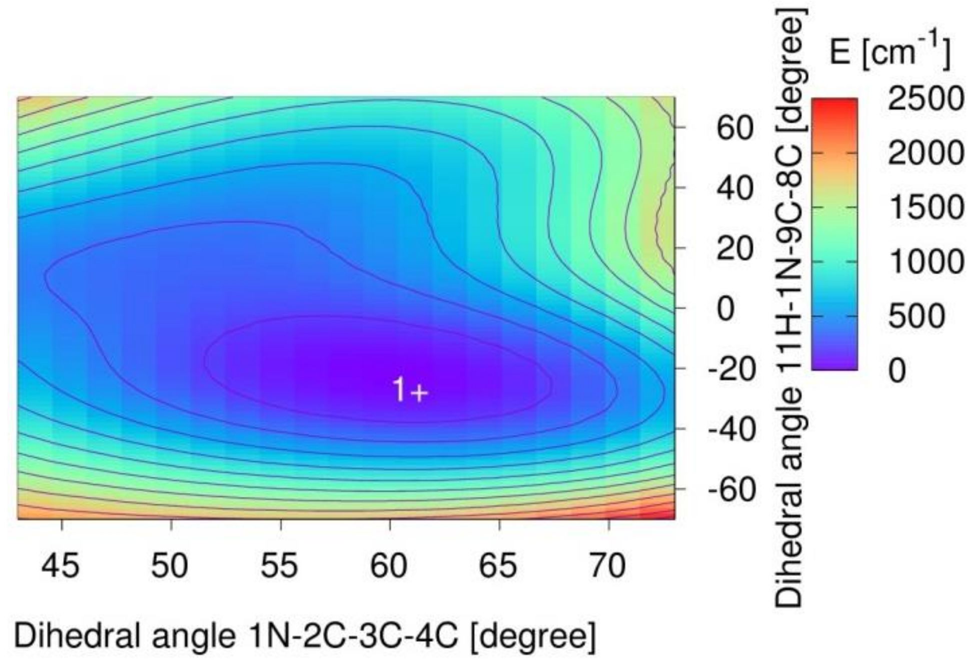

Fig. F6: The 3-dimensional potential energy surface scanned along the dihedral angles 1N-2C-3C-4C and 11H-1N-9C-8C by MP2/cc-pVDZ.

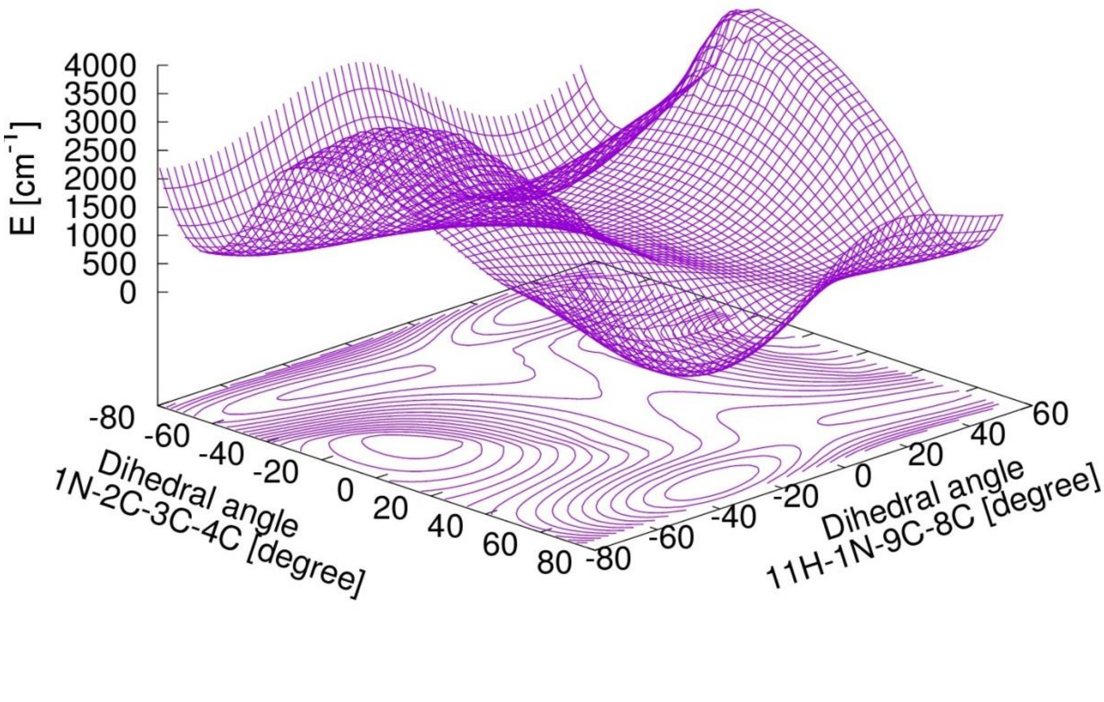

Table T5: The R-branch rotational transitions of 1,2,3,4-tetrahydroquinoline measured by COBRA- and IMPACT-FTMW spectrometers in the frequency range from 7 to 20 GHz. Numbers in parentheses are uncertainties in units of the least significant digit. The uncertainties of the transition frequencies were calculated as $\boldsymbol{U} = \frac{\sqrt{u_1^2+u_2^2}}{2}$, where u_1 and u_2 are the uncertainties of each Doppler doublet component position.

Transition $J_{K_aK_c} \leftarrow J'_{K'_aK'_b}$	F ← F'	Observed frequency [MHz]	Obs.– calc. [MHz]
$3_{13} \leftarrow 4_{14}$	4 ← 5	7314.14205 (82)	-0.00111
	2 ← 3	7314.26421 (687)	0.00098
	3 ← 4	7314.34441 (478)	-0.00192
$3_{03} \leftarrow 4_{04}$	4 ← 5	7645.98744 (231)	-0.00178
	2 ← 3	7646.02776 (136)	-0.00004
	3 ← 4	7646.31967 (27)	-0.00061
$3_{22} \leftarrow 4_{23}$	2 ← 3	7970.31146 (581)	0.00091
	4 ← 5	7970.41357 (94)	0.00082
	3 ← 4	7970.80623 (56)	-0.00002
$3_{21} \leftarrow 4_{22}$	2 ← 3	8324.80906 (325)	-0.00301
	4 ← 5	8324.87508 (185)	0.00054
	3 ← 4	8324.95661 (53)	-0.00013
$3_{12} \leftarrow 4_{13}$	2 ← 3	8531.02745 (800)	0.00108
	4 ← 5	8531.11743 (410)	0.00017
	3 ← 4	8531.30264 (430)	0.00039
$4_{14} \leftarrow 5_{15}$	5 ← 6	9088.60619 (510)	-0.00027
	3 ← 4	9088.68394 (490)	-0.00002
	4 ← 5	9088.76515 (310)	-0.00091
$4_{04} \leftarrow 5_{05}$	5 ← 6	9362.11192 (156)	-0.00065
	3 ← 4	9362.13467 (282)	0.00156
	4 ← 5	9362.42018 (211)	-0.00164
$1_{11} \leftarrow 2_{21}$	2 ← 3	9680.16662 (810)	0.00648
$4_{04} \leftarrow 5_{15}$	3 ← 4	9838.48222 (93)	0.00336
	5 ← 6	9838.51500 (38)	-0.00155
	4 ← 5	9839.11112 (38)	0.00030
$4_{23} \leftarrow 5_{24}$	3 ← 4	9915.02587 (96)	0.00049
	5 ← 6	9915.05545 (315)	-0.00051
	4 ← 5	9915.30920 (31)	0.00080
$4_{41} \leftarrow 5_{42}$	3 ← 4	10086.17933 (213)	0.00075
	5 ← 6	10086.36369 (350)	-0.00780
	4 ← 5	10086.98618 (136)	-0.00180
$4_{32} \leftarrow 5_{33}$	5 ← 5	10104.46301 (39)	-0.00248
	5 ← 6	10104.55421 (29)	-0.00060
	4 ← 5	10104.89744 (29)	-0.00045
$4_{31} \leftarrow 5_{32}$	3 ← 4	10166.41800 (87)	-0.00177
	5 ←6	10166.49968 (24)	-0.00041
	4 ← 5	10166.76803 (20)	-0.00069

Table T5: *(Continued)*

Transition $J_{K_aK_c} \leftarrow J'_{K'_aK'_b}$	F ← F'	Observed frequency [MHz]	Obs.– calc. [MHz]
	4 ← 5	10552.14093 (345)	0.00089
$4_{22} \leftarrow 5_{23}$	3 ← 4	10552.16680 (412)	-0.00429
	5 ← 6	10552.18324 (550)	0.00128
	3 ← 4	10570.41118 (19)	-0.00082
$4_{13} \leftarrow 5_{14}$	5 ← 6	10570.46771 (33)	0.00048
	4 ← 5	10570.66490 (30)	0.00044
	6 ← 7	10839.38368 (69)	-0.00190
$5_{15} \leftarrow 6_{16}$	4 ← 5	10839.44312 (431)	0.00315
	5 ← 6	10839.52137 (66)	-0.00022
	6 ← 7	11033.69231 (92)	-0.00076
$5_{05} \leftarrow 6_{06}$	4 ← 5	11033.71525 (924)	-0.00203
	5 ← 6	11033.94694 (51)	-0.00152
$2_{11} \leftarrow 3_{21}$	3 ← 4	11251.70644 (140)	-0.01057
	2 ← 3	11251.98234 (750)	-0.00512
	4 ← 5	11315.78152 (831)	-0.00420
$5_{05} \leftarrow 6_{16}$	6 ← 7	11315.78884 (778)	-0.00072
	5 ← 6	11316.21105 (601)	0.00046
	4 ← 5	11829.02240 (45)	0.00065
$5_{24} \leftarrow 6_{25}$	6 ← 7	11829.03455 (66)	0.00180
	5 ← 6	11829.23053 (52)	-0.00008
	4 ← 5	12129.93148 (65)	-0.00350
$5_{42} \leftarrow 6_{43}$	6 ← 7	12130.01793 (65)	0.00259
	5 ← 6	12130.35926 (24)	0.00117
	4 ← 5	12136.97587 (50)	0.00011
$5_{41} \leftarrow 6_{42}$	6 ← 7	12137.05442 (35)	-0.00032
	5 ← 6	12137.38822 (21)	-0.00042
	4 ← 5	12138.98304 (85)	0.00013
$5_{33} \leftarrow 6_{34}$	6 ← 7	12139.01921 (65)	-0.00071
	5 ← 6	12139.22205 (39)	0.00021
	4 ← 5	12297.26631 (45)	-0.00093
$5_{32} \leftarrow 6_{33}$	6 ← 7	12297.28529 (62)	-0.00212
	5 ← 6	12297.36497 (51)	0.00159
	4 ← 5	12533.52109 (71)	0.00037
$5_{14} \leftarrow 6_{15}$	6 ← 7	12533.56470 (67)	0.00099
	5 ← 6	12533.79949 (203)	0.00056
	7 ← 8	12570.41586 (22)	-0.00008
$6_{16} \leftarrow 7_{17}$	5 ← 6	12570.45504 (372)	-0.00175
	6 ← 7	12570.53398 (442)	-0.00030
	7 ← 8	12693.99840 (92)	-0.00097
$6_{06} \leftarrow 7_{07}$	5 ← 6	12694.02404 (31)	-0.00101
	6 ← 7	12694.19254 (88)	-0.00181
	5 ← 6	12789.24975 (16)	0.00049
$5_{23} \leftarrow 6_{24}$	4 ← 5	12789.27962 (26)	-0.00102
	6 ← 7	12789.29006 (31)	0.00187

Table T5: *(Continued)*

Transition $J_{K_aK_c} \leftarrow J'_{K'_aK'_b}$	F ← F'	Observed frequency [MHz]	Obs.– calc. [MHz]
	7 ← 8	12852.51146 (52)	-0.00097
$6_{06} \leftarrow 7_{17}$	5 ← 6	12852.52792 (91)	0.00269
	6 ← 7	12852.79629 (39)	-0.00013
	2 ← 3	13138.77488 (940)	0.00725
$3_{12} \leftarrow 4_{22}$	4 ← 5	13138.84343 (710)	0.00605
	3 ← 4	13138.94048 (490)	0.00020
	5 ← 6	13708.52850 (686)	-0.00236
$6_{25} \leftarrow 7_{26}$	7 ← 8	13708.53689 (417)	0.00156
	6 ← 7	13708.70974 (54)	-0.00002
	5 ← 6	14164.10890 (89)	-0.00084
$6_{34} \leftarrow 7_{35}$	7 ← 8	14164.12750 (45)	0.00019
	6 ← 7	14164.26852 (39)	0.00054
	5 ← 6	14184.70803 (78)	0.00222
$6_{43} \leftarrow 7_{44}$	7 ← 8	14184.74249 (36)	-0.00006
	6 ← 7	14184.94680 (68)	0.00122
	5 ← 6	14207.69935 (98)	0.00241
$6_{42} \leftarrow 7_{43}$	7 ← 8	14207.73149 (52)	0.00054
	6 ← 7	14207.91304 (71)	0.00004
	8 ← 9	14286.61268 (214)	0.00222
$7_{17} \leftarrow 8_{18}$	6 ← 7	14286.64321 (416)	0.00044
	7 ← 8	14286.71402 (498)	0.00068
	8 ← 9	14359.38911 (13)	0.00065
$7_{07} \leftarrow 8_{08}$	6 ← 7	14359.41231 (33)	-0.00133
	7 ← 8	14359.53507 (11)	0.00020
	5 ← 6	14400.28347 (83)	0.00120
$6_{15} \leftarrow 7_{16}$	7 ← 8	14400.31791 (38)	-0.00015
	6 ← 7	14400.59626 (73)	0.00077
	8 ← 9	14445.12112 (711)	-0.00241
$7_{07} \leftarrow 8_{18}$	6 ← 7	14445.14651 (798)	0.00356
	7 ← 8	14445.31635 (659)	0.00094
	6 ← 7	14494.85825 (42)	0.00047
$6_{33} \leftarrow 7_{34}$	7 ← 8	14494.89584 (588)	0.00009
	5 ← 6	14494.89852 (622)	0.00060
	5 ← 6	14992.67470 (201)	-0.00417
$6_{24} \leftarrow 7_{25}$	7 ← 8	14992.68897 (105)	-0.00196
	6 ← 7	14992.70237 (131)	0.00353
	4 ← 5	15159.78271 (97)	0.00464
$4_{13} \leftarrow 5_{23}$	5 ← 6	15159.90216 (270)	0.00008
	3 ← 4	15159.91521 (540)	0.00286
	1 ← 2	15196.21086 (760)	0.00031
$2_{20} \leftarrow 3_{30}$	2 ← 3	15196.23667 (620)	-0.00524
	3 ← 4	15196.36148 (580)	-0.00918
	6 ← 7	15551.86396 (484)	0.00026
$7_{26} \leftarrow 8_{27}$	8 ← 9	15551.87141 (424)	0.00578
	7 ← 8	15552.02772 (40)	-0.00081

Table T5: *(Continued)*

Transition $J_{K_aK_c} \leftarrow J'_{K'_aK'_b}$	F ← F'	Observed frequency [MHz]	Obs.– calc. [MHz]
	9 ← 10	15992.62987 (321)	0.00166
$8_{18} \leftarrow 9_{19}$	7 ← 8	15992.65230 (515)	-0.00245
	8 ← 9	15992.71696 (400)	-0.00018
	9 ← 10	16033.28526 (52)	0.00116
$8_{08} \leftarrow 9_{09}$	7 ← 8	16033.30612 (93)	-0.00129
	8 ← 9	16033.39595 (62)	-0.00007
	6 ← 7	16165.11096 (57)	0.00160
$7_{16} \leftarrow 8_{17}$	8 ← 9	16165.13917 (60)	-0.00035
	7 ← 8	16165.44164 (39)	0.00059
	6 ← 7	16190.73816 (161)	0.00442
$7_{53} \leftarrow 8_{54}$	8 ← 9	16190.77113 (155)	0.00149
	7 ← 8	16190.98812 (136)	-0.00061
	6 ← 7	16248.32477 (43)	-0.00082
$7_{44} \leftarrow 8_{45}$	8 ← 9	16248.34283 (39)	-0.00032
	7 ← 8	16248.46853 (45)	-0.00120
	6 ← 7	16309.52438 (256)	-0.00561
$7_{43} \leftarrow 8_{44}$	8 ← 7	16309.54435 (501)	-0.00481
	7 ← 8	16309.62696 (478)	-0.00094
$6_{15} \leftarrow 7_{26}$	7 ← 8	16412.49183 (623)	-0.00164
	7 ← 8	16759.27374 (971)	-0.00624
$7_{34} \leftarrow 8_{35}$	8 ← 9	16759.37456 (787)	-0.00202
	6 ← 7	16759.38840 (602)	0.00282
	6 ← 7	17132.52044 (63)	-0.00080
$7_{25} \leftarrow 8_{26}$	8 ← 9	17132.53771 (61)	0.00036
	7 ← 8	17132.59899 (89)	-0.00267
	7 ← 8	17359.88891 (270)	-0.00013
$8_{27} \leftarrow 9_{28}$	9 ← 10	17359.88952 (203)	-0.00013
	8 ← 9	17360.04338 (120)	-0.00133
	10 ← 11	17692.18580 (59)	-0.00011
$9_{19} \leftarrow 10_{110}$	8 ← 9	17692.20702 (33)	-0.00127
	9 ← 10	17692.26270 (41)	0.00020
	10 ← 11	17714.07241 (378)	0.00305
$9_{09} \leftarrow 10_{010}$	8 ← 9	17714.08789 (409)	-0.00242
	9 ← 10	17714.15705 (383)	-0.00051
	7 ← 8	17847.64494 (65)	0.00120
$8_{17} \leftarrow 9_{18}$	9 ← 10	17847.66644 (40)	0.00007
	8 ← 9	17847.96139 (27)	0.00013
	7 ← 8	18148.92995 (68)	-0.00338
$8_{36} \leftarrow 9_{37}$	9 ← 10	18148.94264 (77)	0.00229
	8 ← 9	18149.05072 (83)	0.00105
	7 ← 8	18316.00821 (213)	0.00315
$8_{45} \leftarrow 9_{46}$	9 ← 10	18316.01795 (77)	0.00359
	8 ← 9	18316.09668 (83)	-0.00279

Table T5:*(Continued)*

Transition $J_{K_aK_c} \leftarrow J'_{K'_aK'_b}$	F ← F'	Observed frequency [MHz]	Obs.– calc. [MHz]
$8_{44} \leftarrow 9_{45}$	7 ← 8	18455.77296 (340)	0.00436
	9 ← 10	18455.77549 (531)	0.00485
	8 ← 9	18455.78694 (503)	0.00417
$8_{35} \leftarrow 9_{36}$	8 ← 9	19064.56091 (321)	-0.00083
	9 ← 10	19064.67056 (333)	0.00492
	7 ← 8	19064.68323 (212)	0.00979
$9_{28} \leftarrow 10_{29}$	10 ← 11	19135.98506 (233)	-0.00297
	8 ← 9	19135.98542 (99)	-0.00287
	9 ← 10	19136.14035 (343)	0.00514
$8_{26} \leftarrow 9_{27}$	7 ← 8	19188.05863 (161)	-0.00504
	9 ← 10	19188.07886 (127)	-0.00328
	8 ← 9	19188.20100 (78)	-0.00238
$10_{110} \leftarrow 11_{111}$	11 ← 12	19387.89949 (185)	-0.00195
	9 ← 10	19387.92080 (126)	0.00014
	10 ← 11	19387.96712 (100)	-0.00027
$10_{010} \leftarrow 11_{011}$	11 ← 12	19399.36149 (92)	-0.00202
	9 ← 10	19399.38272 (118)	0.00061
	10 ← 11	19399.43601 (890)	0.00085
$9_{18} \leftarrow 10_{19}$	8 ← 9	19486.19676 (116)	-0.00278
	10 ← 11	19486.21732 (117)	0.00306
	9 ← 10	19486.47488 (196)	-0.00097

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