Cold Snapshot of a Molecular Rotary Motor Captured by High-Resolution Rotational Spectroscopy

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1 Experimental details

We use broadband rotational spectroscopy to investigate the rotational spectrum of molecular motor 1-A using chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). The spectrum was recorded using the Hamburg COMPACT spectrometer as described elsewhere.[1] The sample was synthesised and purified as previously described.[2] A supersonic expansion brings the sample into the vacuum chamber where a 4 µs chirp spanning 2–4 GHz polarises the ensemble of molecules. The seeding of molecules into a supersonic expansion is done using a pulsed nozzle (Parker General Valve Series 9) operating at 3 Hz with a constant flow of Ne at stagnation pressures of 0.5 bar to generate a cold molecular jet. To create sufficient vapour pressure the sample was heated to 180°C directly at the nozzle. The chirp is generated with an arbitrary waveform generator and amplified in a 300 W traveling wave tube amplifier (2.5–7.5 GHz) before being broadcast into the vacuum chamber using a horn antenna. For this particular molecular system, a shorter chirp was produced in the arbitrary waveform generator covering only 2 GHz instead of the 6 GHz normally utilised in our spectrometer. In this way we effectively allocate the entire 300 W amplification power over the frequency region of interest and improve our signal-to-noise ratio. Upon chirped microwave excitation we record the free induction decay (FID) of the macroscopic dipole moment of the ensemble of molecules. In our experiments we used a new data acquisition scheme using the ‘fast frame’ option of the digital oscilloscope.[3] In short, eight back-to-back excitation chirps are performed on each sample pulse, and the subsequent eight FID acquisitions are co-added and averaged. This scheme decreases the measurement time and sample consumption, resulting in an effective repetition rate of 24 Hz for this particular experiment. We record 40 µs of the FIDs which, after a Fourier transformation (FT), gives a resolution of 25 kHz in the microwave spectrum. 1.5 M FIDs (equivalent to 13 hours of measurement time) were co-added to obtain the final spectrum.

2 Theoretical details

Geometry optimisations were performed using second-order Møller-Plesset perturbation theory (MP2), and Density Functional Theory using the hybrids B3LYP (Becke, three-parameter, LeeYangParr), B3LYP-D3BJ (including Grimme’s dispersion correction[4] with Becke-Johnson damping[5]) and the M06-2X exchange-correlation energy functional.[6] Basis sets 6-311++G** and def2-TZVP were used. All calculations were done using Gaussian09.[7]
3 Rotational spectra of the dissociation products

![Graph showing rotational spectra](image)

Figure 1: Broadband rotational spectrum of the molecular motor from 2 to 4 GHz (1.5M averages, 13 h of measurement time). The upper trace (in black) shows the experimental spectrum using neon as carrier gas. The lower trace represents simulations obtained from the fitted spectroscopic parameters of the dissociation structure of the rotor (r-B, see Table 2 in main paper). [*] The simulated spectrum of fluorene was obtained directly using the rotational constants reported in Ref 16 (A=2176.210160(70) MHz, B=586.65338(12) MHz, C=463.568993(63) MHz).

4 Line lists

4.1 Molecular Motor

Table 1: Observed and calculated rotational transitions (MHz) for the molecular motor. A few additional strong transitions above 4 GHz were included in the fit and those are listed at the end of the table.

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4.2 Rotor fragment (r-B)

Table 2: Observed and calculated rotational transitions (MHz) for the rotor fragment. The strong a-type character of r-B allowed observation of rotational transitions up to about 7 GHz.

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