**Supplemental Material for:** "Rotational Constants and Structure of $para$-Difluorobenzene Determined by Femtosecond Raman Coherence Spectroscopy: A New Transient Type"

*Takuya Den*[1], *Hans-Martin Frey*[1], *Peter M. Felker*[2], *and Samuel Leutwyler*[1]

[1]Departement für Chemie und Biochemie, Universität Bern, Freiestrasse 3, CH-3000 Bern 9, Switzerland

[2] Department of Chemistry and Biochemistry, 607 Charles E. Young Drive East, University of California at Los Angeles, USA

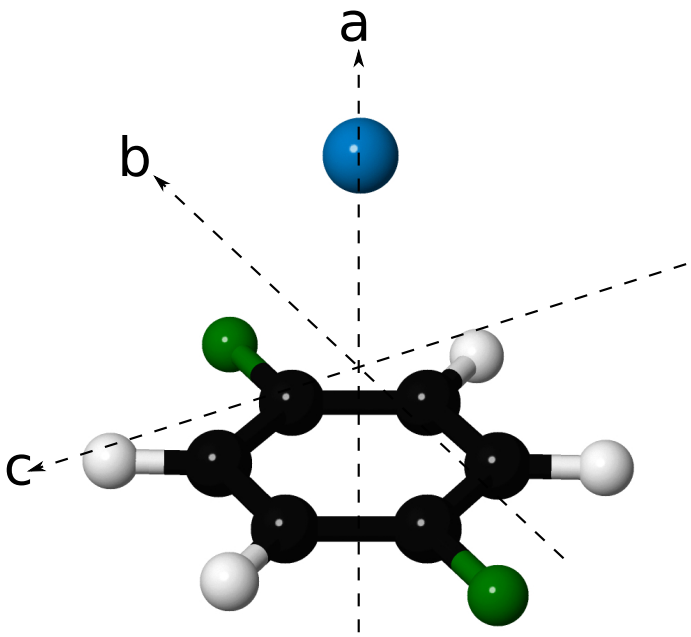


Figure S1. Schematic structure of the para-difluorobenzene-Ar complex with inertial axes, cf. Riehn, Chem. Phys. **283** (2002) 297-320.

source: https://doi.org/10.7892/boris.75046 | downloaded: 2.12.2024

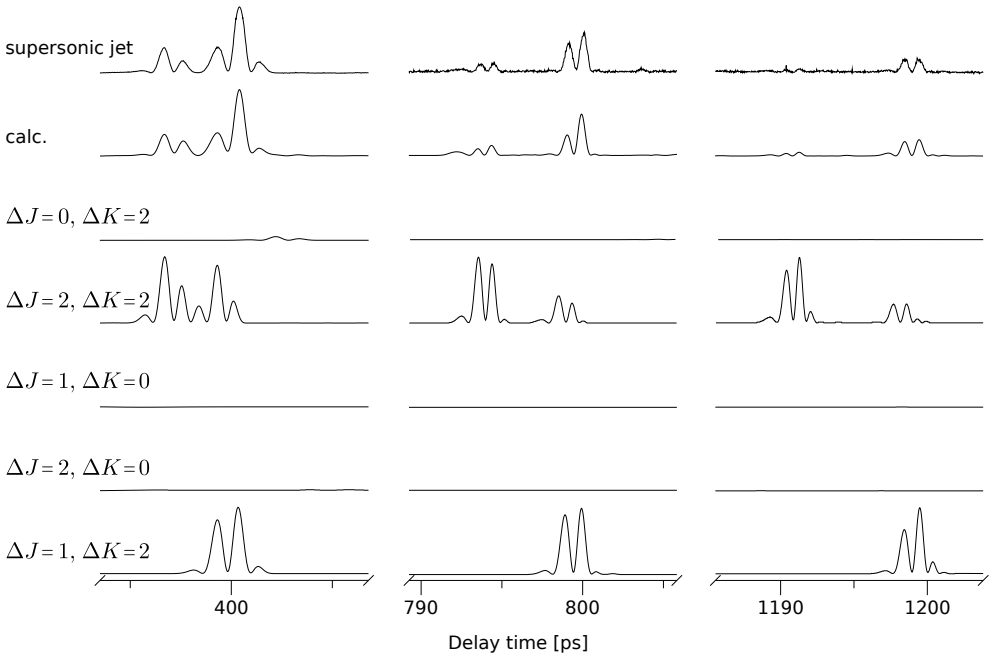


Figure S2. Transients at multiples of $400$ ps are produced by coherences with $\Delta J = 1, \Delta K = 2$. Coherences with $\Delta J = 2, \Delta K = 2$ also contribute but with smaller intensity. Also they are slightly shifted to shorter delay times.

Table S1: CCSD(T)/cc-pwCVDZ calculated vibrational frequencies (in $cm^{-1}$), population in % at 130 K and rotational-vibration coupling constants $\alpha^B_{v,i}$, $i = A, B, C$ (in MHz).

| Normal mode | Wavenumber | Population | Symmetry | $\alpha_1^A$ | $\alpha_1^B$ | $\alpha_1^C$ |
|---|---|---|---|---|---|---|
| $v = 0$ | 0.0 | 81.4 | $A_g$ | 0 | 0 | 0 |
| $\nu_7$ | 159.5 | 12.0 | $B_{1u}$ | 26.15 | -0.64 | -1.06 |
| $\nu_8$ | 342.4 | 1.3 | $B_{2u}$ | -24.23 | 0.08 | 0.47 |
| $\nu_9$ | 377.4 | 0.9 | $B_{2g}$ | 65.06 | -0.88 | -0.82 |
| $\nu_{10}$ | 422.1 | 0.5 | $A_u$ | 5.06 | -0.19 | -0.56 |
| $\nu_{11}$ | 437.3 | 0.4 | $B_{1g}$ | -62.61 | -0.19 | 1.15 |
| $\nu_{12}$ | 448.5 | 0.4 | $A_g$ | -0.81 | -0.11 | -0.65 |
| $\nu_{13}$ | 522.0 | 0.2 | $B_{1u}$ | -0.48 | 0.17 | -0.46 |
| $\nu_{14}$ | 637.6 | 0 | $B_{1g}$ | 6.89 | -0.02 | 0.34 |
| $\nu_{15}$ | 656.6 | 0 | $B_{2g}$ | -5.38 | -0.22 | -0.45 |
| $\nu_{16}$ | 741.9 | 0 | $B_{3u}$ | 2.34 | 0.52 | 0.53 |
| $\nu_{17}$ | 827.3 | 0 | $B_{3g}$ | 9.11 | 0.31 | -0.08 |
| $\nu_{18}$ | 851.5 | 0 | $B_{1u}$ | 7.53 | 0.24 | -0.16 |
| $\nu_{19}$ | 861.1 | 0 | $A_g$ | -4.96 | 1.00 | 0.63 |
| $\nu_{20}$ | 916.9 | 0 | $B_{2g}$ | 5.90 | 0.08 | -0.23 |
| $\nu_{21}$ | 951.4 | 0 | $A_u$ | 5.95 | 0.52 | -0.15 |
| $\nu_{22}$ | 1017.1 | 0 | $B_{3u}$ | 0.64 | -0.38 | 1.09 |
| $\nu_{23}$ | 1093.9 | 0 | $B_{2u}$ | -1.56 | -0.41 | -0.28 |
| $\nu_{24}$ | 1152.0 | 0 | $A_g$ | 1.95 | -0.91 | -0.01 |
| $\nu_{25}$ | 1248.5 | 0 | $B_{3u}$ | 0.30 | 1.30 | 1.98 |
| $\nu_{26}$ | 1287.8 | 0 | $A_g$ | -0.12 | -0.53 | 0.97 |
| $\nu_{27}$ | 1299.8 | 0 | $B_{1g}$ | 3.66 | 2.93 | 1.23 |
| $\nu_{28}$ | 1329.1 | 0 | $B_{2u}$ | 15.95 | 1.91 | 1.27 |
| $\nu_{29}$ | 1441.2 | 0 | $B_{2u}$ | -0.25 | 1.68 | 1.64 |
| $\nu_{30}$ | 1557.0 | 0 | $B_{3u}$ | 10.14 | 0.62 | 0.51 |
| $\nu_{31}$ | 1657.3 | 0 | $B_{1g}$ | 11.50 | 1.61 | 5.85 |
| $\nu_{32}$ | 678.0 | 0 | $A_g$ | 9.99 | 1.65 | -2.62 |
| $\nu_{33}$ | 3190.9 | 0 | $B_{3u}$ | 2.75 | 0.49 | 0.42 |
| $\nu_{34}$ | 3192.8 | 0 | $B_{1g}$ | 2.78 | 0.48 | 0.41 |
| $\nu_{35}$ | 3206.0 | 0 | $B_{2u}$ | 2.80 | 0.53 | 0.43 |
| $\nu_{36}$ | 3206.8 | 0 | $A_g$ | 2.88 | 0.52 | 0.43 |

[a] vibrational partition function truncated at 1000 $cm^{-1}$.