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

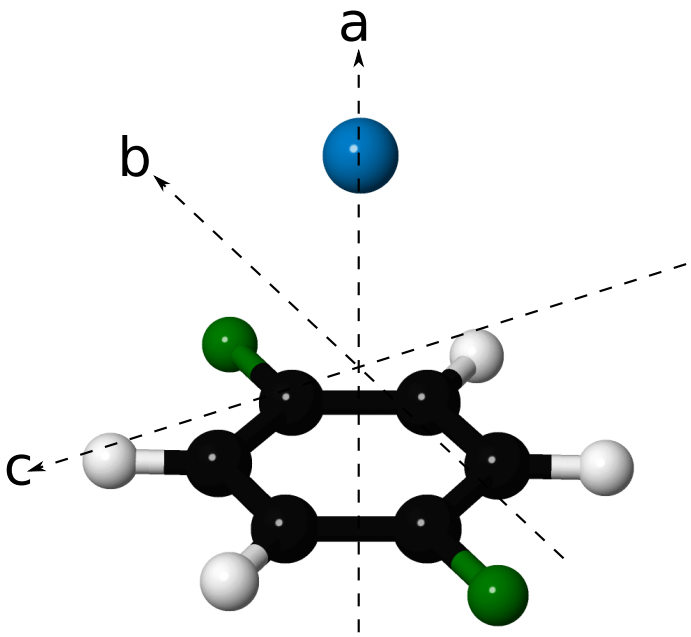

Figure S1. Schematic structure of the para-difluorobenzene-Ar complex with inertial axes, cf. Riehn, Chem. Phys. **283** (2002) 297-320.

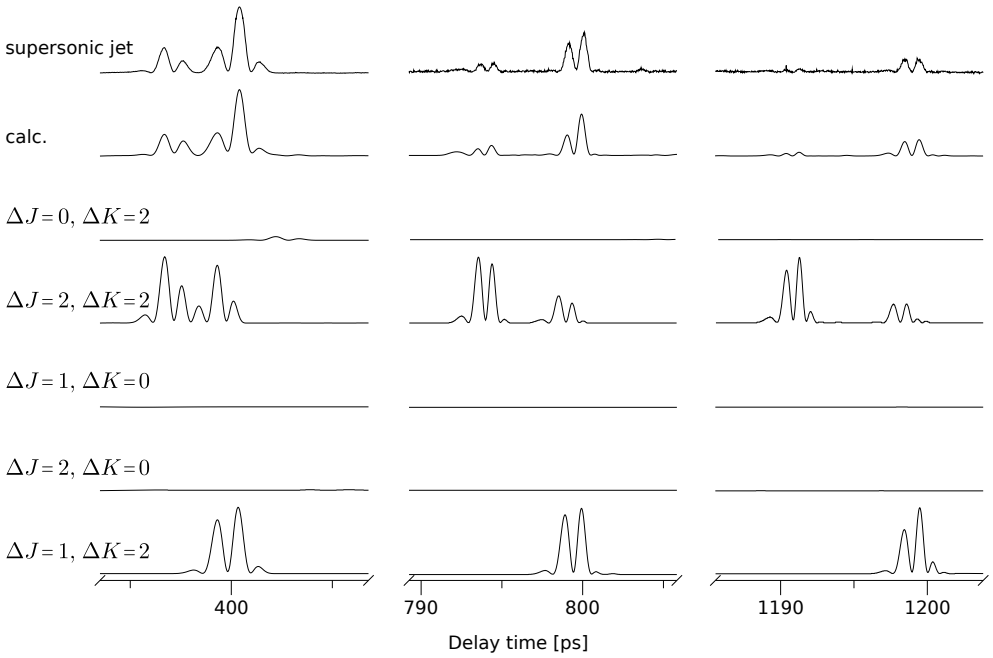

Figure S2. Transients at multiples of 400 ps are produced by coherences with $\Delta J = 1, \Delta K = 2$. Coherences with $\Delta J = 2, \Delta K = 2$ also contribute but with smaller intensity. Also they are slightly shifted to shorter delay times.

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	α_1^A	α_1^B	α_1^C
$v = 0$	0.0	81.4	A_g	0	0	0
ν_7	159.5	12.0	B_{1u}	26.15	-0.64	-1.06
ν_8	342.4	1.3	B_{2u}	-24.23	0.08	0.47
ν_9	377.4	0.9	B_{2g}	65.06	-0.88	-0.82
ν_{10}	422.1	0.5	A_u	5.06	-0.19	-0.56
ν_{11}	437.3	0.4	B_{1g}	-62.61	-0.19	1.15
ν_{12}	448.5	0.4	A_g	-0.81	-0.11	-0.65
ν_{13}	522.0	0.2	B_{1u}	-0.48	0.17	-0.46
ν_{14}	637.6	0	B_{1g}	6.89	-0.02	0.34
ν_{15}	656.6	0	B_{2g}	-5.38	-0.22	-0.45
ν_{16}	741.9	0	B_{3u}	2.34	0.52	0.53
ν_{17}	827.3	0	B_{3g}	9.11	0.31	-0.08
ν_{18}	851.5	0	B_{1u}	7.53	0.24	-0.16
ν_{19}	861.1	0	A_g	-4.96	1.00	0.63
ν_{20}	916.9	0	B_{2g}	5.90	0.08	-0.23
ν_{21}	951.4	0	A_u	5.95	0.52	-0.15
ν_{22}	1017.1	0	B_{3u}	0.64	-0.38	1.09
ν_{23}	1093.9	0	B_{2u}	-1.56	-0.41	-0.28
ν_{24}	1152.0	0	A_g	1.95	-0.91	-0.01
ν_{25}	1248.5	0	B_{3u}	0.30	1.30	1.98
ν_{26}	1287.8	0	A_g	-0.12	-0.53	0.97
ν_{27}	1299.8	0	B_{1g}	3.66	2.93	1.23
ν_{28}	1329.1	0	B_{2u}	15.95	1.91	1.27
ν_{29}	1441.2	0	B_{2u}	-0.25	1.68	1.64
ν_{30}	1557.0	0	B_{3u}	10.14	0.62	0.51
ν_{31}	1657.3	0	B_{1g}	11.50	1.61	5.85
ν_{32}	678.0	0	A_g	9.99	1.65	-2.62
ν_{33}	3190.9	0	B_{3u}	2.75	0.49	0.42
ν_{34}	3192.8	0	B_{1g}	2.78	0.48	0.41
ν_{35}	3206.0	0	B_{2u}	2.80	0.53	0.43
ν_{36}	3206.8	0	A_g	2.88	0.52	0.43

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