

ARS (Ar = *p*-FC₆H₄) Monomer Radical [neutral, doublet] at UB3LYP/6-311++G(2d,p).

Mode No.	Frequency cm ⁻¹	IR Intensity 10 ⁻⁴⁰ esu ² cm ²	Raman Activity A ² /AMU	Scaled Freq. x0.98	bond/group	Assign motion	direction	activity	type
1	111.8	2.0	1.2	110	S-CCCC-F	single bend	out-of-plane		a
2	267.7	1.3	2.2	262	C-C-S	head-waving skew	in-plane		b
3	308.1	0.5	1.0	302	S-CCCC-F	dolphin kick	out-of-plane		c
4	383.4	5.7	16.4	376	S-CCCC-F	ring squaring	in-plane	IR/Raman	d
5	397.4	0.0	0.2	389	C-C-C	skew	out-of-plane		e
6	423.2	3.4	0.0	415	C-C-F	tail-waving skew	in-plane		f
7	517.7	15.5	1.5	507	C-C-C	butterfly	out-of-plane	IR	g
8	638.4	0.0	5.3	626	C-C-C	ring squeeze	in-plane	Raman	h
9	658.0	12.9	9.6	645	C-S	stretch	in-plane	IR/Raman	i
10	727.0	0.0	0.2	712	C-C-C	ring chairing	out-of-plane		j
11	818.0	0.0	0.0	802	C-C-H	padding	out-of-plane		k
12	835.1	13.7	42.9	818	C-S/C-F	ring squaring	in-plane	IR/Raman	l
13	856.7	62.2	0.2	840	C-C-H	zigzag bend	out-of-plane	IR	m
14	972.3	0.0	0.0	953	C-C-H	butterflying	out-of-plane		n
15	978.5	0.0	0.0	959	C-C-H	crawling	out-of-plane		o
16	1024.0	2.0	1.6	1004	C-C	ring triangularing	in-plane		p
17	1077.9	32.0	20.4	1056	C-C/C-S	stretch/ring breathing	in-plane	IR/Raman	q
18	1112.8	4.0	0.9	1091	C-C	anti-sym ring defoem	in-plane		r
19	1175.9	40.3	8.2	1152	C-C	sym-ring defoem	in-plane	IR/Raman	s
20	1255.7	153.4	15.2	1231	S-F	stretch	in-plane	IR/Raman	t
21	1293.7	0.1	1.4	1268	C-C/C-S	2-fold ring twist	in-plane		u
22	1313.1	7.3	3.8	1287	C-C/C-F	1-fold ring twist	in-plane	IR	v
23	1431.5	7.1	1.3	1403	C-C	ring defoem	in-plane	IR	w
24	1496.9	45.4	3.9	1467	C-C/C-F/C-S	ring defoem	in-plane	IR	x
25	1576.1	7.8	1.4	1545	C-C	2-fold ring twist	in-plane	IR	y
26	1601.8	213.9	123.8	1570	C-C/C-F	ring squaring	in-plane	IR/Raman	z
27	3190.4	1.1	20.2	3127	C-H	stretch	in-plane	Raman	
28	3191.3	0.1	97.9	3127	C-H	stretch	in-plane	Raman	
29	3202.9	0.5	14.0	3139	C-H	stretch	in-plane	Raman	
30	3204.7	2.4	250.7	3141	C-H	sym-stretch breathing	in-plane	Raman	

*Colours distinguish prominent Raman modes (yellow) or in-plane (green) or out-of-plane (orange) vibrational modes.

*Type depicts each of the 26 vibrational modes other than four C-H stretching modes as a-z from low frequencies.