ArSSAr (Ar = *p*-FC_6H_4) Disulfide [neutral, singlet] at B3LYP/6-311++G(2d,p).

Mode	Frequency	IR Intensity	Raman Activity	Scaled Freq.	Assign				activity	type
No.	cm^{-1}	10^{-40} esu^2 cm^2	Å^2/AMU	x0.98	bond/group	motion	direction	phase		
1	17.9	0.0	5.1	18	S-S	rotation Z	inter molecular	ring overlap	Raman	
2	22.1	0.1	3.0	22	C-S	rotation anti-sym	inter molecular	dihedral angle		
3	25.3	0.0	5.3	25	C-S	rotation sym	inter molecular	dihedral angle	Raman	
4	67.2	0.3	3.9	66	S-S	rotation X	inter molecular			
5	76.8	0.2	4.1	75	S-S	rotation Y	inter molecular			
6	138.9	0.1	3.7	136	S-CCCC-F	single bend	out-of-plane	sym		a
7	194.4	1.2	2.3	191	S-CCCC-F			anti-sym		a
8	249.2	1.5	0.0	244	C-C-S	head-waiving skew	in-plane	anti-sym		b
9	277.0	1.5	4.1	271	C-C-S			sym		b
10	321.0	0.4	8.1	315	S-CCCC-F/S-S	dolphin kick	out-of-plane	sym	Raman	c
11	346.4	10.0	1.9	339	S-CCCC-F/S-S			anti-sym	IR	c
12	383.5	10.1	3.9	376	S-CCCC-F/S-S	ring squaring	in-plane	sym	IR	d
13	395.6	8.3	0.2	388	S-CCCC-F/S-S		/out-of-plane	anti-sym	IR	d
14	421.2	3.5	0.0	413	C-C-C	tail-waving skew	in-plane	anti-sym		f
15	423.2	0.5	4.5	415	C-C-C			sym		f
16	427.5	0.1	1.0	419	C-C-C	skew	out-of-plane	sym		e
17	429.3	0.2	0.0	421	C-C-C			anti-sym		e
18	460.1	3.0	100.0	451	S-S	stretch	inter molecular	sym	Raman	
19	529.5	8.0	0.9	519	C-C-C	butterfly	out-of-plane	sym	IR	g
20	529.5	32.7	0.5	519	C-C-C			anti-sym	IR	g
21	632.0	4.3	13.8	619	C-S	stretch	in-plane	sym	Raman	i
22	633.1	11.2	3.7	620	C-S			anti-sym	IR	i
23	645.6	0.1	1.3	633	C-C-C	ring squeeze	in-plane	anti-sym		h
24	645.8	0.0	8.8	633	C-C-C			sym	Raman	h
25	730.1	0.4	1.1	715	C-C-C	ring chairing	out-of-plane	sym		j
26	732.1	0.2	0.3	717	C-C-C			anti-sym		j
27	824.6	0.1	0.2	808	C-C-H	paddling	out-of-plane	anti-sym		k
28	825.6	1.0	0.5	809	C-C-H			sym		k
29	834.8	21.1	42.8	818	C-S/C-F	ring-squaring	in-plane	sym	IR/Raman	l
30	835.1	14.5	1.8	818	C-S/C-F			anti-sym	IR	l
31	854.9	6.3	3.2	838	C-C-H	zigzag bend	out-of-plane	sym	IR	m
32	855.3	93.5	0.2	838	C-C-H			anti-sym	IR	m
33	964.9	0.2	0.2	946	C-C-H	butterflying	out-of-plane	sym		n
34	967.2	0.1	0.1	948	C-C-H			anti-sym		n
35	975.1	0.2	0.1	956	C-C-H	crawling	out-of-plane	anti-sym		o
36	975.3	0.1	0.4	956	C-C-H			sym		o
37	1033.1	6.9	0.2	1012	C-C	ring triangularing	in-plane	anti-sym	IR	p
38	1033.4	2.3	2.7	1013	C-C			sym		p
39	1089.4	1.8	195.2	1068	C-C/C-S	stretch/ring breathing	in-plane	sym	Raman	q
40	1094.4	2.4	30.9	1072	C-C/C-S			anti-sym	Raman	q
41	1113.6	6.7	0.2	1091	C-C	anti-sym ring deform	in-plane	anti-sym	IR	r
42	1114.1	3.9	4.1	1092	C-C			sym		r
43	1176.5	62.3	3.6	1153	C-C	sym-ring deform	in-plane	anti-sym	IR	s
44	1178.6	21.7	25.4	1155	C-C			sym	IR/Raman	s
45	1244.0	168.9	0.6	1219	C-F	stretch	in-plane	anti-sym	IR	t
46	1244.9	136.2	24.8	1220	C-F			sym	IR/Raman	t
47	1305.6	0.6	0.9	1279	C-C/C-S	2-fold ring twist	in-plane	anti-sym		u
48	1306.0	0.0	5.0	1280	C-C/C-S			sym	Raman	u
49	1319.5	6.9	0.7	1293	C-C/C-F	1-fold ring twist	in-plane	anti-sym	IR	v
50	1319.7	2.6	3.4	1293	C-C/C-F			sym		v
51	1425.8	4.5	0.9	1397	C-C	ring deform	in-plane	anti-sym		w
52	1427.1	1.6	3.1	1399	C-C			sym		w
53	1520.0	72.0	15.7	1490	C-C/C-F/C-S	ring deform	in-plane	sym	IR/Raman	x
54	1520.6	95.4	6.7	1490	C-C/C-F/C-S			anti-sym	IR	x
55	1618.9	2.9	8.1	1587	C-C	2-fold ring twist	in-plane	anti-sym	Raman	y
56	1619.1	21.9	30.0	1587	C-C			sym	IR/Raman	y
57	1623.1	53.2	84.4	1591	C-S/C-F	ring squaring	in-plane	sym	IR/Raman	z
58	1623.5	84.5	68.0	1591	C-S/C-F			anti-sym	IR/Raman	z
59	3186.6	1.7	31.2	3123	C-H	stretch	in-plane	sym	Raman	
60	3186.7	1.3	12.4	3123	C-H	stretch	in-plane	anti-sym	Raman	
61	3187.8	1.6	19.7	3124	C-H	stretch	in-plane	anti-sym	Raman	
62	3187.9	0.0	106.3	3124	C-H	stretch	in-plane	sym	Raman	
63	3200.2	2.4	9.7	3136	C-H	stretch	in-plane	anti-sym	Raman	
64	3200.3	0.3	118.7	3136	C-H	sym-stretch breathing	in-plane	sym	Raman	
65	3201.5	3.5	68.1	3138	C-H	stretch	in-plane	anti-sym	Raman	
66	3201.6	1.7	394.7	3138	C-H	sym-stretch breathing	in-plane	sym	Raman	

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

*On colours in red are the intermolecular vibrational modes including an S-S stretching mode, all associated with the dimer.

*Phase denotes the distinction of the relative motion in the two ArS moieties in the disulfide ArSSAr.

*Type depicts each of the 26 vibrational modes of a-z from low frequencies as deffined for the monomer radical ArS.

*Each type in the a-z modes is doubly degenerated in the disulfide ArSSAr.