

ArS(ArSSAr)⁺ (Ar = p-FC₆H₄) Trimer Cation [mono-cation, 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	7.4	0.1	6.1	7		inter molecular	libration	S ₃ translation	Raman	
2	17.7	0.1	1.6	17		inter molecular	libration	S ₃ translation	Raman	
3	25.3	0.3	3.9	25		inter molecular	libration	S ₃ translation		
4	33.1	0.2	5.0	32	C-S	rotation	all		Raman	
5	36.8	0.1	2.4	36	C-S	rotation	center			
6	39.0	0.2	3.8	38	C-S	rotation	sides			
7	57.7	0.2	6.6	57		inter molecular	swing	S ₃ rotation	Raman	
8	63.2	0.0	7.5	62		inter molecular	swing	S ₃ rotation	Raman	
9	102.7	1.2	11.0	101		inter molecular	swing	S ₃ bend	Raman	
10	117.0	0.3	12.2	115		inter molecular	swing	S ₃ bend	Raman	
11	131.4	0.5	19.5	129	S-CCCC-F		centre-side1	Raman	a	
12	145.8	0.2	36.8	143	S-CCCC-F	single bend	out-of-plane	centre-side2	Raman	a
13	162.2	0.6	16.0	179	S-CCCC-F		all	Raman	a	
14	241.1	4.5	53.5	236	C-C-S		centre	Raman	b	
15	262.0	2.8	1.0	257	C-C-S	head-waiving skew	in-plane	side2	Raman	b
16	265.0	0.5	23.2	260	C-C-S		side1	Raman	b	
17	303.8	1.9	83.3	298	S-CCCC-F/S-S		S ₃ anti-sym str	Raman	c	
18	322.4	1.4	10.5	316	S-CCCC-F/S-S	dolphin kick	out-of-plane	S ₃ bend	Raman	c
19	341.8	20.8	24.4	335	S-CCCC-F/S-S		S ₃ translation	IR/Raman	c	
20	370.2	59.2	95.2	363	S-CCCC-F/S-S		side2/S ₃ anti-sym str	IR/Raman	d	
21	371.9	17.9	77.4	364	S-CCCC-F/S-S	ring squaring	in-plane	side1/S ₃ anti-sym str	IR/Raman	d
22	386.1	6.6	151.5	378	S-CCCC-F/S-S		centre/S ₃ anti-sym str	IR/Raman	d	
23	419.9	1.4	15.9	412	C-C-C		centre out-of-plane	Raman	e,f	
24	422.4	0.7	19.9	414	C-C-C		center in-plane/all	Raman	e,f	
25	424.7	0.1	6.5	416	C-C-C	tail-waving skew	in-plane	side2 out-of-plane	Raman	e,f
26	425.9	3.3	2.3	417	C-C-C	/skew	/out-of-plane	side1 in-plane	Raman	e,f
27	426.7	2.6	0.8	418	C-C-C		side2 in-plane	Raman	e,f	
28	429.4	2.1	26.7	421	C-C-C		side1 out-of-plane	Raman	e,f	
29	443.0	13.1	64.6	434	S-S		S ₃ anti-sym str	IR/Raman		
30	467.7	1.3	146.3	458	S-S	stretch	inter molecular	S ₃ sym str (breathing)	Raman	
31	524.5	31.6	0.4	514	C-C-C		centre	IR	g	
32	533.4	11.4	3.2	523	C-C-C	butterfly	out-of-plane	side1	IR	g
33	537.5	8.6	3.6	527	C-C-C		side2	IR	g	
34	631.9	1.7	33.4	619	C-S	stretch	in-plane	centre	Raman	h
35	640.5	0.7	7.5	628	C-C-C		centre	Raman	h	
36	641.8	0.3	4.8	629	C-C-C	ring squeeze	in-plane	side2	Raman	h
37	642.0	0.3	5.4	629	C-C-C		side1	Raman	h	
38	643.3	2.7	10.1	630	C-S	stretch	in-plane	side1	Raman	i
39	645.2	1.9	17.6	632	C-S		side2	Raman	i	
40	723.2	0.3	2.3	709	C-C-C		center	Raman	j	
41	732.8	1.2	6.3	718	C-C-C	ring chairing	out-of-plane	side1	Raman	j
42	734.2	1.6	9.5	719	C-C-C		side2	Raman	j	
43	825.3	0.1	0.9	809	C-C-H		centre		k	
44	829.9	0.2	0.1	813	C-C-H	padding	out-of-plane	side2		k
45	830.5	0.1	0.1	814	C-C-H		side1		k	
46	839.3	7.9	20.5	823	C-S/C-F		center	IR/Raman	i	
47	841.1	14.3	23.2	824	C-S/C-F	ring-squaring	in-plane	side1	IR/Raman	i
48	841.3	9.5	11.5	824	C-S/C-F		side2	IR/Raman	i	
49	859.8	46.9	5.0	843	C-C-H		centre	IR/Raman	m	
50	865.5	57.3	2.6	848	C-C-H	zigzag bend	out-of-plane	side2	IR	m
51	865.8	46.3	2.6	848	C-C-H		side1	IR	m	
52	972.9	2.3	0.7	953	C-C-H		centre		n	
53	979.1	0.2	0.0	960	C-C-H	butterflying	out-of-plane	side2		n
54	979.7	0.6	0.0	960	C-C-H		side1		n	
55	979.7	0.2	0.2	960	C-C-H		centre		o	
56	984.7	0.1	0.1	965	C-C-H	crawling	out-of-plane	side2		o
57	984.9	0.1	0.0	965	C-C-H		side1		o	
58	1025.7	1.3	28.7	1005	C-C		centre	Raman	p	
59	1028.3	0.5	18.7	1008	C-C	ring triangularing	in-plane	side2	Raman	p
60	1028.4	0.2	26.1	1008	C-C		side1	Raman	p	
61	1069.0	34.0	338.9	1048	C-C/C-S		centre	IR/Raman	q	
62	1078.8	96.7	216.1	1057	C-C/C-S	stretch/ring breathing	in-plane	anti-sym sedes	IR/Raman	q
63	1081.4	75.9	336.0	1060	C-C/C-S		sym sides	IR/Raman	q	
64	1123.2	3.4	1.1	1101	C-C		side1		r	
65	1123.9	4.3	1.4	1101	C-C	anti-sym ring deform	in-plane	side2		r
66	1130.1	5.9	3.8	1107	C-C		center	IR	r	
67	1181.0	88.8	12.8	1157	C-C		anti-sym sides	IR/Raman	s	
68	1182.1	127.2	13.3	1158	C-C	sym-ring deform	in-plane	sym sides	IR/Raman	s
69	1185.4	11.4	26.8	1162	C-C		sym all	Raman	s	
70	1273.9	225.7	8.0	1248	C-F		anti-sym sides	IR/Raman	t	
71	1274.7	292.6	24.6	1249	C-F	stretch	in-plane	sym sides	IR/Raman	t
72	1278.1	118.8	24.9	1253	C-F		centre	IR/Raman	t	
73	1315.9	0.2	2.8	1290	C-C/C-S		side1		u	
74	1316.9	0.0	2.5	1291	C-C/C-S	2-fold ring twist	in-plane	side2		u
75	1323.6	7.9	5.8	1297	C-C/C-S		side1+centre	IR/Raman	u	
76	1324.3	8.7	6.4	1298	C-C/C-F		side2	IR/Raman	v	
77	1324.9	0.9	4.0	1298	C-C/C-F	1-fold ring twist	in-plane	all		v
78	1327.7	8.0	3.4	1301	C-C/C-F		centre	IR	v	
79	1436.8	8.0	3.8	1408	C-C		side1	IR	w	
80	1437.0	8.4	5.3	1408	C-C	ring deform	in-plane	side2	IR/Raman	w
81	1438.2	7.6	7.4	1409	C-C		centre	IR/Raman	w	
82	1518.3	54.7	28.5	1488	C-C/C-F/C-S		anti-sym sides	IR/Raman	x	
83	1518.8	58.9	32.9	1488	C-C/C-F/C-S	ring deform	in-plane	sym sides	IR/Raman	x
84	1521.8	84.3	25.3	1491	C-C/C-F/C-S		centre	IR/Raman	x	
85	1605.2	5.1	2.7	1573	C-C		anti-sym sides	IR	y	
86	1605.5	6.9	1.9	1573	C-C	2-fold ring twist	in-plane	sym sides	IR	y
87	1613.1	18.5	12.2	1581	C-C		centre	IR/Raman	y	
88	1618.8	314.9	336.5	1586	C-S/C-F		anti-sym sides	IR/Raman	z	
89	1620.0	338.3	146.8	1588	C-S/C-F	ring squaring	in-plane	centre	IR/Raman	z
90	1620.8	35.0	482.3	1588	C-S/C-F		sym all	IR/Raman	z	
91	3189.2	0.2	24.9	3125	C-H	stretch	in-plane	centre	Raman	
92	3193.6	0.2	32.4	3130	C-H	stretch	in-plane	side2	Raman	
93	3194.0	0.2	21.8	3130	C-H	stretch	in-plane	side1	Raman	
94	3194.8	0.2	16.3	3131	C-H	stretch	in-plane	centre	Raman	
95	3194.9	0.4	55.0	3131	C-H	stretch	in-plane	side1	Raman	
96	3196.8	0.2	45.9	3133	C-H	stretch	in-plane	side2	Raman	
97	3207.7	2.0	69.4	3144	C-H	stretch	in-plane	side1	Raman	
98	3207.8	2.4	105.7	3144	C-H	stretch	in-plane	side2	Raman	
99	3208.5	4.0	192.3	3144	C-H	stretch	in-plane	centre	Raman	
100	3208.5	0.6	155.2	3144	C-H	stretch	in-plane	side1	Raman	
101	3209.0	0.7	172.9	3145	C-H	stretch	in-plane	side2	Raman	
102	3209.1	1.2	259.8	3145	C-H	stretch	in-plane	centre	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 S₃-oriented modes, all associated with the trimer cation.

*On colours in purple or gray are the coupled modes between S₃ modes and phenyl-ring deformation modes, some of which have substantial Raman activities.

*Phase denotes the distinction of the ArS moiety(ies) having major displacements in the trimer cation ArS(ArSSAr)⁺.

*Types depict each of the 26 vibrational modes of a-z from low frequencies as defined for the monomer radical ArS.

*Each type in the a-z modes is triply degenerated in the trimer cation ArS(ArSSAr)⁺.