Supplementary Material for Adsorption Geometry of Alizarin on Silver Nanoparticles: a Computational and Spectroscopic Study

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Table S1: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of alizarin (AZ) at B3LYP/6-311++G(d,p) level of theory.

	sym	frequencies	scaled	IR	Raman
1	$a^{"}$	44.14	43.30	2.851	0.0595
2	$a^{"}$	90.41	88.70	0.4488	0.246
3	$a^{"}$	118.73	116.48	1.1292	1.0575
4	$a^{"}$	136.32	133.73	0.0047	0.2759
5	$a^{"}$	179.00	175.60	0.0843	0.8
6	$a^{'}$	195.58	191.86	0.5979	0.2548
7	$a^{"}$	250.06	245.31	0.2788	2.9736
8	$a^{'}$	290.09	284.58	1.3719	1.0208
9	$a^{'}$	327.13	320.91	0.2414	0.572
10	$a^{"}$	331.98	325.67	0.6504	1.1007
11	$a^{'}$	348.72	342.09	7.1482	3.3885
12	$a^{'}$	393.43	385.95	5.6536	6.1083
13	$a^{'}$	424.45	416.39	21.2545	2.7208
14	$a^{"}$	424.98	416.91	0.2631	0.0801
15	$a^{"}$	448.69	440.17	17.1066	0.223
16	$a^{"}$	461.80	453.02	102.871	0.9913
17	$a^{'}$	473.89	464.89	0.2902	44.1586
18	$a^{'}$	486.64	477.39	12.9854	6.7051
19	$a^{"}$	497.55	488.10	14.4248	1.3458
20	$a^{"}$	574.94	564.01	0.3491	0.0961
21	$a^{'}$	584.13	573.04	6.1636	3.1088
22	$a^{'}$	626.70	614.79	13.7296	3.6714

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	sym	frequencies	scaled	IR	Raman
23	$a^{'}$	671.61	658.85	16.0475	17.2867
24	$a^{"}$	679.07	666.16	2.748	0.0539
25	$a^{'}$	698.79	685.52	3.3622	9.3186
26	$a^{"}$	704.36	690.98	0	0.0281
27	$a^{"}$	733.37	719.44	65.674	0.0272
28	$a^{'}$	767.18	752.60	6.0587	1.4809
29	$a^{"}$	781.52	766.67	5.5618	0.0073
30	$a^{"}$	789.83	774.82	91.1058	0.9505
31	$a^{"}$	809.33	793.96	3.3673	0.5505
32	$a^{'}$	843.81	827.77	42.8969	19.8975
33	$a^{"}$	862.44	846.06	22.6535	0.0147
34	$a^{'}$	906.70	889.47	8.0215	2.7556
35	$a^{"}$	916.24	898.83	0.119	0.0056
36	$a^{"}$	977.65	959.07	0.0235	0.3715
37	$a^{"}$	1002.83	983.78	1.802	0.0015
38	$a^{"}$	1019.37	1000.00	0.0728	0.0713
39	$a^{'}$	1026.99	1007.47	58.1284	43.6985
40	$a^{'}$	1045.79	1025.92	12.2582	33.7089
41	$a^{'}$	1066.53	1046.26	8.6225	17.6141
42	$a^{'}$	1113.34	1092.19	0.7614	5.6626
43	$a^{'}$	1171.48	1149.22	1.6341	12.7164
44	$a^{'}$	1182.32	1159.85	14.819	15.4238
45	$a^{'}$	1205.26	1182.36	38.6992	115.446
46	$a^{'}$	1216.27	1193.16	75.66	58.3112
47	$a^{'}$	1244.28	1220.64	21.0452	138.201

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	sym	frequencies	scaled	IR	Raman
48	$a^{'}$	1285.69	1261.26	92.8893	4.4616
49	$a^{'}$	1307.20	1282.36	981.339	6.1249
50	$a^{'}$	1317.97	1292.93	84.4023	16.9421
51	$a^{'}$	1344.86	1319.31	98.709	74.5836
52	$a^{'}$	1357.81	1332.01	46.4758	2.0527
53	$a^{'}$	1376.18	1350.03	161.081	24.3862
54	$a^{'}$	1431.95	1404.74	2.5511	75.1676
55	$a^{'}$	1481.71	1453.56	33.024	20.7032
56	$a^{'}$	1486.11	1457.87	392.353	31.5884
57	$a^{'}$	1504.29	1475.71	1.5085	33.4658
58	$a^{'}$	1514.60	1485.83	6.5626	27.8741
59	$a^{'}$	1608.01	1577.46	6.6202	43.565
60	$a^{'}$	1622.42	1591.60	142.884	127.476
61	$a^{'}$	1625.42	1594.53	23.5782	282.478
62	$a^{'}$	1631.62	1600.62	45.0388	44.2299
63	$a^{'}$	1673.11	1641.33	168.551	190.936
64	$a^{'}$	1717.99	1685.35	173.787	226.781
65	$a^{'}$	3171.57	3111.31	3.2176	79.5562
66	$a^{'}$	3185.91	3125.38	10.6523	204.84
67	$a^{'}$	3191.08	3130.45	2.7183	123.036
68	$a^{'}$	3201.51	3140.68	0.9182	45.3003
69	$a^{'}$	3204.27	3143.39	10.2783	204.014
70	$a^{'}$	3207.48	3146.54	1.5462	149.579
71	$a^{'}$	3286.48	3224.04	288.442	316.46
72	$a^{'}$	3755.57	3684.21	129.611	137.057

Table S2: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of alizarin anion (AZ^-; oxygen atom bound to C1) at B3LYP/6-311++G(d,p) level of theory.

	sym	frequencies	scaled	IR	Raman
1	$a^{"}$	31.18	30.59	3.8961	0.0952
2	$a^{"}$	68.79	67.48	1.2237	0.1324
3	$a^{"}$	114.81	112.63	0.0288	0.9421
4	$a^{"}$	118.53	116.28	1.2284	0.7696
5	$a^{"}$	179.22	175.81	1.0344	0.6799
6	$a^{'}$	188.50	184.92	1.1011	2.015
7	$a^{"}$	249.19	244.46	0.2241	1.6838
8	$a^{'}$	285.68	280.25	0.0141	0.7197
9	$a^{'}$	328.21	321.97	8.2527	1.8033
10	$a^{"}$	336.75	330.35	0.1273	0.7733
11	$a^{'}$	360.70	353.85	16.5302	1.7495
12	$a^{'}$	392.14	384.69	16.6803	3.4891
13	$a^{'}$	398.44	390.87	12.4168	14.3167
14	$a^{"}$	426.97	418.86	0.0882	0.2197
15	$a^{"}$	446.92	438.43	0.4519	0.822
16	$a^{'}$	463.59	454.79	10.6986	38.6951
17	$a^{"}$	484.80	475.59	0.9441	1.1471
18	$a^{'}$	491.83	482.49	8.4769	20.8947
19	$a^{'}$	581.20	570.15	8.7639	1.8176
20	$a^{"}$	587.71	576.54	0.1304	0.1817
21	$a^{'}$	633.34	621.30	12.1194	9.3967
22	$a^{'}$	672.50	659.72	16.7615	18.6607

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	sym	frequencies	scaled	IR	Raman
23	$a^{"}$	683.12	670.15	0.4118	0.041
24	$a^{'}$	697.12	683.87	0.5067	6.7338
25	$a^{"}$	726.13	712.34	63.6441	0.0601
26	$a^{"}$	758.51	744.10	20.8848	0.3024
27	$a^{'}$	767.31	752.73	15.7565	4.7423
28	$a^{"}$	790.84	775.81	0.3639	0.5088
29	$a^{"}$	804.39	789.11	5.7316	3.1319
30	$a^{'}$	818.36	802.81	22.7283	62.4171
31	$a^{"}$	833.85	818.01	49.9212	0.6037
32	$a^{"}$	841.39	825.40	64.4045	2.0521
33	$a^{"}$	899.43	882.35	0.1133	0.0449
34	$a^{'}$	910.87	893.57	2.0557	15.9749
35	$a^{"}$	925.11	907.53	0.185	1.9292
36	$a^{"}$	987.61	968.85	1.9158	0.0394
37	$a^{"}$	997.41	978.46	0.7701	0.0161
38	$a^{'}$	1031.03	1011.44	103.801	20.0399
39	$a^{'}$	1044.74	1024.89	3.3757	12.9018
40	$a^{'}$	1060.40	1040.25	0.0669	60.0929
41	$a^{'}$	1105.88	1084.86	2.603	4.5584
42	$a^{'}$	1157.79	1135.80	2.4642	39.0581
43	$a^{'}$	1166.21	1144.06	4.0128	73.6021
44	$a^{'}$	1195.24	1172.53	26.1115	226.522
45	$a^{'}$	1212.20	1189.17	21.3985	51.8313
46	$a^{'}$	1247.83	1224.13	99.4757	582.968
47	$a^{'}$	1272.12	1247.95	66.9965	90.9234

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	sym	frequencies	scaled	IR	Raman
48	$a^{'}$	1299.28	1274.59	116.796	93.6388
49	$a^{'}$	1320.59	1295.50	819.115	146.61
50	$a^{'}$	1348.71	1323.09	1.8248	1.0948
51	$a^{'}$	1380.90	1354.66	74.8788	15.1621
52	$a^{'}$	1425.03	1397.95	40.7999	352.63
53	$a^{'}$	1449.62	1422.08	159.444	67.137
54	$a^{'}$	1474.24	1446.23	16.0163	6.685
55	$a^{'}$	1496.95	1468.51	1.8154	38.8283
56	$a^{'}$	1532.94	1503.82	775.33	841.518
57	$a^{'}$	1559.23	1529.61	25.9943	109.009
58	$a^{'}$	1606.35	1575.83	4.2272	38.3643
59	$a^{'}$	1626.14	1595.24	102.846	71.593
60	$a^{'}$	1646.32	1615.04	3.5622	22.9616
61	$a^{'}$	1664.78	1633.15	106.938	323.598
62	$a^{'}$	1680.80	1648.86	405.008	14.2514
63	$a^{'}$	3143.06	3083.35	10.7184	104.458
64	$a^{'}$	3155.06	3095.11	42.7974	220.682
65	$a^{'}$	3161.66	3101.59	47.9196	322.527
66	$a^{'}$	3188.82	3128.23	6.784	49.3152
67	$a^{'}$	3191.35	3130.72	25.9394	174.241
68	$a^{'}$	3193.40	3132.72	5.7425	144.694
69	$a^{'}$	3259.83	3197.89	167.853	191.564

Table S3: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of alizarin anion (AZ^-; oxygen atom bound to C2) at B3LYP/6-311++G(d,p) level of theory.

	sym	frequencies	scaled	IR	Raman
1	$a^{"}$	32.58	31.96	1.2902	0.6277
2	$a^{"}$	46.21	45.33	0.0158	0.1256
3	$a^{"}$	83.47	81.88	6.248	1.3956
4	$a^{"}$	119.44	117.17	0.2223	1.972
5	$a^{"}$	169.53	166.31	3.1068	0.0457
6	$a^{'}$	193.17	189.50	0.5355	2.3154
7	$a^{"}$	240.76	236.19	0.3131	0.7893
8	$a^{'}$	295.73	290.11	6.3298	8.993
9	$a^{"}$	316.88	310.86	0.1525	4.8761
10	$a^{'}$	324.97	318.80	17.0677	22.8551
11	$a^{'}$	369.57	362.55	3.5472	14.0155
12	$a^{'}$	387.78	380.41	9.37	59.0981
13	$a^{'}$	389.97	382.56	0.1928	69.3055
14	$a^{"}$	429.81	421.64	0.7012	0.1122
15	$a^{"}$	443.73	435.30	0.1044	0.3981
16	$a^{'}$	458.98	450.26	14.0791	13.1729
17	$a^{'}$	494.84	485.44	22.6782	5.6087
18	$a^{"}$	516.93	507.11	0.001	2.6982
19	$?_a$	564.68	553.96	1.3429	0.4296
20	$?_a$	564.77	554.04	6.9985	4.9125
21	$a^{'}$	630.70	618.72	12.5797	4.3666
22	$a^{'}$	651.92	639.54	1.0371	52.746

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	sym	frequencies	scaled	IR	Raman
23	$a^{"}$	661.66	649.08	2.2602	0.1605
24	$a^{'}$	673.58	660.78	13.2368	8.6184
25	$a^{"}$	707.52	694.08	79.193	0.2982
26	$a^{"}$	754.45	740.11	4.3611	1.0215
27	$a^{'}$	767.64	753.05	10.5448	7.3731
28	$a^{"}$	775.57	760.83	27.4762	0.5352
29	$a^{"}$	780.43	765.60	6.7229	11.284
30	$a^{'}$	783.33	768.44	4.6632	76.3495
31	$a^{"}$	838.26	822.33	5.6799	0.7663
32	$a^{"}$	853.85	837.63	0.0784	0.3514
33	$a^{'}$	910.69	893.38	3.5163	30.2864
34	$a^{"}$	956.86	938.68	0.0402	0.1859
35	$a^{"}$	960.96	942.70	1.3158	0.3577
36	$a^{"}$	972.32	953.85	3.2398	1.3919
37	$a^{'}$	1007.43	988.29	21.5091	212.389
38	$a^{'}$	1038.42	1018.69	54.6952	303.68
39	$a^{'}$	1062.46	1042.27	48.3218	26.8255
40	$a^{'}$	1096.04	1075.21	5.2231	6.9097
41	$a^{'}$	1131.76	1110.25	33.6968	886.615
42	$a^{'}$	1152.30	1130.40	6.0397	11.0982
43	$a^{'}$	1177.02	1154.66	66.7028	294.216
44	$a^{'}$	1196.68	1173.95	13.6863	52.8464
45	$a^{'}$	1228.64	1205.30	157.253	638.981
46	$a^{'}$	1253.30	1229.49	48.8139	75.6257
47	$a^{'}$	1297.89	1273.23	41.9029	1580.73

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	sym	frequencies	scaled	IR	Raman
48	$a^{'}$	1348.92	1323.29	58.8135	544.974
49	$a^{'}$	1357.01	1331.23	37.0754	454.275
50	$a^{'}$	1376.04	1349.89	194.241	247.26
51	$a^{'}$	1439.15	1411.81	229.262	28.9484
52	$a^{'}$	1469.66	1441.73	151.888	294.789
53	$a^{'}$	1478.01	1449.93	18.1084	219.217
54	$a^{'}$	1517.35	1488.52	933.753	696.004
55	$a^{'}$	1521.21	1492.31	73.5935	198.648
56	$a^{'}$	1576.29	1546.34	377.021	57.5633
57	$a^{'}$	1585.06	1554.95	988.443	296.351
58	$a^{'}$	1610.65	1580.05	131.937	148.389
59	$a^{'}$	1615.38	1584.69	23.0591	297.187
60	$a^{'}$	1648.26	1616.94	356.582	71.2014
61	$a^{'}$	3095.84	3037.02	136.155	599.965
62	$a^{'}$	3102.90	3043.95	25.7331	167.228
63	$a^{'}$	3126.19	3066.79	128.883	469.437
64	$a^{'}$	3150.42	3090.56	31.7905	80.4318
65	$a^{'}$	3168.92	3108.71	15.508	39.8514
66	$a^{'}$	3171.14	3110.89	48.3127	232.33

Table S4: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of alizarin dianion (AZ^{2-}) at B3LYP/6-311++G(d,p) level of theory.

	sym	frequencies	scaled	IR	Raman
1	$a^{"}$	32.58	31.96	1.2902	0.6277
2	$a^{"}$	46.21	45.33	0.0158	0.1256
3	$a^{"}$	83.47	81.88	6.248	1.3956
4	$a^{"}$	119.44	117.17	0.2223	1.972
5	$a^{"}$	169.53	166.31	3.1068	0.0457
6	$a^{'}$	193.17	189.50	0.5355	2.3154
7	$a^{"}$	240.76	236.19	0.3131	0.7893
8	$a^{'}$	295.73	290.11	6.3298	8.993
9	$a^{"}$	316.88	310.86	0.1525	4.8761
10	$a^{'}$	324.97	318.80	17.0677	22.8551
11	$a^{'}$	369.57	362.55	3.5472	14.0155
12	$a^{'}$	387.78	380.41	9.37	59.0981
13	$a^{'}$	389.97	382.56	0.1928	69.3055
14	$a^{"}$	429.81	421.64	0.7012	0.1122
15	$a^{"}$	443.73	435.30	0.1044	0.3981
16	$a^{'}$	458.98	450.26	14.0791	13.1729
17	$a^{'}$	494.84	485.44	22.6782	5.6087
18	$a^{"}$	516.93	507.11	0.001	2.6982
19	$?_a$	564.68	553.96	1.3429	0.4296
20	$?_a$	564.77	554.04	6.9985	4.9125
21	$a^{'}$	630.70	618.72	12.5797	4.3666
22	$a^{'}$	651.92	639.54	1.0371	52.746

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	sym	frequencies	scaled	IR	Raman
23	$a^{"}$	661.66	649.08	2.2602	0.1605
24	$a^{'}$	673.58	660.78	13.2368	8.6184
25	$a^{"}$	707.52	694.08	79.193	0.2982
26	$a^{"}$	754.45	740.11	4.3611	1.0215
27	$a^{'}$	767.64	753.05	10.5448	7.3731
28	$a^{"}$	775.57	760.83	27.4762	0.5352
29	$a^{"}$	780.43	765.60	6.7229	11.284
30	$a^{'}$	783.33	768.44	4.6632	76.3495
31	$a^{"}$	838.26	822.33	5.6799	0.7663
32	$a^{"}$	853.85	837.63	0.0784	0.3514
33	$a^{'}$	910.69	893.38	3.5163	30.2864
34	$a^{"}$	956.86	938.68	0.0402	0.1859
35	$a^{"}$	960.96	942.70	1.3158	0.3577
36	$a^{"}$	972.32	953.85	3.2398	1.3919
37	$a^{'}$	1007.43	988.29	21.5091	212.389
38	$a^{'}$	1038.42	1018.69	54.6952	303.68
39	$a^{'}$	1062.46	1042.27	48.3218	26.8255
40	$a^{'}$	1096.04	1075.21	5.2231	6.9097
41	$a^{'}$	1131.76	1110.25	33.6968	886.615
42	$a^{'}$	1152.30	1130.40	6.0397	11.0982
43	$a^{'}$	1177.02	1154.66	66.7028	294.216
44	$a^{'}$	1196.68	1173.95	13.6863	52.8464
45	$a^{'}$	1228.64	1205.30	157.253	638.981
46	$a^{'}$	1253.30	1229.49	48.8139	75.6257
47	$a^{'}$	1297.89	1273.23	41.9029	1580.73

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	sym	frequencies	scaled	IR	Raman
48	$a^{'}$	1348.92	1323.29	58.8135	544.974
49	$a^{'}$	1357.01	1331.23	37.0754	454.275
50	$a^{'}$	1376.04	1349.89	194.241	247.26
51	$a^{'}$	1439.15	1411.81	229.262	28.9484
52	$a^{'}$	1469.66	1441.73	151.888	294.789
53	$a^{'}$	1478.01	1449.93	18.1084	219.217
54	$a^{'}$	1517.35	1488.52	933.753	696.004
55	$a^{'}$	1521.21	1492.31	73.5935	198.648
56	$a^{'}$	1576.29	1546.34	377.021	57.5633
57	$a^{'}$	1585.06	1554.95	988.443	296.351
58	$a^{'}$	1610.65	1580.05	131.937	148.389
59	$a^{'}$	1615.38	1584.69	23.0591	297.187
60	$a^{'}$	1648.26	1616.94	356.582	71.2014
61	$a^{'}$	3095.84	3037.02	136.155	599.965
62	$a^{'}$	3102.90	3043.95	25.7331	167.228
63	$a^{'}$	3126.19	3066.79	128.883	469.437
64	$a^{'}$	3150.42	3090.56	31.7905	80.4318
65	$a^{'}$	3168.92	3108.71	15.508	39.8514
66	$a^{'}$	3171.14	3110.89	48.3127	232.33

Table S5: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of model (a) in Figure 5 of the manuscript at B3LYP/6-311++G(d,p) level of theory. Silver has been treated with LANL2TZ basis set.

	sym	frequencies	scaled	IR	Raman
1	a	18.35	18.01	0.0652	2.6365
2	a	24.49	24.03	0.8992	1.1039
3	a	39.04	38.29	1.2776	1.86
4	a	42.07	41.27	2.1223	1.621
5	a	58.13	57.02	2.8907	2.5261
6	a	74.98	73.56	2.6813	1.0301
7	a	84.29	82.69	0.3029	2.4485
8	a	94.69	92.89	2.7264	12.7651
9	a	112.99	110.85	0.869	1.9125
10	a	120.75	118.46	0.527	1.7094
11	a	131.17	128.68	2.1643	3.0196
12	a	166.94	163.77	1.8476	8.0364
13	a	170.77	167.53	8.7197	18.9664
14	a	197.13	193.39	16.6179	3.2863
15	a	207.72	203.78	17.3033	3.1981
16	a	267.10	262.02	21.0958	9.6216
17	a	310.51	304.61	5.0021	0.7518
18	a	328.17	321.93	2.7973	2.1402
19	a	332.91	326.58	22.4375	3.2177
20	a	374.91	367.79	63.2867	7.2352
21	a	384.86	377.55	12.1699	5.0108
22	a	406.62	398.89	11.7007	3.468

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	sym	frequencies	scaled	IR	Raman
23	a	418.66	410.71	30.4216	4.1354
24	a	429.12	420.97	2.786	1.4949
25	a	452.92	444.32	0.9962	1.5403
26	a	483.44	474.26	3.8102	35.4882
27	a	497.41	487.96	1.0405	2.1656
28	a	500.64	491.12	10.6825	17.0268
29	a	585.49	574.37	8.3652	2.9503
30	a	592.23	580.98	1.9914	2.3888
31	a	631.15	619.16	5.9558	8.4003
32	a	674.05	661.24	19.3637	20.7449
33	a	691.11	677.98	0.8357	3.8976
34	a	695.23	682.02	4.0326	4.5881
35	a	731.68	717.77	69.2943	0.7954
36	a	767.80	753.21	20.8955	1.4761
37	a	775.96	761.22	17.3501	4.8443
38	a	801.66	786.43	2.3629	1.3715
39	a	817.57	802.04	6.5187	23.6217
40	a	830.40	814.62	27.691	14.8757
41	a	844.64	828.59	29.9333	1.3871
42	a	912.96	895.61	3.12	0.6289
43	a	914.11	896.74	12.1274	7.6571
44	a	947.23	929.23	0.166	1.8455
45	a	998.78	979.80	1.7225	0.0755
46	a	1013.26	994.01	0.0949	0.1907
47	a	1031.00	1011.41	17.6485	19.4309

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	sym	frequencies	scaled	IR	Raman
48	a	1044.66	1024.82	75.068	104.695
49	a	1066.00	1045.75	3.13	29.7348
50	a	1114.16	1093.00	1.0683	5.0188
51	a	1168.89	1146.68	104.989	51.2979
52	a	1172.50	1150.22	204.22	8.7139
53	a	1181.75	1159.30	117.369	29.2332
54	a	1214.40	1191.32	10.5703	73.495
55	a	1232.75	1209.33	128.237	434.615
56	a	1269.89	1245.76	258.567	7.7156
57	a	1281.65	1257.30	266.244	223.72
58	a	1317.40	1292.37	220.643	52.2164
59	a	1356.01	1330.25	3.8361	17.9391
60	a	1381.75	1355.49	87.2856	55.2471
61	a	1421.46	1394.46	61.8626	184.657
62	a	1429.42	1402.26	260.377	132.486
63	a	1468.55	1440.65	101.025	154.383
64	a	1483.58	1455.39	70.3501	19.3025
65	a	1506.09	1477.48	1.0667	31.7676
66	a	1560.23	1530.59	307.245	299.039
67	a	1601.32	1570.90	231.059	304.348
68	a	1621.01	1590.21	20.2938	204.249
69	a	1626.37	1595.47	182.535	172.724
70	a	1647.27	1615.97	213.33	193.376
71	a	1708.26	1675.80	234.211	279.333
72	a	3140.66	3080.98	26.1814	199.001

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	sym	frequencies	scaled	IR	Raman
73	a	3167.08	3106.91	3.5369	83.7609
74	a	3182.30	3121.84	17.3317	267.45
75	a	3200.33	3139.52	6.4474	144.149
76	a	3207.35	3146.41	2.7028	58.6527
77	a	3207.68	3146.74	6.2694	169.336
78	a	3825.88	3753.19	104.295	258.704

Table S6: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of model (b) in Figure 5 of the manuscript at B3LYP/6-311++G(d,p) level of theory. Silver has been treated with LANL2TZ basis set.

	sym	frequencies	scaled	IR	Raman
1	a	12.47	12.23	0.0998	0.0604
2	a	14.53	14.26	0.1394	2.8514
3	a	16.78	16.46	0.3653	0.094
4	a	32.32	31.71	3.0416	0.4235
5	a	64.04	62.82	1.1138	2.4307
6	a	73.66	72.26	6.8602	1.1097
7	a	74.25	72.84	6.7305	0.6897
8	a	95.09	93.28	1.3981	9.1134
9	a	106.57	104.55	0.0447	0.3874
10	a	119.78	117.50	0.0597	0.891
11	a	137.00	134.40	0.416	0.5357
12	a	149.51	146.67	10.475	8.2625
13	a	181.00	177.56	0.9515	0.7692
14	a	190.75	187.12	20.4034	24.3521
15	a	210.17	206.17	2.6045	2.7532
16	a	251.84	247.06	0.0238	2.3867
17	a	310.23	304.34	6.9332	0.1225
18	a	319.54	313.47	26.963	0.3372
19	a	332.57	326.25	0.466	4.6485
20	a	378.98	371.78	63.7779	3.2758
21	a	393.31	385.84	9.0632	10.9753
22	a	411.02	403.21	1.9336	7.8202

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	sym	frequencies	scaled	IR	Raman
23	a	426.08	417.99	40.9319	11.0955
24	a	428.12	419.99	0.3396	0.04
25	a	455.12	446.47	1.2593	0.855
26	a	484.11	474.91	1.133	15.2139
27	a	492.77	483.41	0.2436	1.4927
28	a	497.65	488.19	5.6198	38.142
29	a	585.25	574.13	0.0183	0.3266
30	a	591.35	580.11	14.2809	1.3373
31	a	637.37	625.26	2.1459	2.8764
32	a	675.91	663.07	17.7417	22.6257
33	a	688.55	675.47	1.0185	0.0025
34	a	698.40	685.13	9.1535	10.752
35	a	730.20	716.32	65.6815	0.0322
36	a	767.68	753.09	24.0882	0.4624
37	a	770.57	755.93	23.9687	6.4787
38	a	798.67	783.49	1.6759	0.3857
39	a	816.48	800.96	0.1362	1.4832
40	a	823.86	808.21	16.0605	28.3779
41	a	840.98	825.00	32.436	0.351
42	a	910.11	892.82	0.2142	0.0055
43	a	915.42	898.03	7.3464	5.4722
44	a	943.33	925.40	0.2915	1.616
45	a	996.92	977.98	1.4595	0.0055
46	a	1010.33	991.13	0.1569	0.0957
47	a	1034.05	1014.40	23.819	59.5216

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	sym	frequencies	scaled	IR	Raman
48	a	1046.90	1027.01	128.693	64.2269
49	a	1065.60	1045.35	6.3322	24.7475
50	a	1114.51	1093.33	3.3841	3.6315
51	a	1170.75	1148.50	32.7281	10.3641
52	a	1172.96	1150.67	135.387	41.0343
53	a	1182.13	1159.67	198.651	14.5471
54	a	1214.85	1191.77	8.2359	22.9742
55	a	1230.08	1206.71	109.447	305.654
56	a	1277.15	1252.89	109.934	137.732
57	a	1290.12	1265.61	284.271	24.2564
58	a	1320.71	1295.62	243.493	117.529
59	a	1355.62	1329.87	0.351	3.7844
60	a	1381.49	1355.24	124.671	58.3513
61	a	1416.67	1389.76	0.7757	305.128
62	a	1438.81	1411.47	110.419	51.3319
63	a	1464.33	1436.51	97.8854	197.386
64	a	1483.18	1455.00	40.6722	23.1466
65	a	1505.76	1477.15	0.3289	27.5351
66	a	1560.41	1530.76	405.425	653.737
67	a	1600.71	1570.29	472.527	209.377
68	a	1623.91	1593.05	141.004	200.226
69	a	1627.54	1596.62	107.128	69.4322
70	a	1645.80	1614.53	286.966	142.696
71	a	1700.36	1668.06	226.127	164.376
72	a	3135.20	3075.63	38.9942	260.291

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	sym	frequencies	scaled	IR	Raman
73	a	3163.85	3103.74	4.2314	85.1429
74	a	3179.77	3119.35	20.5971	259.653
75	a	3199.75	3138.95	7.217	140.723
76	a	3205.21	3144.31	0.642	103.57
77	a	3208.98	3148.01	8.8843	100.333
78	a	3821.42	3748.81	91.978	305.059

Table S7: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of model (c) in Figure 5 of the manuscript at B3LYP/6-311++G(d,p) level of theory. Silver has been treated with LANL2TZ basis set.

	sym	frequencies	scaled	IR	Raman
1	a	8.40	8.24	0.5868	0.1588
2	a	14.71	14.43	0.3885	1.4578
3	a	17.02	16.70	0.1963	3.2114
4	a	41.09	40.31	1.1829	1.9396
5	a	58.09	56.99	0.1281	1.8611
6	a	58.73	57.61	6.5082	1.0121
7	a	94.53	92.73	2.2657	3.5708
8	a	100.38	98.48	0.8814	0.0392
9	a	121.28	118.97	0.0427	4.8255
10	a	122.77	120.44	6.6796	1.5503
11	a	140.17	137.50	1.2066	0.238
12	a	153.16	150.25	10.1458	16.3199
13	a	174.48	171.17	0	0.7592
14	a	192.06	188.41	15.9297	9.7813
15	a	245.04	240.38	8.6499	0.6054
16	a	248.91	244.18	0.0045	3.3824
17	a	322.97	316.84	9.4338	8.7193
18	a	332.84	326.51	0.0809	1.4374
19	a	342.92	336.41	28.0759	4.9432
20	a	393.80	386.31	0.4739	5.4732
21	a	426.09	418.00	28.5605	7.417
22	a	426.22	418.13	0.4463	0.0355

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	sym	frequencies	scaled	IR	Raman
23	a	452.14	443.55	11.5285	33.5083
24	a	455.34	446.69	0.0018	0.3367
25	a	477.65	468.58	1.3444	92.5053
26	a	502.74	493.18	0.7116	0.6869
27	a	512.03	502.30	12.1053	29.8241
28	a	569.88	559.05	0.3059	0.0584
29	a	584.75	573.64	12.3437	8.019
30	a	649.72	637.37	11.4448	46.5714
31	a	672.20	659.43	21.3664	10.0339
32	a	683.80	670.81	5.5108	0.0995
33	a	696.07	682.84	2.8701	29.6357
34	a	730.46	716.58	31.7783	0.0146
35	a	734.26	720.31	32.4535	0.097
36	a	773.66	758.96	23.3823	3.0807
37	a	779.74	764.93	0.3333	0.352
38	a	808.30	792.94	11.6035	1.3835
39	a	841.39	825.40	52.5455	25.7532
40	a	854.85	838.61	46.1649	0.4865
41	a	874.32	857.71	57.9665	1.2049
42	a	907.80	890.55	2.056	3.6659
43	a	912.60	895.26	0.5124	0.0158
44	a	980.93	962.29	0.2319	0.6154
45	a	998.39	979.43	1.5298	0.0015
46	a	1014.74	995.46	0.2917	0.0293
47	a	1024.35	1004.89	85.837	2.5139

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	sym	frequencies	scaled	IR	Raman
48	a	1055.65	1035.59	0.4769	134.493
49	a	1074.91	1054.49	1.6918	11.9937
50	a	1112.19	1091.05	1.3748	7.1021
51	a	1175.07	1152.75	49.6624	8.7562
52	a	1178.98	1156.57	0.3803	65.2762
53	a	1203.74	1180.87	23.7499	383.98
54	a	1224.74	1201.47	104.997	27.2462
55	a	1273.45	1249.25	69.6806	293.088
56	a	1298.87	1274.19	747.872	505.446
57	a	1312.77	1287.83	2.0737	212.126
58	a	1338.81	1313.38	141.861	104.386
59	a	1355.67	1329.91	8.3598	24.6846
60	a	1379.95	1353.73	720.497	84.9129
61	a	1399.03	1372.45	452.235	58.4363
62	a	1481.16	1453.01	23.5954	14.3693
63	a	1492.92	1464.56	594.645	522.135
64	a	1503.22	1474.66	156.418	1.4754
65	a	1516.41	1487.60	419.262	50.2126
66	a	1569.32	1539.51	2.8825	233.216
67	a	1593.86	1563.58	278.346	125.834
68	a	1606.00	1575.49	134.261	33.4146
69	a	1625.21	1594.34	109.531	58.8325
70	a	1653.06	1621.66	63.8877	275.675
71	a	1692.49	1660.33	224.703	360.173
72	a	3052.98	2994.97	496.716	1753.16

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	sym	frequencies	scaled	IR	Raman
73	a	3166.31	3106.15	4.7877	100.154
74	a	3178.09	3117.71	5.5793	93.2175
75	a	3181.60	3121.15	16.557	279.743
76	a	3194.70	3134.00	7.0386	149.238
77	a	3199.49	3138.70	1.1823	55.4865
78	a	3202.03	3141.19	14.1246	220.846

Table S8: Calculated and scaled (0.981) normal mode frequencies (cm^1), infrared intensities (IR), and Raman activities (Raman) of model (d) in Figure 5 of the manuscript at B3LYP/6-311++G(d,p) level of theory. Silver has been treated with LANL2TZ basis set.

	sym	frequencies	scaled	IR	Raman
1	a	21.48	21.07	0.838	4.4864
2	a	27.02	26.51	0.2839	5.9423
3	a	34.72	34.06	0.2565	15.3126
4	a	51.53	50.55	0.7606	13.21
5	a	56.43	55.36	1.5046	7.9464
6	a	62.45	61.26	1.2379	14.982
7	a	72.18	70.81	0.8011	1.6814
8	a	80.37	78.85	3.7222	10.3147
9	a	95.67	93.86	0.1136	1.2565
10	a	108.15	106.09	1.1152	54.8805
11	a	119.70	117.42	6.9306	49.346
12	a	123.55	121.20	1.9183	4.494
13	a	126.72	124.31	2.1791	12.3984
14	a	146.28	143.50	0.0733	100.512
15	a	152.21	149.31	0.4312	9.4081
16	a	179.58	176.17	7.863	131.057
17	a	190.69	187.06	8.8344	19.64
18	a	253.75	248.93	1.1531	62.7455
19	a	263.16	258.16	5.9171	83.1521
20	a	323.32	317.18	12.7128	7.3867
21	a	339.23	332.78	9.5781	114.072
22	a	350.87	344.20	7.6884	22.8287

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	sym	frequencies	scaled	IR	Raman
23	a	398.90	391.32	4.4845	297.073
24	a	418.78	410.82	29.7209	64.6409
25	a	430.42	422.24	2.7838	6.7098
26	a	460.15	451.41	0.647	4.2624
27	a	476.02	466.98	1.4585	26.6138
28	a	482.02	472.86	5.4251	84.0392
29	a	515.23	505.44	5.8017	71.3735
30	a	524.43	514.47	1.2078	1.6464
31	a	580.75	569.72	4.3062	8.3651
32	a	591.68	580.44	10.1806	3.1067
33	a	646.06	633.79	1.1221	513.696
34	a	675.56	662.73	19.4457	36.9941
35	a	689.03	675.94	6.481	13.2849
36	a	697.57	684.31	3.9158	8.3256
37	a	733.49	719.55	62.7122	2.2349
38	a	776.02	761.27	13.1421	73.4755
39	a	778.48	763.69	8.9279	18.4308
40	a	802.18	786.93	8.1128	1.5137
41	a	815.89	800.39	4.5907	23.1265
42	a	829.78	814.01	29.4043	54.7626
43	a	860.38	844.03	22.4699	2.377
44	a	911.92	894.59	1.2389	2.0921
45	a	913.57	896.22	14.6769	32.3096
46	a	985.04	966.33	0.2743	1.9626
47	a	996.65	977.72	1.3727	0.0721

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	sym	frequencies	scaled	IR	Raman
48	a	1012.65	993.41	0.2973	0.3109
49	a	1028.55	1009.01	118.591	163.401
50	a	1057.59	1037.50	0.7609	353.643
51	a	1070.71	1050.37	10.7831	32.4347
52	a	1113.87	1092.71	1.1824	4.2597
53	a	1168.42	1146.22	47.0606	876.248
54	a	1177.79	1155.41	5.0793	239.573
55	a	1203.33	1180.47	38.2151	676.604
56	a	1229.64	1206.28	49.784	249.999
57	a	1279.21	1254.91	681.624	774.651
58	a	1287.56	1263.10	3.6786	1407.03
59	a	1323.28	1298.13	44.555	3394.59
60	a	1348.42	1322.80	236.919	1945.94
61	a	1359.67	1333.84	178.592	1327.84
62	a	1379.30	1353.09	360.949	111.564
63	a	1418.32	1391.37	144.18	964.777
64	a	1441.43	1414.04	71.2964	7457.78
65	a	1478.14	1450.05	4.387	415.014
66	a	1503.66	1475.09	2.7631	49.0297
67	a	1535.14	1505.98	150.585	2621.07
68	a	1564.20	1534.48	8.2976	299.05
69	a	1584.10	1554.00	72.4531	422.36
70	a	1618.82	1588.06	53.3548	144.957
71	a	1635.51	1604.44	96.366	273.651
72	a	1682.88	1650.90	557.755	243.194

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	sym	frequencies	scaled	IR	Raman
73	a	3165.04	3104.91	4.3977	101.129
74	a	3176.09	3115.74	9.1869	161.299
75	a	3180.56	3120.13	21.8671	323.739
76	a	3193.87	3133.19	7.6295	191.069
77	a	3199.86	3139.06	6.4301	159.742
78	a	3205.57	3144.66	11.1808	91.9838