Electronic Supplementary Information

Raman and ROA Analysis of Twisted Anthracenes: Connecting Vibrational and Electronic/Photonic Properties

Contents

1. Vibrational assignment

Table S1. Wavenumbers and relative intensities measured in the Raman spectra of **Ant-C5** and their correlation with the calculated B3LYP/6-31G* eigenvalues.

Experimental		Calculated (scaled by 0.975)	Assignment
solid sample	CD_2Cl_2 solution		
1618 w	1615 sh	1617	ν(bz-tether) + ν(bz- central)
1596 m	1601 m	1609	ν(anthr) + ν(bz-tether)
1576 w		1589	ν(bz-tether)
1560 s	1562 s	1566	ν(anthr)
1533 sh		1540	ν(anthr)
1529 m	1534 m	1527	ν(anthr)
1490 vw	1490 vw	1485	$\delta(CH_2)$ + δ(CH),bz-tether
1481 vw	1482 vw	1477	δ(CH),anthr + δ(CH),bz-central
1443 vw	1445 vw	1439	δ(CH),bz-central
1408 s	1410 m	1407	δ(CH),anthr
1373 s	1374 m	1356	$\delta(CH_2)$ + ν(bz-central) + ν(C-CF_3)
1345 m	1348 m	1343	δ(CH),anthr
1277 m	1276 sh	1270	$\omega(CH_2)$ + δ(CH),all
1260 s	1268 s	1256	δ(CH),anthr
1191 w	1196 vw	1185	δ(CH),anthr
1163 vw	1196 vw	1185	δ(CH),anthr
1043 m	1047 sh	1042	δ(CH),anthr + δ(CH),bz-tether
1003 m	1007 w	992	ν(bz- central),breathing
972 w	980 vw	958	γ(CH),anhtr

2. Experimental and theoretical Raman spectra

Figure S1. Experimental (532 nm excitation láser) Raman spectra of the twistacene series.

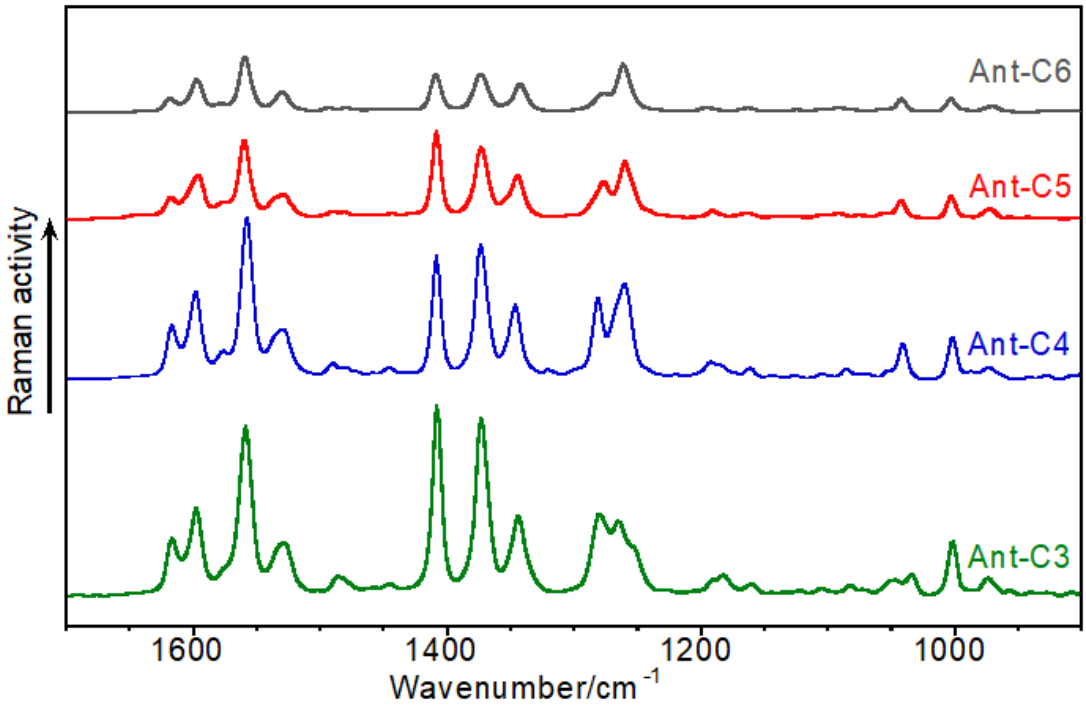
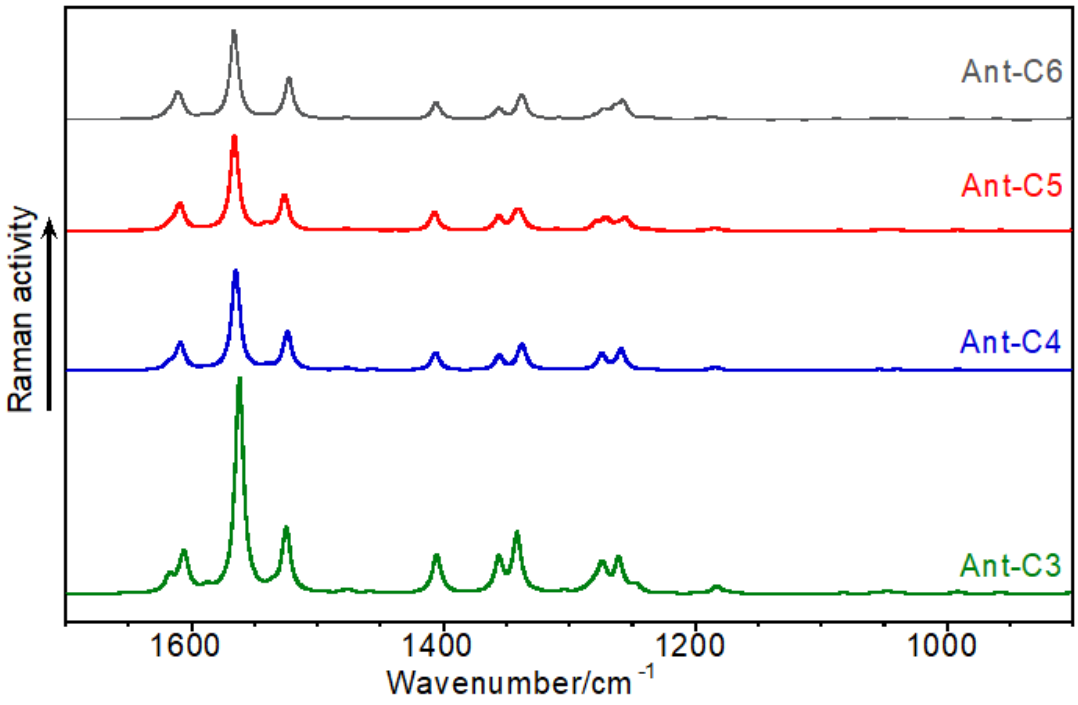


Figure S2. Calculated (B3LYP/6-31G*) Raman spectra of the twistacene series.



3. Z-matrix.

Table S2. Cartesian coordinates of the optimized structures of (*M*) and (*P*) enantiomers of the twistacene series.

(*M*)-Ant-C3

C	1.10097	0.99026	3.36414
C	1.62362	0.50541	2.18427
C	0.82445	0.59524	0.9763
C	-0.59321	0.82677	1.12869
C	-1.0651	1.35879	2.37193
C	-0.22284	1.49386	3.44144
C	1.34454	0.48998	-0.33492
C	-1.46769	0.51591	0.05943
C	-0.94047	0.10011	-1.18504
C	0.46761	0.30448	-1.43066
C	0.91477	0.30303	-2.79327
H	1.94059	0.57526	-3.01038
C	0.06711	-0.03676	-3.81257
C	-1.23662	-0.52462	-3.52178
C	-1.73149	-0.50807	-2.24073
H	1.69488	0.91534	4.26991
H	-2.10467	1.64902	2.46039
H	-0.58728	1.90703	4.37699
H	0.41679	-0.01985	-4.84035
H	-1.82092	-0.99181	-4.30897
C	-2.93488	0.73508	0.23464
C	-3.57934	1.72821	-0.51349
C	-3.69136	-0.00372	1.15352
C	-4.94786	1.95599	-0.3657
H	-3.00831	2.31873	-1.22176
C	-5.05861	0.23069	1.30164
H	-3.21487	-0.78378	1.73655
C	-5.69765	1.20999	0.54218
H	-6.76073	1.38307	0.6508
C	2.80873	0.64466	-0.57551
C	3.45134	1.83667	-0.21491
C	3.57363	-0.37196	-1.16073
C	4.82277	1.99499	-0.40917
H	2.87379	2.64065	0.22803
C	4.94628	-0.20954	-1.35385
H	3.09593	-1.30128	-1.45018
C	5.58186	0.97215	-0.97696
H	6.64674	1.09522	-1.1273
C	2.90076	-0.26223	2.27466
C	2.92129	-1.64266	1.94754
C	4.04898	0.30011	2.84225
C	4.05483	-2.41235	2.22433
C	5.19306	-0.45989	3.09108
H	4.04546	1.3612	3.07294
C	5.18609	-1.81801	2.78905
H	4.06574	-3.47483	2.01524
H	6.07347	0.00697	3.52067
H	6.06048	-2.42996	2.98954
C	-2.92397	-1.34279	-1.89741
C	-2.68334	-2.56552	-1.23072
C	-4.2412	-1.0234	-2.24542
C	-3.74446	-3.38775	-0.84684
C	-5.30195	-1.85162	-1.8751
H	-4.44022	-0.09607	-2.77344
C	-5.05467	-3.02155	-1.15591
H	-3.535	-4.32728	-0.34463
H	-6.31841	-1.57786	-2.14045
H	-5.87743	-3.66436	-0.85749
O	1.78421	-2.13298	1.363
O	-1.37686	-2.98355	-1.10671
C	1.65213	-3.5176	1.03557
H	2.60678	-3.92828	0.6897
H	1.34811	-4.07748	1.93153
C	-0.77101	-3.13923	0.18404
H	-0.7423	-2.17477	0.70214
H	-1.33651	-3.85105	0.8017
C	0.644	-3.6433	-0.10227
H	1.02024	-3.06873	-0.9547
H	0.60435	-4.69198	-0.41886
C	-5.83217	-0.56898	2.31677
C	-5.62329	2.95157	-1.26934
C	5.73938	-1.35987	-1.91483
C	5.48869	3.25374	0.07817
F	5.88247	-2.3498	-1.00298
F	5.12615	-1.9087	-2.98861
F	6.97794	-0.9873	-2.29919
F	6.69128	3.45129	-0.50112
F	5.69458	3.21152	1.41772
F	4.73259	4.34677	-0.16397
F	-7.16345	-0.50889	2.10233
F	-5.61033	-0.11936	3.57428
F	-5.47402	-1.87209	2.30013
F	-5.84519	2.4195	-2.49829
F	-6.81987	3.34824	-0.78885
F	-4.86854	4.05565	-1.45533

(*P*)-Ant-C3

C	1.10097	0.99026	-3.36414
C	1.62362	0.50541	-2.18427
C	0.82445	0.59524	-0.9763
C	-0.59321	0.82677	-1.12869
C	-1.0651	1.35879	-2.37193
C	-0.22284	1.49386	-3.44144
C	1.34454	0.48998	0.33492
C	-1.46769	0.51591	-0.05943
C	-0.94047	0.10011	1.18504
C	0.46761	0.30448	1.43066
C	0.91477	0.30303	2.79327
H	1.94059	0.57526	3.01038
C	0.06711	-0.03676	3.81257
C	-1.23662	-0.52462	3.52178
C	-1.73149	-0.50807	2.24073
H	1.69488	0.91534	-4.26991
H	-2.10467	1.64902	-2.46039
H	-0.58728	1.90703	-4.37699
H	0.41679	-0.01985	4.84035
H	-1.82092	-0.99181	4.30897
C	-2.93488	0.73508	-0.23464
C	-3.57934	1.72821	0.51349
C	-3.69136	-0.00372	-1.15352
C	-4.94786	1.95599	0.3657
H	-3.00831	2.31873	1.22176
C	-5.05861	0.23069	-1.30164
H	-3.21487	-0.78378	-1.73655
C	-5.69765	1.20999	-0.54218
H	-6.76073	1.38307	-0.6508
C	2.80873	0.64466	0.57551
C	3.45134	1.83667	0.21491
C	3.57363	-0.37196	1.16073
C	4.82277	1.99499	0.40917
H	2.87379	2.64065	-0.22803
C	4.94628	-0.20954	1.35385
H	3.09593	-1.30128	1.45018
C	5.58186	0.97215	0.97696
H	6.64674	1.09522	1.1273
C	2.90076	-0.26223	-2.27466
C	2.92129	-1.64266	-1.94754
C	4.04898	0.30011	-2.84225
C	4.05483	-2.41235	-2.22433
C	5.19306	-0.45989	-3.09108
H	4.04546	1.3612	-3.07294
C	5.18609	-1.81801	-2.78905
H	4.06574	-3.47483	-2.01524
H	6.07347	0.00697	-3.52067
H	6.06048	-2.42996	-2.98954
C	-2.92397	-1.34279	1.89741
C	-2.68334	-2.56552	1.23072
C	-4.2412	-1.0234	2.24542
C	-3.74446	-3.38775	0.84684
C	-5.30195	-1.85162	1.8751
H	-4.44022	-0.09607	2.77344
C	-5.05467	-3.02155	1.15591
H	-3.535	-4.32728	0.34463
H	-6.31841	-1.57786	2.14045
H	-5.87743	-3.66436	0.85749
O	1.78421	-2.13298	-1.363
O	-1.37686	-2.98355	1.10671
C	1.65213	-3.5176	-1.03557
H	2.60678	-3.92828	-0.6897
H	1.34811	-4.07748	-1.93153
C	-0.77101	-3.13923	-0.18404
H	-0.7423	-2.17477	-0.70214
H	-1.33651	-3.85105	-0.8017
C	0.644	-3.6433	0.10227
H	1.02024	-3.06873	0.9547
H	0.60435	-4.69198	0.41886
C	-5.83217	-0.56898	-2.31677
C	-5.62329	2.95157	1.26934
C	5.73938	-1.35987	1.91483
C	5.48869	3.25374	-0.07817
F	5.88247	-2.3498	1.00298
F	5.12615	-1.9087	2.98861
F	6.97794	-0.9873	2.29919
F	6.69128	3.45129	0.50112
F	5.69458	3.21152	-1.41772
F	4.73259	4.34677	0.16397
F	-7.16345	-0.50889	-2.10233
F	-5.61033	-0.11936	-3.57428
F	-5.47402	-1.87209	-2.30013
F	-5.84519	2.4195	2.49829
F	-6.81987	3.34824	0.78885
F	-4.86854	4.05565	1.45533

(*M*)-**Ant-C4**

C	1.25231	0.74105	3.49981
C	1.765	0.33763	2.29015
C	0.94782	0.47695	1.09438
C	-0.46899	0.70276	1.265
C	-0.93416	1.1314	2.55206
C	-0.08396	1.20825	3.62016
C	1.45668	0.43711	-0.22346
C	-1.3524	0.51825	0.17348
C	-0.85066	0.21112	-1.11377
C	0.57523	0.34916	-1.32982
C	1.05753	0.41801	-2.67686
H	2.1075	0.61762	-2.84967
C	0.21596	0.23881	-3.73886
C	-1.13834	-0.117	-3.51513
C	-1.6744	-0.17408	-2.24845
H	1.85961	0.62604	4.3927
H	-1.97648	1.39987	2.67107
H	-0.44809	1.55013	4.58426
H	0.59385	0.30572	-4.75454
H	-1.75913	-0.40646	-4.35753
C	-2.81113	0.76891	0.3893
C	-3.39668	1.93221	-0.12218
C	-3.60986	-0.1138	1.12686
C	-4.75414	2.19123	0.07339
H	-2.78914	2.63536	-0.68192
C	-4.96638	0.14782	1.31919
H	-3.16921	-1.01282	1.54272
C	-5.54885	1.30059	0.79158
H	-6.60116	1.50396	0.94513
C	2.91865	0.6264	-0.47514
C	3.51365	1.85442	-0.15927
C	3.7172	-0.37313	-1.04342
C	4.8752	2.06436	-0.3772
H	2.90844	2.64527	0.2704
C	5.07868	-0.15852	-1.2625
H	3.27741	-1.33163	-1.29581
C	5.66836	1.05981	-0.92945
H	6.72644	1.22021	-1.09185
C	3.0406	-0.44368	2.28483
C	2.95529	-1.83485	2.03636
C	4.29124	0.0993	2.58803
C	4.10349	-2.6286	2.01493
C	5.44237	-0.69349	2.58492
H	4.37117	1.16478	2.78102
C	5.34668	-2.05033	2.283
H	4.02743	-3.69177	1.81346
H	6.4071	-0.2469	2.80386
H	6.23777	-2.67081	2.26511
C	-3.03511	-0.78846	-2.12582
C	-3.15621	-2.11032	-1.63283
C	-4.18312	-0.15769	-2.61098
C	-4.40102	-2.74511	-1.60211
C	-5.43052	-0.78661	-2.58273
H	-4.1001	0.8557	-2.99176
C	-5.53444	-2.07696	-2.07242
H	-4.4941	-3.75508	-1.2215
H	-6.30848	-0.26626	-2.95175
H	-6.49744	-2.57737	-2.03729
O	1.69053	-2.32253	1.87496
O	-1.99317	-2.69639	-1.21932
C	1.43308	-3.46813	1.06173
H	2.01403	-3.40495	0.13051
H	1.72761	-4.39109	1.5813
C	-1.99807	-4.03582	-0.72613
H	-2.6765	-4.11984	0.13551
H	-2.35262	-4.72358	-1.50586
C	-5.8194	-0.85995	2.04341
C	-5.36502	3.40343	-0.57587
C	5.89689	-1.25961	-1.88345
C	5.49649	3.3561	0.08007
F	5.63643	-2.45473	-1.30681
F	5.62308	-1.39777	-3.20227
F	7.22257	-1.03434	-1.77255
F	6.68691	3.58807	-0.51119
F	5.71378	3.34514	1.41972
F	4.69846	4.41549	-0.17455
F	-6.9173	-0.29245	2.58843
F	-5.13747	-1.46864	3.03957
F	-6.25054	-1.83663	1.21164
F	-5.57022	3.19516	-1.90053
F	-6.5587	3.72565	-0.03595
F	-4.56301	4.48573	-0.47364
C	-0.06579	-3.41997	0.78057
H	-0.60933	-3.60575	1.71539
H	-0.29497	-2.39488	0.481
C	-0.5635	-4.36512	-0.3176
H	0.07293	-4.28016	-1.20708
H	-0.52687	-5.41329	0.00446

(*P*)-**Ant-C4**

C	1.25231	0.74105	-3.49981
C	1.765	0.33763	-2.29015
C	0.94782	0.47695	-1.09438
C	-0.46899	0.70276	-1.265
C	-0.93416	1.1314	-2.55206
C	-0.08396	1.20825	-3.62016
C	1.45668	0.43711	0.22346
C	-1.3524	0.51825	-0.17348
C	-0.85066	0.21112	1.11377
C	0.57523	0.34916	1.32982
C	1.05753	0.41801	2.67686
H	2.1075	0.61762	2.84967
C	0.21596	0.23881	3.73886
C	-1.13834	-0.117	3.51513
C	-1.6744	-0.17408	2.24845
H	1.85961	0.62604	-4.3927
H	-1.97648	1.39987	-2.67107
H	-0.44809	1.55013	-4.58426
H	0.59385	0.30572	4.75454
H	-1.75913	-0.40646	4.35753
C	-2.81113	0.76891	-0.3893
C	-3.39668	1.93221	0.12218
C	-3.60986	-0.1138	-1.12686
C	-4.75414	2.19123	-0.07339
H	-2.78914	2.63536	0.68192
C	-4.96638	0.14782	-1.31919
H	-3.16921	-1.01282	-1.54272
C	-5.54885	1.30059	-0.79158
H	-6.60116	1.50396	-0.94513
C	2.91865	0.6264	0.47514
C	3.51365	1.85442	0.15927
C	3.7172	-0.37313	1.04342
C	4.8752	2.06436	0.3772
H	2.90844	2.64527	-0.2704
C	5.07868	-0.15852	1.2625
H	3.27741	-1.33163	1.29581
C	5.66836	1.05981	0.92945
H	6.72644	1.22021	1.09185
C	3.0406	-0.44368	-2.28483
C	2.95529	-1.83485	-2.03636
C	4.29124	0.0993	-2.58803
C	4.10349	-2.6286	-2.01493
C	5.44237	-0.69349	-2.58492
H	4.37117	1.16478	-2.78102
C	5.34668	-2.05033	-2.283
H	4.02743	-3.69177	-1.81346
H	6.4071	-0.2469	-2.80386
H	6.23777	-2.67081	-2.26511
C	-3.03511	-0.78846	2.12582
C	-3.15621	-2.11032	1.63283
C	-4.18312	-0.15769	2.61098
C	-4.40102	-2.74511	1.60211
C	-5.43052	-0.78661	2.58273
H	-4.1001	0.8557	2.99176
C	-5.53444	-2.07696	2.07242
H	-4.4941	-3.75508	1.2215
H	-6.30848	-0.26626	2.95175
H	-6.49744	-2.57737	2.03729
O	1.69053	-2.32253	-1.87496
O	-1.99317	-2.69639	1.21932
C	1.43308	-3.46813	-1.06173
H	2.01403	-3.40495	-0.13051
H	1.72761	-4.39109	-1.5813
C	-1.99807	-4.03582	0.72613
H	-2.6765	-4.11984	-0.13551
H	-2.35262	-4.72358	1.50586
C	-5.8194	-0.85995	-2.04341
C	-5.36502	3.40343	0.57587
C	5.89689	-1.25961	1.88345
C	5.49649	3.3561	-0.08007
F	5.63643	-2.45473	1.30681
F	5.62308	-1.39777	3.20227
F	7.22257	-1.03434	1.77255
F	6.68691	3.58807	0.51119
F	5.71378	3.34514	-1.41972
F	4.69846	4.41549	0.17455
F	-6.9173	-0.29245	-2.58843
F	-5.13747	-1.46864	-3.03957
F	-6.25054	-1.83663	-1.21164
F	-5.57022	3.19516	1.90053
F	-6.5587	3.72565	0.03595
F	-4.56301	4.48573	0.47364
C	-0.06579	-3.41997	-0.78057
H	-0.60933	-3.60575	-1.71539
H	-0.29497	-2.39488	-0.481
C	-0.5635	-4.36512	0.3176
H	0.07293	-4.28016	1.20708
H	-0.52687	-5.41329	-0.00446

(*M*)-**Ant-C5**

C	1.29975	1.04568	3.4345
C	1.80369	0.57083	2.24724
C	0.9863	0.65451	1.04835
C	-0.42741	0.89282	1.20874
C	-0.88742	1.39541	2.47126
C	-0.03296	1.52971	3.53047
C	1.49537	0.52366	-0.26163
C	-1.31345	0.63988	0.13477
C	-0.81563	0.24424	-1.13066
C	0.61267	0.35521	-1.35666
C	1.10009	0.31103	-2.70213
H	2.15144	0.49174	-2.88539
C	0.26344	0.04708	-3.74971
C	-1.09731	-0.26105	-3.5033
C	-1.64096	-0.20053	-2.23927
H	1.90627	0.96982	4.33215
H	-1.92943	1.66969	2.57976
H	-0.39312	1.92589	4.47511
H	0.64578	0.02425	-4.76566
H	-1.72583	-0.59117	-4.32468
C	-2.77022	0.90248	0.35514
C	-3.34667	2.07963	-0.13417
C	-3.57314	0.01321	1.07862
C	-4.70225	2.34422	0.06698
H	-2.73555	2.78589	-0.68614
C	-4.92733	0.28204	1.27883
H	-3.14219	-0.90643	1.45835
C	-5.50205	1.44757	0.77262
H	-6.55571	1.64881	0.91911
C	2.95944	0.68559	-0.51911
C	3.56844	1.9175	-0.2532
C	3.74733	-0.34649	-1.04727
C	4.93258	2.10436	-0.48234
H	2.97233	2.73276	0.14217
C	5.10832	-0.15422	-1.28094
H	3.29538	-1.30638	-1.26841
C	5.71225	1.07168	-0.99732
H	6.76867	1.22062	-1.18306
C	3.05852	-0.23797	2.27313
C	2.94478	-1.62752	2.01656
C	4.31005	0.27449	2.61666
C	4.07288	-2.44964	2.04442
C	5.44039	-0.54718	2.66324
H	4.40708	1.33927	2.80685
C	5.31873	-1.90139	2.36474
H	3.98858	-3.50838	1.82768
H	6.40776	-0.12479	2.91553
H	6.19312	-2.54491	2.37908
C	-3.04322	-0.71061	-2.10801
C	-3.28951	-2.00868	-1.60432
C	-4.12192	0.01439	-2.62544
C	-4.58933	-2.5284	-1.61057
C	-5.41962	-0.4987	-2.6291
H	-3.93626	1.00859	-3.02
C	-5.64783	-1.77289	-2.11792
H	-4.78513	-3.51974	-1.22112
H	-6.23668	0.09457	-3.02676
H	-6.64997	-2.19139	-2.11064
O	1.67503	-2.06219	1.77499
O	-2.20765	-2.71002	-1.12966
C	1.40442	-3.38585	1.32839
H	1.82461	-3.5381	0.32259
H	1.86339	-4.12656	1.99863
C	-2.31144	-4.14056	-1.1073
H	-3.04906	-4.45819	-0.35672
C	-5.7582	-0.68461	2.0804
C	-5.312	3.56021	-0.57562
C	5.94912	-1.29914	-1.78123
C	5.5638	3.41303	-0.09118
F	6.45941	-2.02865	-0.76254
F	5.23301	-2.14854	-2.55163
F	6.99651	-0.86667	-2.51744
F	6.76336	3.59864	-0.68056
F	5.76476	3.47654	1.24899
F	4.7807	4.4648	-0.41579
F	-7.0774	-0.55147	1.82613
F	-5.5899	-0.49941	3.41072
F	-5.42019	-1.96784	1.82043
F	-5.54845	3.3474	-1.89439
F	-6.49049	3.89928	-0.01242
F	-4.49554	4.63356	-0.49624
C	-0.11534	-3.5354	1.33736
H	-0.44634	-3.46981	2.37952
H	-0.55342	-2.68133	0.8129
C	-0.59489	-4.8551	0.70221
H	-1.47367	-5.22281	1.2462
H	0.1742	-5.62729	0.83961
C	-0.95588	-4.77619	-0.7931
H	-0.18017	-4.25102	-1.36336
H	-0.99525	-5.79721	-1.19278
H	-2.67007	-4.47754	-2.08919

(*P*)-**Ant-C5**

C	1.29975	1.04568	-3.4345
C	1.80369	0.57083	-2.24724
C	0.9863	0.65451	-1.04835
C	-0.42741	0.89282	-1.20874
C	-0.88742	1.39541	-2.47126
C	-0.03296	1.52971	-3.53047
C	1.49537	0.52366	0.26163
C	-1.31345	0.63988	-0.13477
C	-0.81563	0.24424	1.13066
C	0.61267	0.35521	1.35666
C	1.10009	0.31103	2.70213
H	2.15144	0.49174	2.88539
C	0.26344	0.04708	3.74971
C	-1.09731	-0.26105	3.5033
C	-1.64096	-0.20053	2.23927
H	1.90627	0.96982	-4.33215
H	-1.92943	1.66969	-2.57976
H	-0.39312	1.92589	-4.47511
H	0.64578	0.02425	4.76566
H	-1.72583	-0.59117	4.32468
C	-2.77022	0.90248	-0.35514
C	-3.34667	2.07963	0.13417
C	-3.57314	0.01321	-1.07862
C	-4.70225	2.34422	-0.06698
H	-2.73555	2.78589	0.68614
C	-4.92733	0.28204	-1.27883
H	-3.14219	-0.90643	-1.45835
C	-5.50205	1.44757	-0.77262
H	-6.55571	1.64881	-0.91911
C	2.95944	0.68559	0.51911
C	3.56844	1.9175	0.2532
C	3.74733	-0.34649	1.04727
C	4.93258	2.10436	0.48234
H	2.97233	2.73276	-0.14217
C	5.10832	-0.15422	1.28094
H	3.29538	-1.30638	1.26841
C	5.71225	1.07168	0.99732
H	6.76867	1.22062	1.18306
C	3.05852	-0.23797	-2.27313
C	2.94478	-1.62752	-2.01656
C	4.31005	0.27449	-2.61666
C	4.07288	-2.44964	-2.04442
C	5.44039	-0.54718	-2.66324
H	4.40708	1.33927	-2.80685
C	5.31873	-1.90139	-2.36474
H	3.98858	-3.50838	-1.82768
H	6.40776	-0.12479	-2.91553
H	6.19312	-2.54491	-2.37908
C	-3.04322	-0.71061	2.10801
C	-3.28951	-2.00868	1.60432
C	-4.12192	0.01439	2.62544
C	-4.58933	-2.5284	1.61057
C	-5.41962	-0.4987	2.6291
H	-3.93626	1.00859	3.02
C	-5.64783	-1.77289	2.11792
H	-4.78513	-3.51974	1.22112
H	-6.23668	0.09457	3.02676
H	-6.64997	-2.19139	2.11064
O	1.67503	-2.06219	-1.77499
O	-2.20765	-2.71002	1.12966
C	1.40442	-3.38585	-1.32839
H	1.82461	-3.5381	-0.32259
H	1.86339	-4.12656	-1.99863
C	-2.31144	-4.14056	1.1073
H	-3.04906	-4.45819	0.35672
C	-5.7582	-0.68461	-2.0804
C	-5.312	3.56021	0.57562
C	5.94912	-1.29914	1.78123
C	5.5638	3.41303	0.09118
F	6.45941	-2.02865	0.76254
F	5.23301	-2.14854	2.55163
F	6.99651	-0.86667	2.51744
F	6.76336	3.59864	0.68056
F	5.76476	3.47654	-1.24899
F	4.7807	4.4648	0.41579
F	-7.0774	-0.55147	-1.82613
F	-5.5899	-0.49941	-3.41072
F	-5.42019	-1.96784	-1.82043
F	-5.54845	3.3474	1.89439
F	-6.49049	3.89928	0.01242
F	-4.49554	4.63356	0.49624
C	-0.11534	-3.5354	-1.33736
H	-0.44634	-3.46981	-2.37952
H	-0.55342	-2.68133	-0.8129
C	-0.59489	-4.8551	-0.70221
H	-1.47367	-5.22281	-1.2462
H	0.1742	-5.62729	-0.83961
C	-0.95588	-4.77619	0.7931
H	-0.18017	-4.25102	1.36336
H	-0.99525	-5.79721	1.19278
H	-2.67007	-4.47754	2.08919

(*M*)-Ant-C6

C	-1.13448	-1.44188	3.36662
C	-1.69629	-0.96117	2.20337
C	-0.86805	-0.85845	1.00925
C	0.56515	-1.0135	1.16638
C	1.0722	-1.51698	2.40813
C	0.2402	-1.76853	3.46164
C	-1.36164	-0.66879	-0.30255
C	1.44738	-0.69516	0.10357
C	0.94811	-0.30992	-1.16184
C	-0.47523	-0.45294	-1.38894
C	-0.95789	-0.40882	-2.73829
H	-2.00497	-0.60514	-2.92838
C	-0.11959	-0.14216	-3.78338
C	1.23477	0.19504	-3.53432
C	1.77064	0.15662	-2.26825
H	-1.75836	-1.51504	4.25187
H	2.13381	-1.7029	2.50568
H	0.63665	-2.16235	4.39254
H	-0.49885	-0.13179	-4.80069
H	1.8566	0.54357	-4.35326
C	2.91178	-0.92063	0.32421
C	3.513	-2.07793	-0.18251
C	3.69523	-0.03199	1.06939
C	4.87175	-2.32283	0.02292
H	2.91732	-2.78573	-0.74913
C	5.05282	-0.2798	1.27289
H	3.24576	0.8677	1.47459
C	5.65151	-1.42574	0.74954
H	6.70752	-1.61119	0.89961
C	-2.82251	-0.75693	-0.60741
C	-3.50457	-1.97444	-0.50993
C	-3.53325	0.37325	-1.02843
C	-4.8691	-2.0499	-0.79351
H	-2.96913	-2.86527	-0.19966
C	-4.89735	0.29629	-1.30623
H	-3.01729	1.32258	-1.11248
C	-5.57678	-0.91589	-1.18891
H	-6.63817	-0.97479	-1.39431
C	-3.10419	-0.4683	2.32734
C	-3.38972	0.90952	2.18011
C	-4.13558	-1.31087	2.75261
C	-4.67209	1.40329	2.43306
C	-5.42099	-0.82642	3.00603
H	-3.92662	-2.3704	2.86714
C	-5.68311	0.53123	2.84615
H	-4.88629	2.45863	2.31231
H	-6.20548	-1.50793	3.31828
H	-6.67721	0.92423	3.03835
C	3.13614	0.75227	-2.10341
C	3.2502	2.07032	-1.60729
C	4.29575	0.10385	-2.54142
C	4.50464	2.68054	-1.50475
C	5.54915	0.70838	-2.43883
H	4.21564	-0.90444	-2.93575
C	5.64929	1.99441	-1.91049
H	4.5905	3.69819	-1.14022
H	6.43639	0.17552	-2.76562
H	6.61787	2.47849	-1.8266
O	-2.33671	1.68087	1.78818
O	2.07153	2.71531	-1.33875
C	-2.48403	3.09025	1.61517
H	-3.21351	3.29793	0.81911
H	-2.85106	3.55404	2.54166
C	1.95192	3.66376	-0.27298
H	2.92308	4.08416	0.00672
C	5.86026	0.68519	2.09995
C	5.50468	-3.51847	-0.63534
C	-5.62025	1.53712	-1.75583
C	-5.58785	-3.35401	-0.57452
F	-5.20122	2.63092	-1.07136
F	-5.40373	1.79629	-3.06586
F	-6.95442	1.44066	-1.58433
F	-6.76615	-3.40363	-1.2311
F	-5.85561	-3.55288	0.73895
F	-4.84672	-4.40754	-0.98343
F	7.18341	0.57914	1.85519
F	5.68325	0.47172	3.42511
F	5.50236	1.96722	1.86162
F	5.73397	-3.2846	-1.95193
F	6.69071	-3.84058	-0.07839
F	4.71007	-4.60872	-0.56772
C	-1.09527	3.59837	1.24673
H	-0.42584	3.41172	2.0957
H	-0.73626	2.9725	0.42285
C	-1.04374	5.0751	0.8442
H	-1.72619	5.24211	-0.00085
C	0.99569	4.77048	-0.72537
H	0.2096	4.3055	-1.33197
H	1.53789	5.44299	-1.39883
C	0.36238	5.56202	0.44199
H	0.28918	6.61943	0.16559
H	1.02577	5.53018	1.31789
H	-1.41546	5.70007	1.66698
H	1.5586	3.13672	0.60539

(*P*)-**Ant-C6**

C	-1.13448	-1.44188	-3.36662
C	-1.69629	-0.96117	-2.20337
C	-0.86805	-0.85845	-1.00925
C	0.56515	-1.0135	-1.16638
C	1.0722	-1.51698	-2.40813
C	0.2402	-1.76853	-3.46164
C	-1.36164	-0.66879	0.30255
C	1.44738	-0.69516	-0.10357
C	0.94811	-0.30992	1.16184
C	-0.47523	-0.45294	1.38894
C	-0.95789	-0.40882	2.73829
H	-2.00497	-0.60514	2.92838
C	-0.11959	-0.14216	3.78338
C	1.23477	0.19504	3.53432
C	1.77064	0.15662	2.26825
H	-1.75836	-1.51504	-4.25187
H	2.13381	-1.7029	-2.50568
H	0.63665	-2.16235	-4.39254
H	-0.49885	-0.13179	4.80069
H	1.8566	0.54357	4.35326
C	2.91178	-0.92063	-0.32421
C	3.513	-2.07793	0.18251
C	3.69523	-0.03199	-1.06939
C	4.87175	-2.32283	-0.02292
H	2.91732	-2.78573	0.74913
C	5.05282	-0.2798	-1.27289
H	3.24576	0.8677	-1.47459
C	5.65151	-1.42574	-0.74954
H	6.70752	-1.61119	-0.89961
C	-2.82251	-0.75693	0.60741
C	-3.50457	-1.97444	0.50993
C	-3.53325	0.37325	1.02843
C	-4.8691	-2.0499	0.79351
H	-2.96913	-2.86527	0.19966
C	-4.89735	0.29629	1.30623
H	-3.01729	1.32258	1.11248
C	-5.57678	-0.91589	1.18891
H	-6.63817	-0.97479	1.39431
C	-3.10419	-0.4683	-2.32734
C	-3.38972	0.90952	-2.18011
C	-4.13558	-1.31087	-2.75261
C	-4.67209	1.40329	-2.43306
C	-5.42099	-0.82642	-3.00603
H	-3.92662	-2.3704	-2.86714
C	-5.68311	0.53123	-2.84615
H	-4.88629	2.45863	-2.31231
H	-6.20548	-1.50793	-3.31828
H	-6.67721	0.92423	-3.03835
C	3.13614	0.75227	2.10341
C	3.2502	2.07032	1.60729
C	4.29575	0.10385	2.54142
C	4.50464	2.68054	1.50475
C	5.54915	0.70838	2.43883
H	4.21564	-0.90444	2.93575
C	5.64929	1.99441	1.91049
H	4.5905	3.69819	1.14022
H	6.43639	0.17552	2.76562
H	6.61787	2.47849	1.8266
O	-2.33671	1.68087	-1.78818
O	2.07153	2.71531	1.33875
C	-2.48403	3.09025	-1.61517
H	-3.21351	3.29793	-0.81911
H	-2.85106	3.55404	-2.54166
C	1.95192	3.66376	0.27298
H	2.92308	4.08416	-0.00672
C	5.86026	0.68519	-2.09995
C	5.50468	-3.51847	0.63534
C	-5.62025	1.53712	1.75583
C	-5.58785	-3.35401	0.57452
F	-5.20122	2.63092	1.07136
F	-5.40373	1.79629	3.06586
F	-6.95442	1.44066	1.58433
F	-6.76615	-3.40363	1.2311
F	-5.85561	-3.55288	-0.73895
F	-4.84672	-4.40754	0.98343
F	7.18341	0.57914	-1.85519
F	5.68325	0.47172	-3.42511
F	5.50236	1.96722	-1.86162
F	5.73397	-3.2846	1.95193
F	6.69071	-3.84058	0.07839
F	4.71007	-4.60872	0.56772
C	-1.09527	3.59837	-1.24673
H	-0.42584	3.41172	-2.0957
H	-0.73626	2.9725	-0.42285
C	-1.04374	5.0751	-0.8442
H	-1.72619	5.24211	0.00085
C	0.99569	4.77048	0.72537
H	0.2096	4.3055	1.33197
H	1.53789	5.44299	1.39883
C	0.36238	5.56202	-0.44199
H	0.28918	6.61943	-0.16559
H	1.02577	5.53018	-1.31789
H	-1.41546	5.70007	-1.66698
H	1.5586	3.13672	-0.60539

4. Analogue molecule

Fig. S3. Optimized structure of the (*M*)-enantiomer

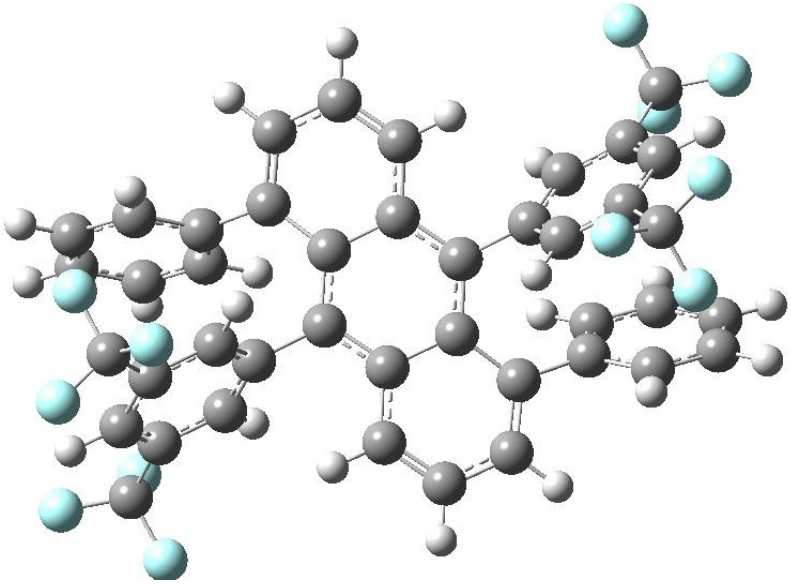


Fig. S4. Raman and ROA spectra

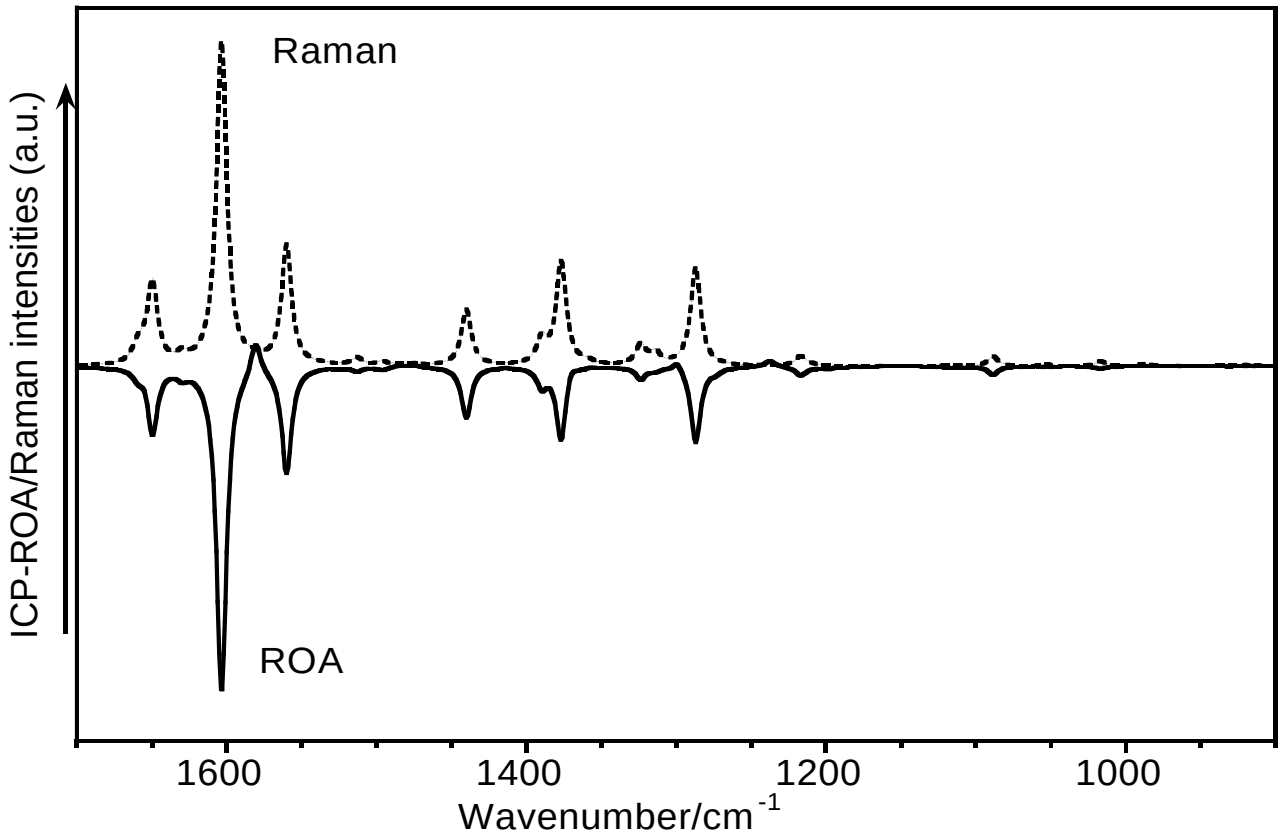


Table S3. Z-matrix of the optimized structure

C	1.17472	-3.54424	-0.25113
C	1.71738	-2.29603	-0.46806
C	0.89432	-1.11831	-0.24614
C	-0.53328	-1.30691	-0.07743
C	-1.0196	-2.6335	0.15845
C	-0.18248	-3.71376	0.11688
C	1.40922	0.19313	-0.10102
C	-1.40915	-0.19278	-0.10112
C	-0.89426	1.11871	-0.24574
C	0.53336	1.30724	-0.07696
C	1.01973	2.63373	0.15926
H	2.07018	2.77824	0.37534
C	0.18266	3.71405	0.11797
C	-1.17456	3.54465	-0.25002
C	-1.71727	2.2965	-0.46725
H	1.79252	-4.41973	-0.4258
H	-2.07003	-2.77812	0.37453
H	-0.56787	-4.71108	0.30524
H	0.56809	4.71131	0.3065
H	-1.79237	4.42019	-0.42439
C	-2.86018	-0.4132	0.1906
C	-3.39365	0.06243	1.3948
C	-3.70447	-1.10994	-0.68181
C	-4.73955	-0.13222	1.7055
H	-2.7533	0.59521	2.08937
C	-5.04914	-1.30728	-0.36561
H	-3.31584	-1.47825	-1.62474
C	-5.57769	-0.81816	0.8281
H	-6.62352	-0.96383	1.0665
C	2.86024	0.41332	0.19086
C	3.39355	-0.06289	1.39492
C	3.70471	1.11033	-0.68114
C	4.73946	0.13141	1.7058
H	2.75306	-0.59583	2.08923
C	5.0494	1.30732	-0.36475
H	3.31618	1.47918	-1.62391
C	5.57779	0.81758	0.82875
H	6.62361	0.96303	1.06731
C	3.08168	-2.24937	-1.07381
C	3.26356	-1.67751	-2.34374
C	4.17643	-2.87558	-0.45943
C	4.50465	-1.72252	-2.97618
C	5.41946	-2.919	-1.09175
H	4.05846	-3.3067	0.53026
C	5.58811	-2.34411	-2.35199
H	4.62487	-1.27626	-3.95897
H	6.25765	-3.39818	-0.59428
H	6.5557	-2.37844	-2.84366
C	-3.08165	2.25014	-1.07289
C	-3.26365	1.67886	-2.34307
C	-4.17632	2.87608	-0.45812
C	-4.5048	1.72418	-2.97536
C	-5.41942	2.9198	-1.09029
H	-4.05824	3.30682	0.53172
C	-5.58821	2.34549	-2.35076
H	-4.62515	1.27839	-3.95835
H	-6.25755	3.39875	-0.59249
H	-6.55584	2.38005	-2.84233
C	-5.91531	-2.07844	-1.32608
C	-5.29506	0.48506	2.96069
C	5.91562	2.07842	-1.32521
C	5.29467	-0.48642	2.96085
F	5.69531	1.69807	-2.60402
F	5.66002	3.40656	-1.26518
F	7.23033	1.91329	-1.07114
F	6.45953	0.08161	3.33674
F	5.53382	-1.80991	2.79005
F	4.43271	-0.37794	3.99555
F	-7.2301	-1.90965	-1.0748
F	-5.66306	-3.40707	-1.26262
F	-5.69173	-1.70143	-2.60529
F	-5.53528	1.80837	2.79005
F	-6.45941	-0.08393	3.33669
F	-4.43285	0.37715	3.99526
H	2.41968	-1.20621	-2.83936
H	-2.41983	1.20777	-2.83898

5. Raman spectra at different excitation laser

Figure S5. Raman spectra of **Ant-C3** at different laser excitations.

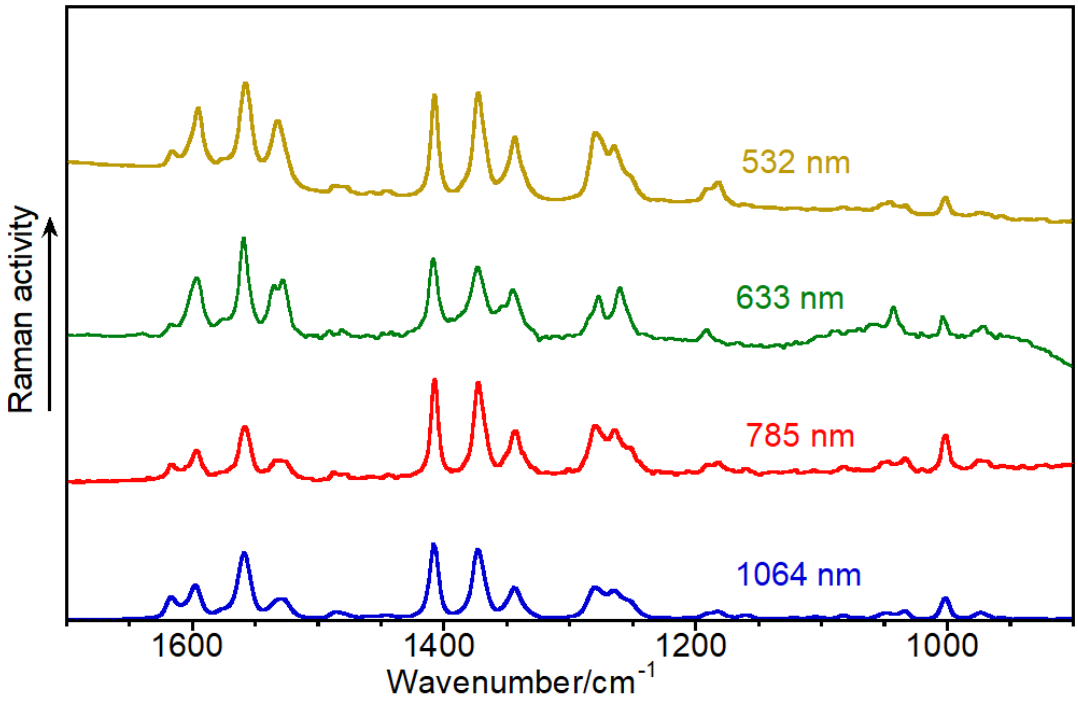


Figure S6. Raman spectra of **Ant-C4** at different laser excitations.

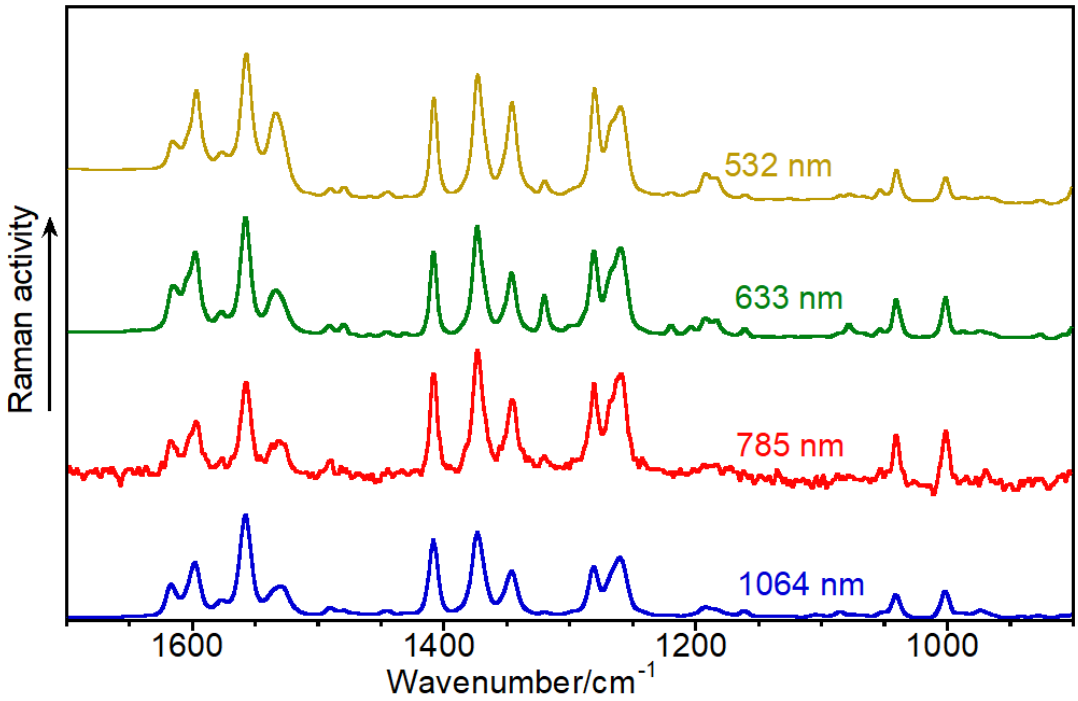


Figure S7. Raman spectra of **Ant-C5** at different laser excitations.

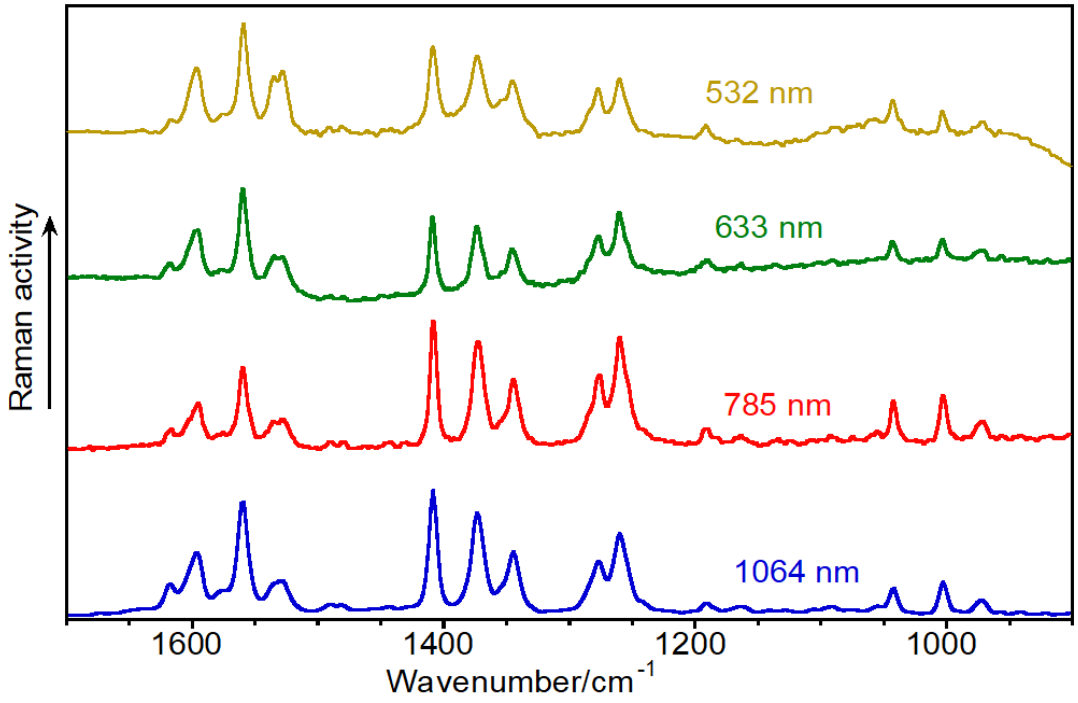


Figure S8. Raman spectra of **Ant-C6** at different laser excitations.