SUPPORTING INFORMATION

Structures and Chiroptical Properties of the BINAS-monosubstituted $Au_{38}(SCH_3)_{24}$ cluster

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Part I. Figure S1. Comparison of experimental and calculated UV-vis and CD spectra of *A*-38.

Part II. Figure S2. Comparison of bond distances of four regioisomers with $Au_{38}(SCH_3)_{24}$ cluster.

Part III. Figure S3-S6. Kohn-Sham orbitals of 5 studied clusters.

Part IV. Tables S1. Excitation energy, oscillator strength, electronic transitions and their weights for peaks of studied regioisomers.

Part V. Relaxed Cartesian coordinates of studied regioisomers.

PART I

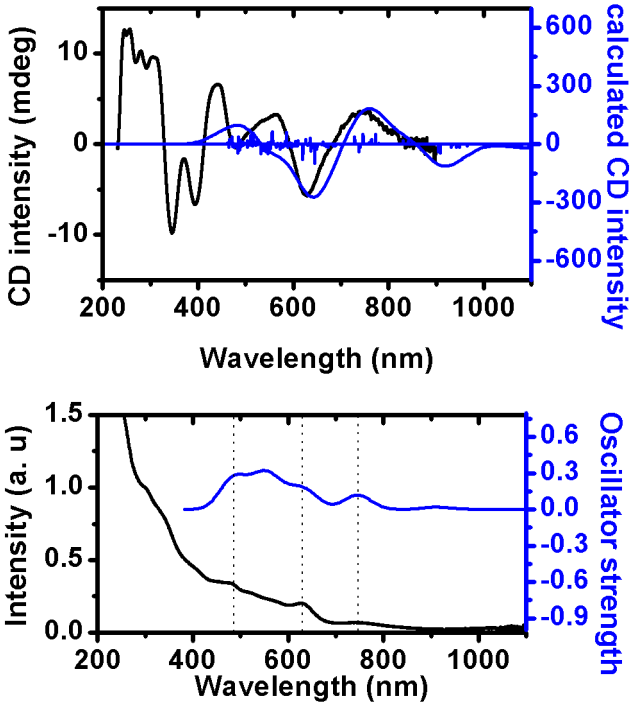


Figure S1. Comparison of experimental and calculated CD and UV-vis spectra of *A*-38.

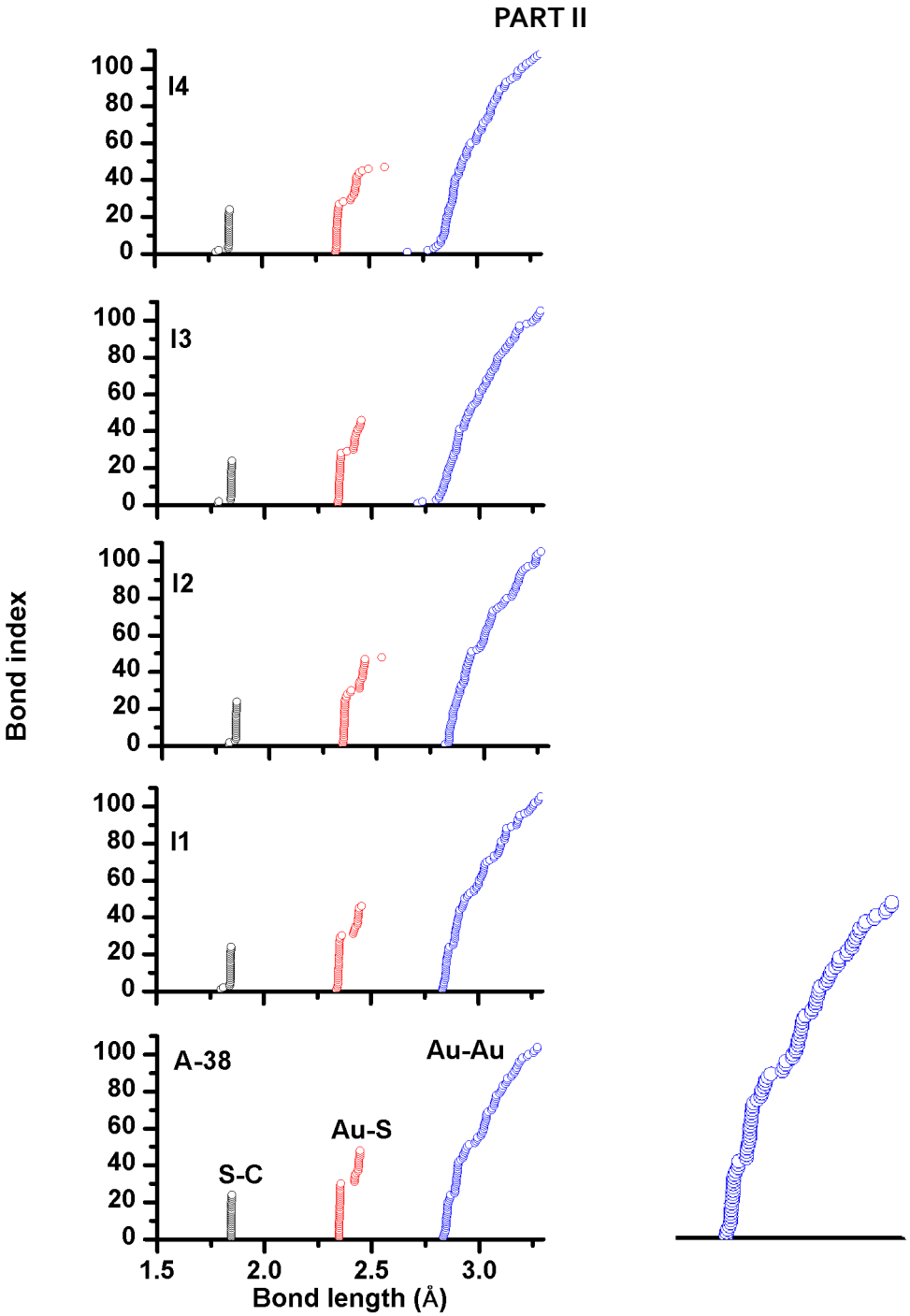


Figure S2. Comparison of distances of four regioisomers with $Au_{38}(SCH_3)_{24}$ cluster. The Au-Au bonds (blue circles) exhibit more structure in the *A*-38 cluster, while I3 and I4 show less symmetry in their Au-Au and Au-S bonds. Au-Au bonding of the *A*-38 cluster is displayed at right.

PART III

Kohn-Sham orbitals of 5 studied clusters.

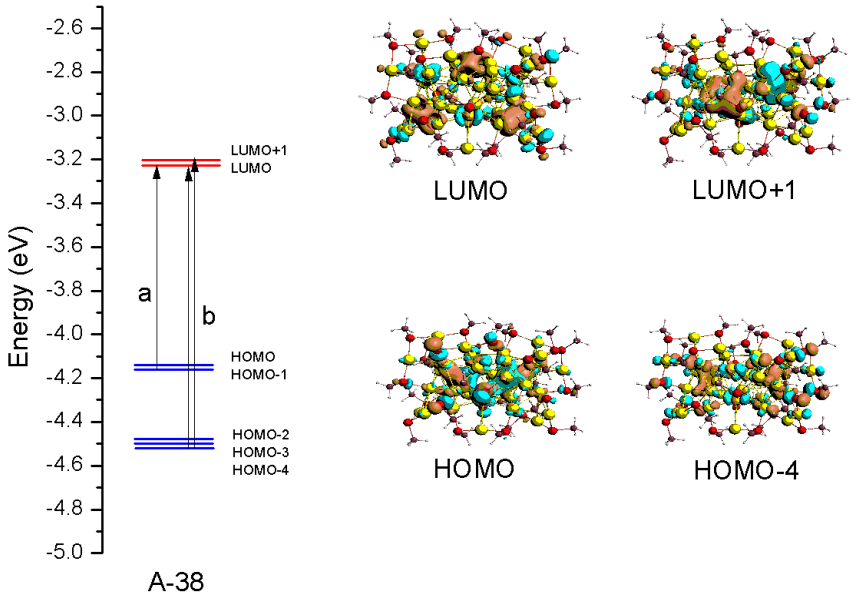


Figura S3. K-S orbitals of the *A*-38 cluster.

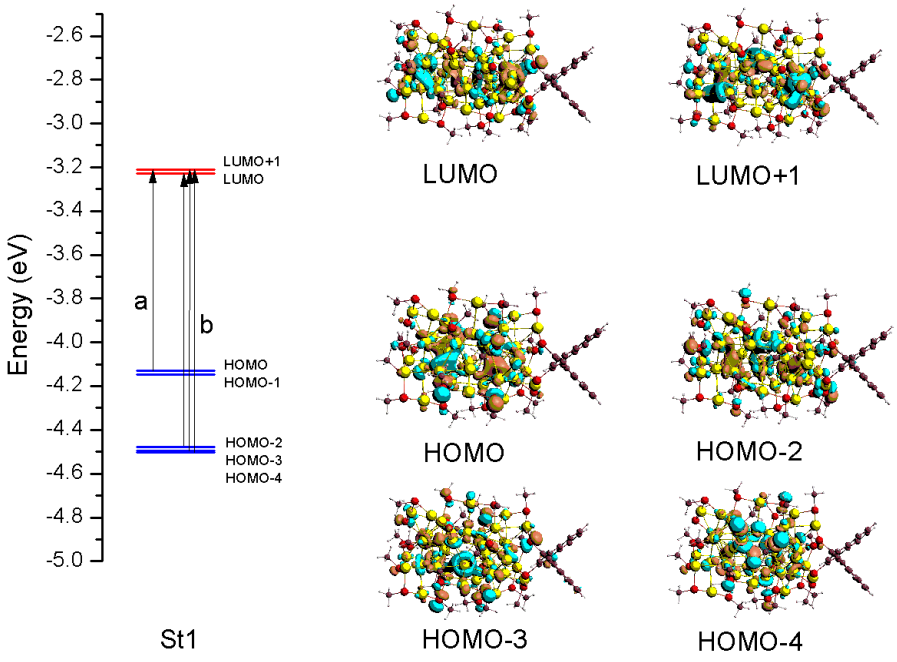


Figura S4. K-S orbitals of the I1 cluster.

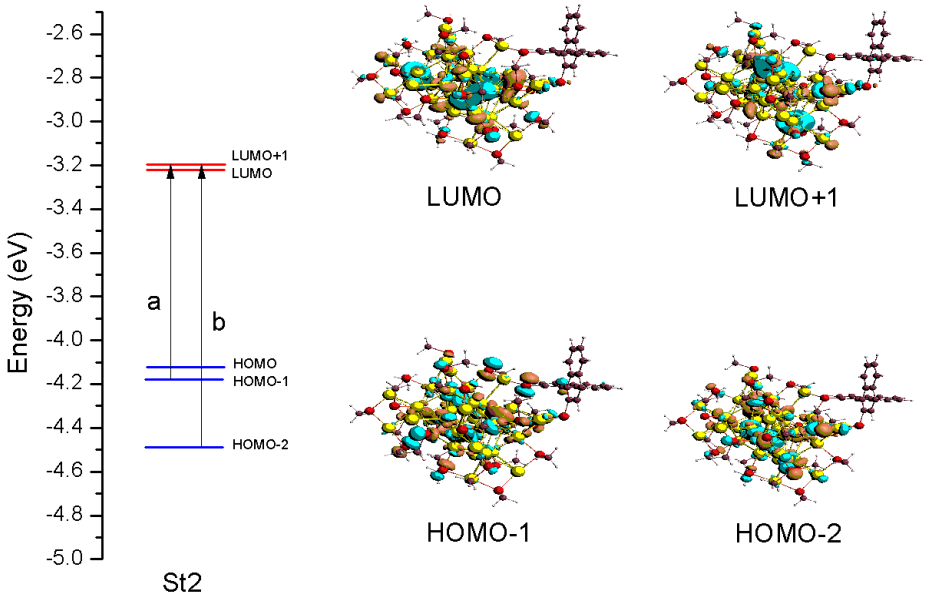


Figura S5. K-S orbitals of the I2 cluster.

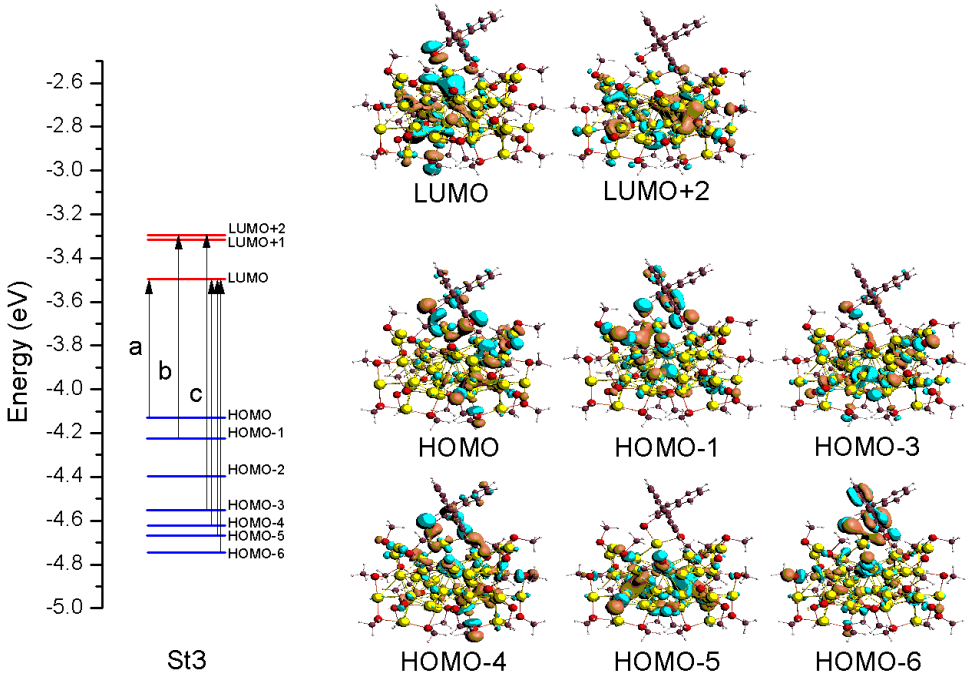


Figura S6. K-S orbitals of the I3 cluster.

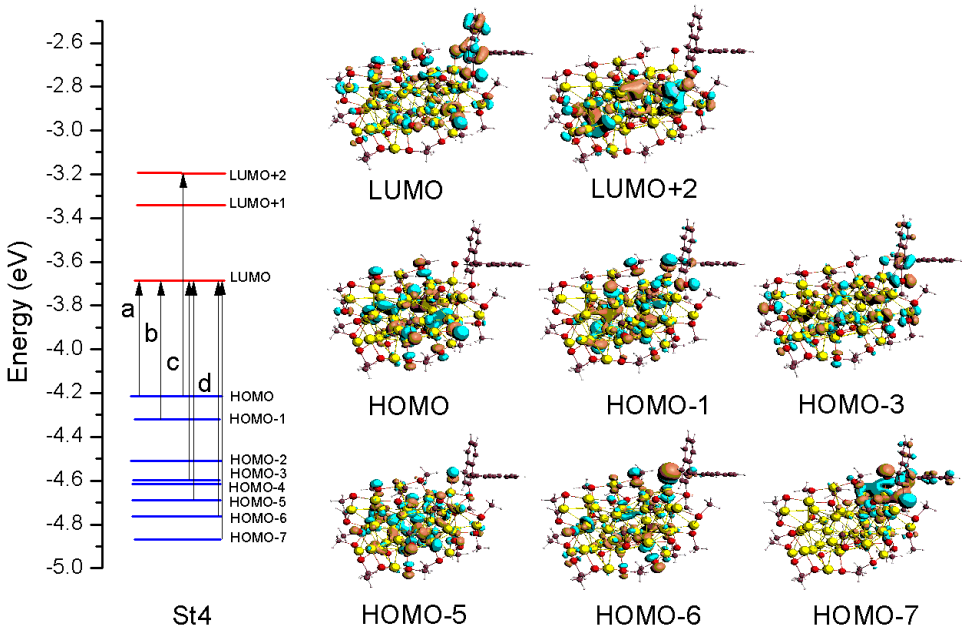


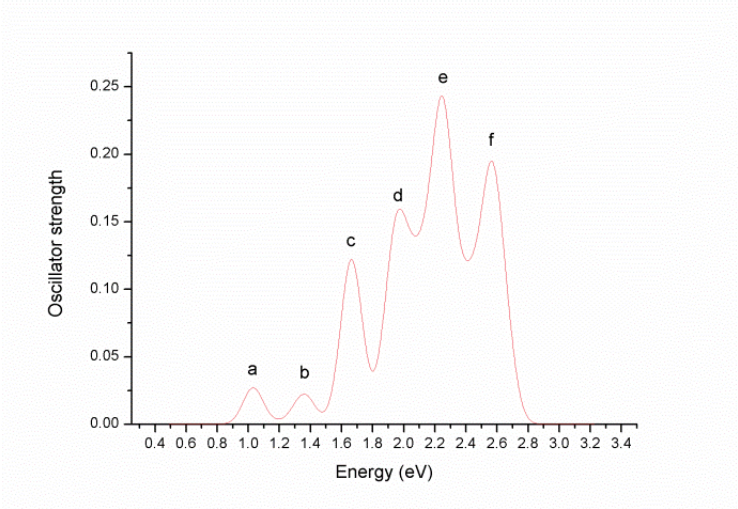
Figura S7. K-S orbitals of the I4 cluster.

PART IV

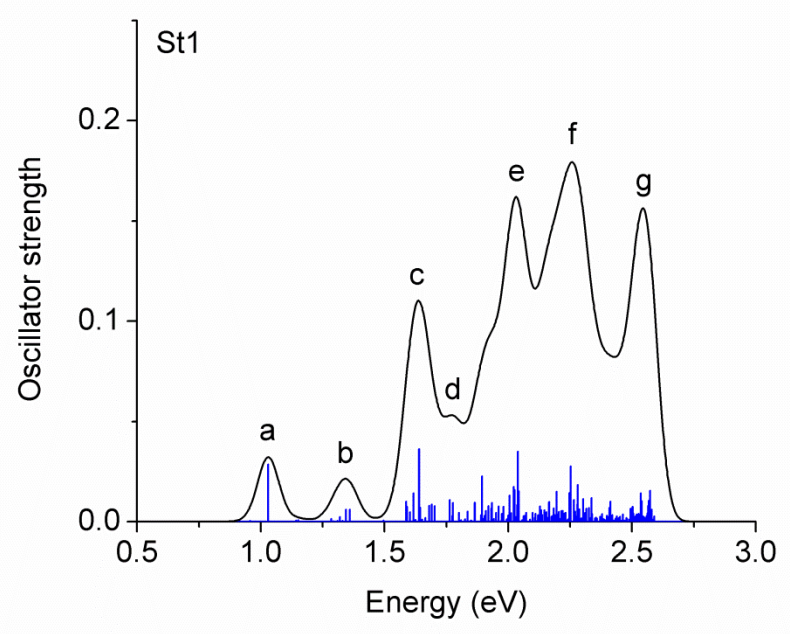
Table S1. Excitation energy, oscillator strength, electronic transitions and their weights for peaks of studied regioisomers.

A-38 enantiomer

Peak	E_{peak}, eV	f	Transition from occupied -> unoccupied orbital	Weigth, %
a	1.030	0.0264	HOMO-1 -> LUMO	54.2
			HOMO -> LUMO+1	38.5
b	1.365	0.0094	HOMO-4 -> LUMO	78.0
			HOMO-4 -> LUMO+1	6.6
	1.369	0.0092	HOMO-4 -> LUMO+1	79.9
			HOMO-4 -> LUMO	6.3
c	1.659	0.0305	HOMO-2 -> LUMO+3	36.3
			HOMO-4 -> LUMO+2	15.9
	1.661	0.0376	HOMO-4 -> LUMO+2	19.0
			HOMO-2 -> LUMO+3	16.3
d	1.967	0.0210	HOMO-12 -> LUMO+1	27.4
			HOMO-12 -> LUMO	18.5
	1.996	0.0173	HOMO-8 -> LUMO+2	37.7
			HOMO-13 -> LUMO	37.7
	2.001	0.0263	HOMO-13 -> LUMO+1	48.2
			HOMO-8 -> LUMO+2	17.7
e	2.234	0.0380	HOMO-11 -> LUMO+4	26.3
			HOMO-11 -> LUMO+3	14.4
	2.235	0.0482	HOMO-20 -> LUMO+1	25.0
			HOMO-3 -> LUMO+6	12.0
f	2.565	0.0271	HOMO-6 -> LUMO+5	19.6
			HOMO-1 -> LUMO+14	15.1
	2.568	0.0197	HOMO-6 -> LUMO+6	41.4
			HOMO-32 -> LUMO+1	15.4



R-BINAS/ 2 dimer motifs



HOMO-LUMO: 0.91 eV

	E_{peak} (eV)	f	Transition from occupied -> unoccupied orbital	Weigth
Peak a				
	1.03033	0.3203E-01	HOMO -> LUMO+1	0.5652
			HOMO-1 -> LUMO	0.3502
Peak b				
	1.31917	0.3808E-02	HOMO-3 -> LUMO+1	0.4527
			HOMO-4 -> LUMO+1	0.2140
			HOMO -> LUMO+3	0.1167
	1.34393	0.6782E-02	HOMO-2 -> LUMO	0.3129
			HOMO-3 -> LUMO	0.2613
			HOMO-4 -> LUMO+1	0.2481
	1.35927	0.9611E-02	HOMO-4 -> LUMO+1	0.7599
Peak c				
	1.58692	0.1036E-01	HOMO-5 -> LUMO	0.4659
			HOMO-2 -> LUMO+3	0.1882
	1.61716	0.2226E-01	HOMO-6 -> LUMO	0.2813
			HOMO-3 -> LUMO+3	0.1737
			HOMO-5 -> LUMO	0.1709
	1.63978	0.4652E-01	HOMO-2 -> LUMO+2	0.2000
			HOMO-2 -> LUMO+3	0.1560
			HOMO-4 -> LUMO+4	0.1275
			HOMO-3 -> LUMO+3	0.0978
	1.64395	0.1106E-01	HOMO-6 -> LUMO+1	0.7331

1.68085	0.1247E-01	HOMO-4 -> LUMO+4	0.4033
		HOMO-2 -> LUMO+3	0.0775
		HOMO-3 -> LUMO+3	0.0765

Peak d

1.76348	0.1397E-01	HOMO-8 -> LUMO	0.6387
		HOMO-8 -> LUMO+1	0.2357
1.77636	0.1892E-01	HOMO-8 -> LUMO+1	0.3510
		HOMO-5 -> LUMO+2	0.2785
		HOMO-8 -> LUMO	0.1435

Peak e

1.89422	0.2341E-01	HOMO-11 -> LUMO+1	0.3308
		HOMO-5 -> LUMO+4	0.1832
		HOMO-1 -> LUMO+5	0.1097
1.91967	0.1223E-01	HOMO-1 -> LUMO+6	0.2665
		HOMO-6 -> LUMO+4	0.1596
		HOMO -> LUMO+6	0.1393
1.93358	0.1048E-01	HOMO-6 -> LUMO+4	0.2229
		HOMO-11 -> LUMO+1	0.1110
		HOMO-8 -> LUMO+2	0.1080
		HOMO-12 -> LUMO	0.1044
2.00553	0.1475E-01	HOMO-1 -> LUMO+7	0.4167
		HOMO-9 -> LUMO+2	0.1766
2.02213	0.1948E-01	HOMO-10 -> LUMO+2	0.3856
		HOMO-15 -> LUMO+1	0.1701
		HOMO-1 -> LUMO+7	0.1009
2.02599	0.1768E-01	HOMO-15 -> LUMO+1	0.2814
		HOMO-7 -> LUMO+3	0.2080
		HOMO-15 -> LUMO	0.0911
2.03951	0.3506E-01	HOMO-1 -> LUMO+8	0.3589
		HOMO-14 -> LUMO+1	0.1325
		HOMO-10 -> LUMO+2	0.1161
2.04226	0.3050E-01	HOMO-1 -> LUMO+8	0.3681
		HOMO-10 -> LUMO+2	0.1814

Peak f

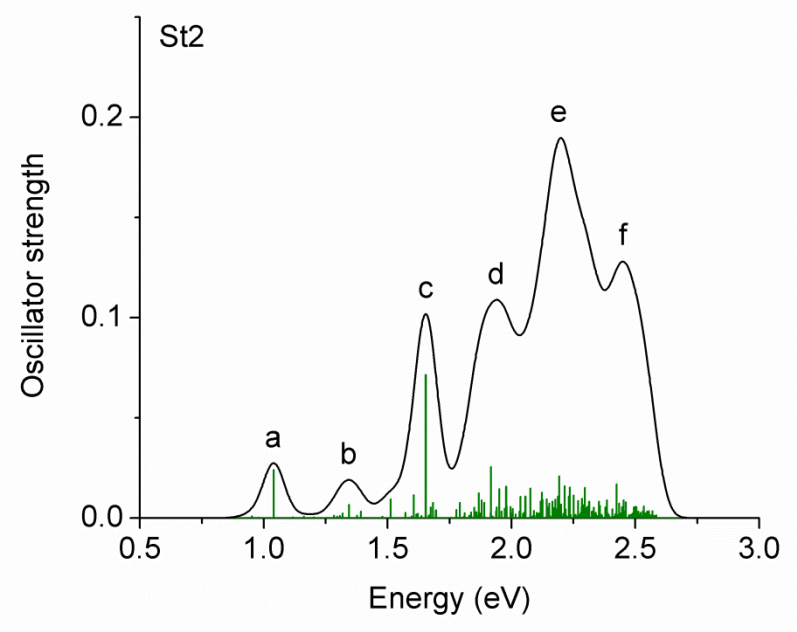
2.12758	0.1001E-01	HOMO-19 -> LUMO	0.2516
		HOMO-1 -> LUMO+10	0.2173
		HOMO-12 -> LUMO+2	0.1361
2.16400	0.1011E-01	HOMO-10 -> LUMO+4	0.4022
		HOMO-18 -> LUMO+1	0.1182
2.16584	0.1271E-01	HOMO-20 -> LUMO	0.6244
2.18397	0.1050E-01	HOMO-20 -> LUMO+1	0.3626
		HOMO-1 -> LUMO+11	0.1677
		HOMO-15 -> LUMO+2	0.1103
2.19563	0.1684E-01	HOMO -> LUMO+12	0.4199
		HOMO-11 -> LUMO+3	0.2237
2.22006	0.1093E-01	HOMO-21 -> LUMO	0.2645
		HOMO-21 -> LUMO+1	0.1492
		HOMO-12 -> LUMO+3	0.1004

2.24631	0.1441E-01	HOMO-3 -> LUMO+6	0.2385
		HOMO-21 -> LUMO+1	0.1638
		HOMO-12 -> LUMO+3	0.1050
		HOMO-13 -> LUMO+3	0.1033
2.25094	0.1046E-01	HOMO-4 -> LUMO+6	0.2554
		HOMO-12 -> LUMO+3	0.2259
		HOMO-12 -> LUMO+4	0.0814
2.25171	0.2772E-01	HOMO-21 -> LUMO+1	0.2679
		HOMO-12 -> LUMO+3	0.1929
		HOMO-22 -> LUMO	0.1615
2.26552	0.1128E-01	HOMO-22 -> LUMO+1	0.6709
		HOMO-4 -> LUMO+6	0.1062
2.27904	0.1129E-01	HOMO-12 -> LUMO+4	0.2775
		HOMO-16 -> LUMO+2	0.1697
		HOMO-14 -> LUMO+4	0.1034
2.28049	0.2058E-01	HOMO-14 -> LUMO+3	0.6964
2.30305	0.2279E-01	HOMO-14 -> LUMO+4	0.5675
2.33663	0.1326E-01	HOMO-23 -> LUMO+1	0.2911
		HOMO-15 -> LUMO+4	0.2287
		HOMO-20 -> LUMO+2	0.1344
2.41222	0.1042E-01	HOMO-2 -> LUMO+9	0.2932
		HOMO-3 -> LUMO+9	0.2778
		HOMO-4 -> LUMO+9	0.1130

Peak g

2.49417	0.1036E-01	HOMO-5 -> LUMO+5	0.3300
		HOMO-24 -> LUMO+2	0.1617
		HOMO-23 -> LUMO+2	0.1509
		HOMO-31 -> LUMO+1	0.1216
2.50255	0.1175E-01	HOMO-31 -> LUMO+1	0.4046
		HOMO-5 -> LUMO+5	0.2701
2.53604	0.1834E-01	HOMO-6 -> LUMO+6	0.3562
		HOMO-21 -> LUMO+4	0.0957
		HOMO-35 -> LUMO	0.0870
2.53860	0.1068E-01	HOMO-1 -> LUMO+15	0.2173
		HOMO-34 -> LUMO	0.1707
		HOMO-21 -> LUMO+4	0.1032
		HOMO-4 -> LUMO+11	0.0804
2.56566	0.1611E-01	HOMO-4 -> LUMO+12	0.2373
		HOMO-22 -> LUMO+4	0.1377
		HOMO-36 -> LUMO	0.1057
		HOMO-3 -> LUMO+12	0.0909
2.56829	0.1089E-01	HOMO-22 -> LUMO+4	0.2555
		HOMO-33 -> LUMO+1	0.1412
		HOMO-1 -> LUMO+16	0.1142
2.57369	0.1731E-01	HOMO-36 -> LUMO	0.1493
		HOMO-35 -> LUMO+1	0.1454
		HOMO-1 -> LUMO+16	0.1110
		HOMO-36 -> LUMO+1	0.0983
2.57466	0.1178E-01	HOMO-25 -> LUMO+2	0.1910
		HOMO-3 -> LUMO+2	0.1582
		HOMO-33 -> LUMO+1	0.1005

R-BINAS/ 1 monomer and 1 dimer motif



HOMO-LUMO: 0.89 eV

E_{peak} (eV)	f	Transition from occupied -> unoccupied orbital	Weigth
Peak a			
1.04022	0.2695E-01	HOMO-1 -> LUMO+1	0.4334
		HOMO-1 -> LUMO	0.3120
		HOMO -> LUMO+1	0.1178
Peak b			
1.34360	0.1059E-01	HOMO-2 -> LUMO+1	0.5969
		HOMO-2 -> LUMO	0.1429
		HOMO-3 -> LUMO+1	0.1073
Peak c			
1.60535	0.1190E-01	HOMO-3 -> LUMO+3	0.3202
		HOMO-2 -> LUMO+4	0.1432
		HOMO-4 -> LUMO+2	0.1425
		HOMO-3 -> LUMO+4	0.1072
1.65414	0.7156E-01	HOMO-2 -> LUMO+4	0.2310
		HOMO-6 -> LUMO+1	0.1849
		HOMO-2 -> LUMO+2	0.1601
		HOMO-4 -> LUMO+2	0.1211
Peak d			
1.86769	0.2496E-01	HOMO-11 -> LUMO+1	0.2274
		HOMO-6 -> LUMO+3	0.1518
		HOMO -> LUMO+6	0.1470

		HOMO-1 -> LUMO+5	0.1198
1.87970	0.1143E-01	HOMO-6 -> LUMO+3	0.5539
		HOMO-1 -> LUMO+6	0.0954
1.91683	0.2629E-01	HOMO-1 -> LUMO+6	0.5348
		HOMO-6 -> LUMO+3	0.0508
1.95148	0.2284E-01	HOMO-13 -> LUMO	0.3020
		HOMO-7 -> LUMO+3	0.2567
		HOMO-12 -> LUMO+1	0.2506
1.97856	0.1777E-01	HOMO-13 -> LUMO+1	0.2964
		HOMO-7 -> LUMO+3	0.2169
		HOMO-9 -> LUMO+2	0.1155

Peak e

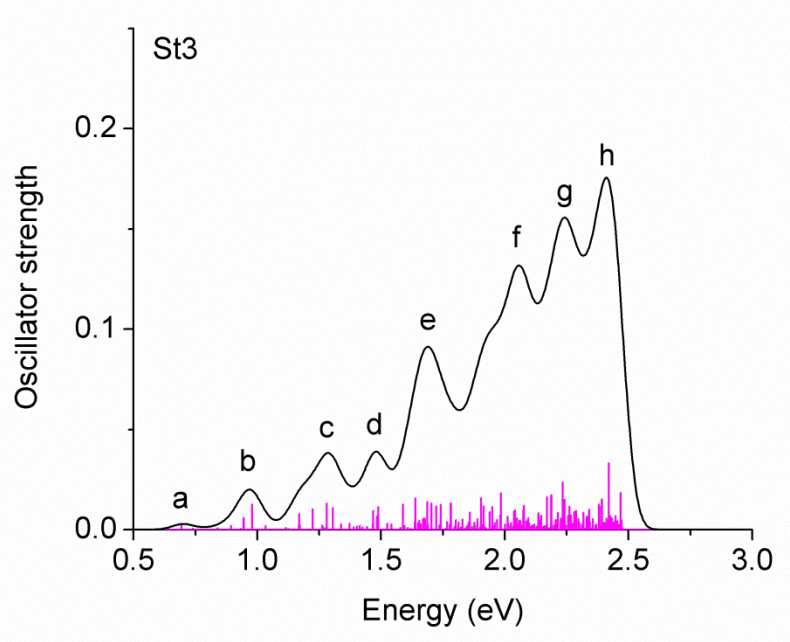
2.03597	0.1370E-01	HOMO-1 -> LUMO+8	0.2929
		HOMO-15 -> LUMO	0.2439
		HOMO-14 -> LUMO+1	0.1864
2.05633	0.1115E-01	HOMO-8 -> LUMO+3	0.4652
		HOMO-1 -> LUMO+8	0.1089
		HOMO-15 -> LUMO+1	0.1058
2.07586	0.1665E-01	HOMO-15 -> LUMO+1	0.2680
		HOMO-8 -> LUMO+3	0.1489
		HOMO-16 -> LUMO	0.1080
2.12214	0.1283E-01	HOMO-17 -> LUMO	0.1917
		HOMO -> LUMO+11	0.1664
		HOMO-13 -> LUMO+2	0.1391
2.12408	0.1002E-01	HOMO-17 -> LUMO+1	0.2167
		HOMO-13 -> LUMO+2	0.1912
		HOMO -> LUMO+11	0.1027
2.12602	0.1015E-01	HOMO-18 -> LUMO+1	0.4503
		HOMO-3 -> LUMO+5	0.0771
2.17698	0.1855E-01	HOMO-19 -> LUMO+1	0.1122
		HOMO-12 -> LUMO+3	0.1074
		HOMO-1 -> LUMO+10	0.1002
		HOMO -> LUMO+12	0.0768
		HOMO-10 -> LUMO+3	0.0671
		HOMO-11 -> LUMO+3	0.0599
2.18827	0.1384E-01	HOMO-11 -> LUMO+4	0.2521
		HOMO -> LUMO+11	0.1690
		HOMO-20 -> LUMO	0.0944
2.19330	0.3272E-01	HOMO-20 -> LUMO	0.2442
		HOMO-21 -> LUMO	0.1215
		HOMO-21 -> LUMO+1	0.0950
		HOMO-4 -> LUMO+5	0.0873
2.21523	0.1643E-01	HOMO-21 -> LUMO	0.3021
		HOMO-15 -> LUMO+2	0.1487
		HOMO-20 -> LUMO	0.0967
2.23108	0.1697E-01	HOMO-3 -> LUMO+6	0.1215
		HOMO-4 -> LUMO+5	0.1098
		HOMO-12 -> LUMO+4	0.1058
		HOMO-15 -> LUMO+2	0.1042
		HOMO-2 -> LUMO+6	0.0837
2.23574	0.1539E-01	HOMO-21 -> LUMO+1	0.4016
		HOMO-3 -> LUMO+6	0.2530

2.25060	0.1761E-01	HOMO-13 -> LUMO+4	0.6329
		HOMO-16 -> LUMO+2	0.0629
2.28485	0.1012E-01	HOMO-17 -> LUMO+2	0.2477
		HOMO-18 -> LUMO+2	0.1699
		HOMO-22 -> LUMO+1	0.1492
		HOMO-4 -> LUMO+6	0.1406
2.29578	0.2369E-01	HOMO-22 -> LUMO+1	0.3634
		HOMO-3 -> LUMO+7	0.2060
		HOMO-2 -> LUMO+7	0.0934
2.31370	0.1290E-01	HOMO-23 -> LUMO	0.5409
		HOMO-24 -> LUMO	0.1283
		HOMO-15 -> LUMO+3	0.1078
2.35290	0.1284E-01	HOMO-3 -> LUMO+8	0.2388
		HOMO-4 -> LUMO+7	0.2229
		HOMO-16 -> LUMO+3	0.2196
		HOMO-1 -> LUMO+13	0.1042

Peak f

2.38470	0.1385E-01	HOMO-16 -> LUMO+4	0.4068
		HOMO-17 -> LUMO+4	0.1527
		HOMO-17 -> LUMO+3	0.1029
2.42424	0.1701E-01	HOMO-27 -> LUMO+1	0.3084
		HOMO-5 -> LUMO+5	0.2488
		HOMO-3 -> LUMO+9	0.1292
2.43529	0.1475E-01	HOMO-27 -> LUMO+1	0.3325
		HOMO-5 -> LUMO+5	0.1317
		HOMO-19 -> LUMO+4	0.1038
2.46231	0.1026E-01	HOMO-28 -> LUMO+1	0.2689
		HOMO-6 -> LUMO+5	0.1624
		HOMO-29 -> LUMO+1	0.0938

_R_-BINAS/ 1 monomer motif



HOMO-LUMO: 0.63 eV

E_{peak} (eV)	f	Transition from occupied -> unoccupied orbital	Weigth
Peak a			
0.69311	0.2386E-02	HOMO -> LUMO	0.9572
Peak b			
0.97990	0.1344E-01	HOMO-1 -> LUMO+2	0.5153
		HOMO-1 -> LUMO+1	0.3203
Peak c			
1.16908	0.1011E-01	HOMO-4 -> LUMO	0.6966
		HOMO-5 -> LUMO	0.1032
1.22433	0.1145E-01	HOMO-5 -> LUMO	0.5707
		HOMO-6 -> LUMO	0.1311
		HOMO-3 -> LUMO+1	0.1043
1.28130	0.1361E-01	HOMO-6 -> LUMO	0.4980
		HOMO-3 -> LUMO+2	0.1229
		HOMO-2 -> LUMO+3	0.1209
		HOMO-1 -> LUMO+4	0.1141
1.30554	0.1409E-01	HOMO-3 -> LUMO+2	0.4908
		HOMO-3 -> LUMO+1	0.0876
Peak d			
1.46768	0.1221E-01	HOMO-6 -> LUMO+1	0.4943
		HOMO-3 -> LUMO+3	0.1944
1.48843	0.1277E-01	HOMO-6 -> LUMO+2	0.5941
		HOMO-9 -> LUMO	0.1831

Peak e

1.58881	0.1300E-01	HOMO-5 -> LUMO+3	0.5163
		HOMO-6 -> LUMO+3	0.2028
1.63920	0.1575E-01	HOMO-8 -> LUMO+1	0.3573
		HOMO-4 -> LUMO+4	0.1951
		HOMO -> LUMO+5	0.1217
1.68780	0.1437E-01	HOMO-13 -> LUMO	0.2597
		HOMO-10 -> LUMO+1	0.1914
		HOMO-9 -> LUMO+2	0.1334
1.70415	0.2057E-01	HOMO-9 -> LUMO+2	0.2757
		HOMO-14 -> LUMO	0.2320
1.72370	0.1196E-01	HOMO-5 -> LUMO+4	0.5342
		HOMO-15 -> LUMO	0.1382
1.74081	0.1259E-01	HOMO-10 -> LUMO+1	0.3155
		HOMO-10 -> LUMO+2	0.2960
		HOMO-15 -> LUMO	0.2292
1.78229	0.1490E-01	HOMO-10 -> LUMO+2	0.2139
		HOMO-11 -> LUMO+2	0.1864
		HOMO -> LUMO+6	0.1172

Peak f

1.90361	0.1584E-01	HOMO-20 -> LUMO	0.3071
		HOMO-19 -> LUMO	0.1884
		HOMO-12 -> LUMO+2	0.1403
1.91553	0.1302E-01	HOMO-20 -> LUMO	0.3187
		HOMO-7 -> LUMO+4	0.1351
		HOMO-10 -> LUMO+3	0.1073
1.93887	0.1379E-01	HOMO -> LUMO+8	0.4435
		HOMO-10 -> LUMO+3	0.2941
1.94949	0.1275E-01	HOMO-8 -> LUMO+4	0.2294
		HOMO-15 -> LUMO+1	0.1486
		HOMO-15 -> LUMO+2	0.1109
1.98473	0.2040E-01	HOMO -> LUMO+9	0.4761
		HOMO-1 -> LUMO+8	0.1066
2.03793	0.1017E-01	HOMO-23 -> LUMO	0.3363
		HOMO -> LUMO+10	0.1961
		HOMO-16 -> LUMO+2	0.1576
2.04106	0.1958E-01	HOMO-17 -> LUMO+1	0.2619
		HOMO-16 -> LUMO+2	0.2129
		HOMO-14 -> LUMO+3	0.1137
2.04886	0.1179E-01	HOMO -> LUMO+10	0.3485
		HOMO-1 -> LUMO+9	0.1046
		HOMO-23 -> LUMO	0.0937
2.07564	0.1249E-01	HOMO-18 -> LUMO+1	0.2164
		HOMO -> LUMO+11	0.1646
		HOMO-14 -> LUMO+3	0.0769
		HOMO-13 -> LUMO+3	0.0676
2.07832	0.1235E-01	HOMO -> LUMO+11	0.5038
		HOMO-18 -> LUMO+1	0.1010

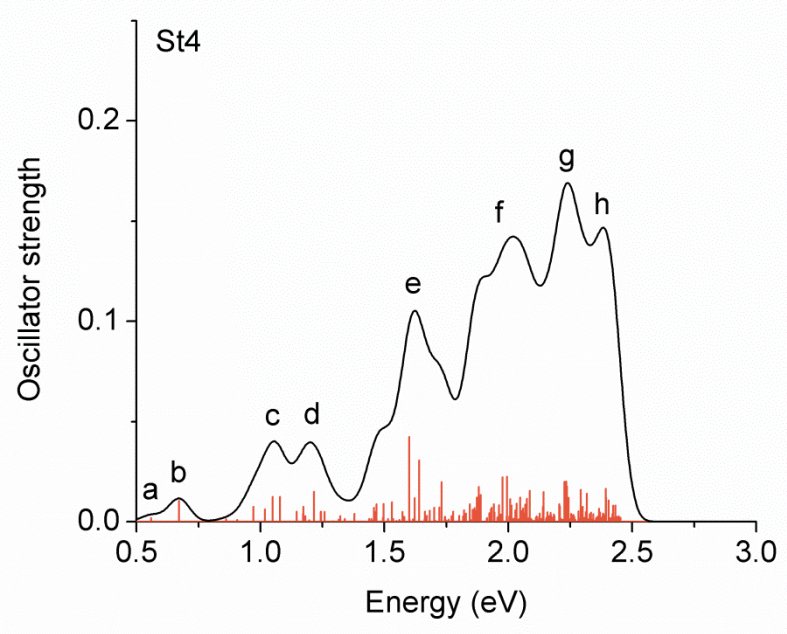
Peak g

2.17092	0.1684E-01	HOMO-21 -> LUMO+2	0.2466
		HOMO-1 -> LUMO+11	0.1425
		HOMO-22 -> LUMO+1	0.1230
2.18839	0.1932E-01	HOMO-22 -> LUMO+2	0.3965
		HOMO-17 -> LUMO+3	0.0712
		HOMO-27 -> LUMO	0.0579
2.23424	0.3050E-01	HOMO-23 -> LUMO+1	0.2960
		HOMO-2 -> LUMO+9	0.1624
		HOMO-29 -> LUMO	0.1000
2.24141	0.1506E-01	HOMO-18 -> LUMO+3	0.4708
		HOMO-23 -> LUMO+1	0.1342
		HOMO-29 -> LUMO	0.1075
2.25627	0.1087E-01	HOMO-15 -> LUMO+4	0.3273
		HOMO-23 -> LUMO+2	0.2407
2.26190	0.1188E-01	HOMO-31 -> LUMO	0.5962
2.28108	0.1148E-01	HOMO-4 -> LUMO+6	0.6196

Peak h

2.31858	0.1099E-01	HOMO-5 -> LUMO+6	0.4083
		HOMO -> LUMO+12	0.1367
		HOMO-16 -> LUMO+4	0.1196
2.34203	0.1139E-01	HOMO-7 -> LUMO+5	0.2373
		HOMO-2 -> LUMO+11	0.2026
		HOMO-17 -> LUMO+4	0.1725
2.38033	0.1425E-01	HOMO -> LUMO+13	0.4775
		HOMO-18 -> LUMO+4	0.2640
		HOMO-6 -> LUMO+6	0.1035
2.38292	0.1194E-01	HOMO-8 -> LUMO+5	0.3786
		HOMO-3 -> LUMO+9	0.2096
		HOMO-6 -> LUMO+6	0.1500
2.39270	0.1572E-01	HOMO-18 -> LUMO+4	0.3500
		HOMO-23 -> LUMO+3	0.1915
2.41970	0.3415E-01	HOMO-6 -> LUMO+6	0.1656
		HOMO-20 -> LUMO+4	0.0922
		HOMO-9 -> LUMO+5	0.0904
		HOMO -> LUMO+13	0.0810
		HOMO-4 -> LUMO+8	0.0713
2.44805	0.1077E-01	HOMO-21 -> LUMO+4	0.4423
		HOMO-4 -> LUMO+9	0.0903
2.46811	0.1840E-01	HOMO-4 -> LUMO+9	0.2870
		HOMO-30 -> LUMO+2	0.2422

R-BINAS/ 1 dimer motif



HOMO-LUMO: 0.53 eV

	E_{peak} (eV)	f	Transition from occupied -> unoccupied orbital	Weigth
Peak a				
	0.55906	0.3333E-02	HOMO -> LUMO	0.9543
Peak b				
	0.67139	0.1155E-01	HOMO-1 -> LUMO	0.9406
Peak c				
	0.97136	0.1320E-01	HOMO-3 -> LUMO	0.6628
			HOMO-1 -> LUMO+1	0.1474
			HOMO-4 -> LUMO	0.1013
	1.04946	0.1936E-01	HOMO-5 -> LUMO	0.5958
			HOMO -> LUMO+2	0.1827
			HOMO-1 -> LUMO+1	0.1028
	1.07907	0.1598E-01	HOMO -> LUMO+2	0.7725
Peak d				
	1.17306	0.1165E-01	HOMO-6 -> LUMO	0.5034
			HOMO-1 -> LUMO+2	0.1700
			HOMO-7 -> LUMO	0.1339

1.21628	0.1685E-01	HOMO-7 -> LUMO	0.7087
		HOMO-6 -> LUMO	0.1172

Peak e

1.49642	0.1015E-01	HOMO-13 -> LUMO	0.4666
		HOMO-5 -> LUMO+2	0.2110
		HOMO-3 -> LUMO+2	0.1165
1.60079	0.4352E-01	HOMO-4 -> LUMO+3	0.5328
		HOMO-1 -> LUMO+5	0.1598
1.62253	0.1535E-01	HOMO-5 -> LUMO+3	0.4262
		HOMO-4 -> LUMO+4	0.1168
1.64041	0.3163E-01	HOMO-5 -> LUMO+3	0.2772
		HOMO-17 -> LUMO	0.1666
		HOMO-15 -> LUMO	0.0920
		HOMO-3 -> LUMO+3	0.0915
1.72256	0.1137E-01	HOMO-5 -> LUMO+4	0.4974
		HOMO-19 -> LUMO	0.1512
1.73044	0.3087E-01	HOMO-18 -> LUMO	0.3469
		HOMO-7 -> LUMO+2	0.0914
		HOMO-6 -> LUMO+3	0.0884

Peak f

1.86464	0.1071E-01	HOMO-7 -> LUMO+4	0.2343
		HOMO-14 -> LUMO+1	0.1814
		HOMO-23 -> LUMO	0.1279
		HOMO-8 -> LUMO+3	0.1202
1.87296	0.1561E-01	HOMO-14 -> LUMO+1	0.5961
		HOMO-3 -> LUMO+5	0.0702
1.88173	0.2234E-01	HOMO-7 -> LUMO+4	0.3838
		HOMO-4 -> LUMO+5	0.0943
1.88827	0.1728E-01	HOMO-4 -> LUMO+5	0.4181
		HOMO -> LUMO+6	0.1506
1.92946	0.1019E-01	HOMO-24 -> LUMO	0.2961
		HOMO -> LUMO+7	0.1522
		HOMO-16 -> LUMO+1	0.1274
		HOMO-5 -> LUMO+5	0.1008
1.97728	0.2489E-01	HOMO-11 -> LUMO+2	0.3342
		HOMO-1 -> LUMO+7	0.1150
		HOMO-5 -> LUMO+5	0.1060
1.99510	0.2260E-01	HOMO-13 -> LUMO+2	0.4214
		HOMO-9 -> LUMO+4	0.1564
		HOMO -> LUMO+8	0.1130
2.00800	0.1141E-01	HOMO-27 -> LUMO	0.4699
		HOMO-1 -> LUMO+7	0.1071
2.03388	0.1018E-01	HOMO-14 -> LUMO+2	0.4878
		HOMO-10 -> LUMO+3	0.1157
2.04793	0.1566E-01	HOMO-10 -> LUMO+3	0.3933
		HOMO-6 -> LUMO+5	0.1242
		HOMO-14 -> LUMO+2	0.1078
2.06786	0.1355E-01	HOMO-15 -> LUMO+2	0.3205
		HOMO-16 -> LUMO+2	0.1317

2.07539	0.1188E-01	HOMO-12 -> LUMO+3	0.5080
		HOMO-18 -> LUMO+1	0.1127
2.08621	0.1588E-01	HOMO-10 -> LUMO+4	0.2449
		HOMO-16 -> LUMO+2	0.1949
		HOMO-30 -> LUMO	0.1359

Peak g

2.13976	0.1173E-01	HOMO-21 -> LUMO+1	0.2044
		HOMO-14 -> LUMO+3	0.1271
		HOMO-1 -> LUMO+9	0.1085
		HOMO-33 -> LUMO	0.1007
2.14289	0.1535E-01	HOMO-33 -> LUMO	0.2039
		HOMO-21 -> LUMO+1	0.1532
		HOMO-11 -> LUMO+4	0.1079
2.22580	0.1193E-01	HOMO-38 -> LUMO	0.2439
		HOMO-15 -> LUMO+4	0.1910
		HOMO-3 -> LUMO+6	0.1282
		HOMO-23 -> LUMO+1	0.1084
2.22632	0.2240E-01	HOMO-16 -> LUMO+4	0.1725
		HOMO-19 -> LUMO+2	0.1682
		HOMO-23 -> LUMO+1	0.1021
2.23358	0.2262E-01	HOMO-15 -> LUMO+4	0.3204
		HOMO-23 -> LUMO+1	0.1272
2.23710	0.1757E-01	HOMO-19 -> LUMO+2	0.4052
		HOMO-9 -> LUMO+5	0.1464
		HOMO-23 -> LUMO+1	0.1354
2.24378	0.1350E-01	HOMO-16 -> LUMO+4	0.4222
		HOMO-2 -> LUMO+8	0.0722
2.29297	0.2057E-01	HOMO-25 -> LUMO+1	0.4733
		HOMO-17 -> LUMO+3	0.1934
2.31761	0.1452E-01	HOMO-42 -> LUMO	0.3669
		HOMO-22 -> LUMO+2	0.1399
		HOMO-5 -> LUMO+6	0.0907

Peak h

2.39281	0.1691E-01	HOMO-21 -> LUMO+3	0.1603
		HOMO-28 -> LUMO+1	0.1402
		HOMO-45 -> LUMO	0.1301
		HOMO-46 -> LUMO	0.0900
2.39380	0.1226E-01	HOMO-28 -> LUMO+1	0.4840
		HOMO-19 -> LUMO+4	0.1576
2.40473	0.1672E-01	HOMO-2 -> LUMO+10	0.6044
2.42315	0.1650E-01	HOMO-20 -> LUMO+4	0.2348
		HOMO-22 -> LUMO+3	0.1541
		HOMO-3 -> LUMO+9	0.0967
		HOMO-47 -> LUMO	0.0927

PART V

Cartesian coordinates of four regioisomers

I1 regioisomer

Au -1.3169 -0.864329 -0.860744

Au -0.329817 1.75521 -0.131795

Au -0.201996 1.60837 2.74852

Au 1.59662 3.49121 1.07406

Au 4.21767 -0.405321 -0.314549

Au -2.58058 0.504845 1.28312

Au 1.96454 0.609229 1.20999

Au -0.251886 -1.14958 1.80691

Au -2.60028 -2.59099 1.07112

Au -2.7927 1.54791 -1.5532

Au 2.3202 1.82346 -1.33764

Au 1.55849 -0.971061 -1.16677

Au 2.41823 -2.18797 1.35066

Au 4.22571 -0.286947 2.6949

Au -0.114997 0.764423 -2.84415

Au -0.094616 -2.21714 -3.12332

Au 2.60328 2.25358 3.45167

Au -4.17715 -0.972599 -0.683405

Au 4.29192 2.21475 0.825024

Au 0.064659 -3.26034 -0.200702

Au -5.43294 1.00006 -3.18916

Au 1.63828 -0.538751 3.86561

Au 0.641246 4.59292 3.97604

Au -2.37332 -3.33449 -1.83125

Au -2.45819 2.18225 -4.78961

Au -5.37793 -1.19956 2.19934

Au 3.98544 5.02284 2.72263

Au -2.68441 -0.66248 -3.35415

Au -2.15813 -3.57157 -5.04886

Au -1.16984 -2.62819 4.2792

Au 3.95107 0.376798 5.85465

Au 3.8196 -2.90829 4.35958

Au 5.64343 2.00274 -2.04889

Au -0.197942 -5.47919 -2.76368

Au -5.16888 -4.00986 -0.020455

Au 7.00711 0.420002 0.844025

Au 3.40953 -2.21378 -3.21437

S -0.109716 2.17371 -4.83328

S -4.78487 2.47428 -4.90006

S 0.705208 -5.58628 -0.594081

S 3.23503 -4.19625 2.47849

S -1.27395 3.25183 4.19821

S 0.388217 -1.57268 5.69322

S 5.64888 4.15734 1.31172

S -4.44127 0.864316 2.82997

S 7.71025 1.22479 -1.25022

S -6.42406 -3.26926 1.82398

S -6.37216 -0.423949 -1.57093

S -2.83944 -3.84837 3.15511

S -4.13559 -4.99762 -1.88363

S 4.644 -1.82837 6.27997

S 3.41393 2.6685 5.7328

S 2.40249 6.16975 4.01071

S -0.889092 -5.55349 -5.00698

S 5.36482 -1.78596 -1.97366

S -3.53752 -1.69822 -5.37009

S 1.67833 -2.79821 -4.69717

S 3.69475 2.77157 -3.11585

C -0.525373 -0.187077 6.50085

H -0.952597 0.491016 5.75472

H 0.198219 0.357019 7.12077

C -5.21357 -2.33792 -4.9271

H -5.57191 -2.94969 -5.76409

H -5.87136 -1.47046 -4.78106

C -5.28317 1.62034 -6.45976

H -4.85288 0.613545 -6.50799

H -4.91609 2.22505 -7.298

C 8.67346 2.74194 -0.822846

H 8.12381 3.36745 -0.110385

H 8.86624 3.29307 -1.7513

S 6.62892 -0.384557 3.01324

C 5.52724 5.21472 -0.197706

H 4.49036 5.30197 -0.535228

H 6.1257 4.74034 -0.987411

C 3.574 -2.41904 7.6616

H 2.5141 -2.30358 7.40718

H 3.82441 -1.82744 8.55025

C -2.09773 -5.50594 2.82391

H -1.2021 -5.42328 2.19891

H -2.86311 -6.09728 2.30531

C -7.11965 0.747528 -0.354277

H -8.01641 1.1847 -0.810289

H -6.41039 1.53363 -0.078379

C -3.38488 -6.54028 -1.19762

H -2.85784 -6.33662 -0.260582

H -2.66869 -6.92315 -1.93679

C 0.304651 3.89111 -4.2941

H -0.22168 4.14711 -3.36685

H 0.015241 4.57847 -5.09788

C 2.52138 -5.61828 -0.927427

C -3.82963 0.529125 4.53899

H -3.22919 1.39293 4.85256

H -3.21368 -0.377671 4.56002

C -8.07194 -2.87112 1.0915

H -7.96359 -2.25759 0.190198

H -8.66038 -2.34115 1.85035

C 7.11106 -2.16513 2.93544

H 8.19836 -2.2151 2.80114

H 6.60129 -2.67567 2.11238

C 1.74918 -5.13824 3.03415

H 1.33697 -5.6495 2.15443

H 0.994622 -4.46436 3.45869

C 3.5785 1.65382 -4.58078

H 3.64967 0.603175 -4.27466

H 4.39582 1.90654 -5.26655

C -2.1822 -6.87087 -5.08619

H -2.57537 -6.8867 -6.11001

H -2.99545 -6.67087 -4.38005

C -2.55042 4.12606 3.1941

H -2.17684 4.33939 2.18469

H -2.80843 5.05896 3.70941

C 1.65133 -1.47312 -5.98171

H 2.59783 -1.50699 -6.53408

H 1.503 -0.485399 -5.53288

C 5.74848 -3.37048 -1.10763

H -1.31483 -0.611134 7.13255

H -5.17924 -2.93647 -4.01068

H -6.37859 1.57375 -6.48434

H 9.62245 2.41716 -0.379001

H 5.93431 6.20302 0.04895

H 3.81111 -3.47568 7.83533

H -1.85395 -5.9798 3.78205

H -7.38743 0.173651 0.543096

H -4.19048 -7.26626 -1.03303

H 1.38897 3.93667 -4.12831

H 2.80457 -4.80556 -1.60658

H 2.7687 -6.58934 -1.3726

H 3.03907 -5.49784 0.032996

H -4.69974 0.413092 5.19601

H -8.5594 -3.82041 0.838316

H 6.82476 -2.62618 3.8892

H 2.06983 -5.87288 3.78243

H 2.60893 1.83416 -5.06285

H -1.70285 -7.83038 -4.85712

H -3.42936 3.47109 3.13368

H 0.817185 -1.70244 -6.65655

H 6.64963 -3.19358 -0.506782

H 5.95274 -4.14067 -1.86074

H 4.92176 -3.67924 -0.458833

C 4.9443 5.15278 8.64479

C 4.98088 5.25746 10.0216

C 3.96664 5.95047 10.7197

C 2.9261 6.52545 10.0201

C 2.85827 6.43073 8.60586

C 3.88718 5.73312 7.8899

C 1.78862 7.01119 7.87563

C 1.72833 6.88554 6.51291

C 2.73656 6.1825 5.79139

C 3.82488 5.621 6.45112

C 4.97254 4.93779 5.77067

C 6.18242 5.68111 5.53677

C 7.34337 5.01011 5.02606

C 7.27363 3.61508 4.77158

C 6.11252 2.91669 4.98646

C 4.95258 3.57193 5.48138

C 6.27239 7.07744 5.7927

C 7.44178 7.77113 5.55112

C 8.58293 7.10625 5.04617

C 8.53047 5.75127 4.79083

H 2.13209 7.06187 10.5448

H 4.00733 6.02728 11.8075

H 5.80223 4.7985 10.5743

H 5.73447 4.61221 8.12311

H 1.00775 7.55345 8.41289

H 0.899012 7.32122 5.95503

H 5.39806 7.60188 6.1806

H 7.48459 8.84291 5.75217

H 9.50142 7.66563 4.86032

H 9.40442 5.2246 4.40052

H 8.1567 3.09732 4.39161

H 6.06604 1.84734 4.77928

H 2.50518 6.58999 -0.8585

C 1.5953 6.08359 -1.20426

H 0.988387 6.78275 -1.79136

H 1.85893 5.2078 -1.80758

S 0.641266 5.59959 0.301504

Au -1.30618 4.58555 -0.553157

S -3.36315 3.92091 -1.48339

H -4.60964 5.16497 0.190139

C -4.59121 4.11316 -0.118499

H -4.34407 3.46988 0.733178

H -5.56958 3.83371 -0.529583

I2 regioisomer

Au -1.32914 -0.773971 -0.931092

Au -0.337148 1.83011 -0.108469

Au -0.311182 1.62174 2.81667

Au 1.41779 3.58108 1.27736

Au 4.18103 -0.436618 -0.150391

Au -2.6501 0.616961 1.17756

Au 1.87445 0.648676 1.28689

Au -0.381093 -1.09978 1.76887

Au -2.72281 -2.50158 0.92019

Au -2.70074 1.63307 -1.68097

Au 2.32407 1.90959 -1.21639

Au 1.55212 -0.911033 -1.12301

Au 2.28387 -2.16872 1.39957

Au 4.07163 -0.343023 2.85704

Au -0.009254 0.844361 -2.85548

Au -0.03692 -2.13498 -3.15633

Au 2.54192 2.22277 3.55317

Au -4.18492 -0.830036 -0.875161

Au 4.23339 2.16415 0.97799

Au -0.020766 -3.19916 -0.245582

Au -5.27006 1.17385 -3.47281

Au 1.43579 -0.563536 3.90823

Au 0.553193 4.74587 4.00785

Au -2.39581 -3.22019 -1.97446

Au -2.20499 2.23808 -4.99633

Au -5.50603 -1.06006 1.96735

Au 3.88595 4.83012 2.81101

Au -2.55526 -0.57805 -3.50886

Au -2.06387 -3.48046 -5.19136

Au -1.40334 -2.65532 4.17108

Au 3.65189 0.127596 6.03793

Au 3.59101 -3.0364 4.43526

Au 5.71063 1.89364 -1.80493

Au -0.243852 -5.4193 -2.83544

Au -5.3023 -3.82205 -0.318663

Au 6.94049 0.344121 1.14912

Au 3.46185 -2.2633 -3.05859

S 0.137408 2.2041 -4.87216

S -4.51983 2.56479 -5.21412

S 0.576183 -5.5387 -0.636358

S 3.03472 -4.21748 2.48313

S -1.16778 3.19951 4.46625

S 0.152417 -1.69875 5.65377

S 5.6557 4.06067 1.46346

S -4.4961 0.915406 2.75181

S 7.73263 1.05261 -0.948309

S -6.63896 -3.05235 1.45409

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S -3.06872 -3.80003 2.96353

S -4.19258 -4.84089 -2.12083

S 4.31989 -2.08497 6.45777

S 3.26093 2.43435 5.85523

S 2.43504 6.17251 4.13447

S -0.835524 -5.48458 -5.1067

S 5.36456 -1.87712 -1.72774

S -3.39048 -1.5774 -5.54995

S 1.78985 -2.80226 -4.62372

S 3.83503 2.73567 -2.94486

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H -0.023967 0.10469 7.23466

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H -5.45304 -2.76251 -5.99954

H -5.72753 -1.28217 -5.00964

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H -4.5813 0.666569 -6.77599

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C 8.73562 2.54853 -0.537701

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H 8.98451 3.05676 -1.47725

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H -2.9856 -6.56681 -4.5726

C -2.7214 3.95997 3.83675

H -2.64303 4.17261 2.76771

H -2.89744 4.88788 4.3932

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H 2.85449 -1.57196 -6.42337

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C -0.131487 9.47448 4.08171

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C 1.58015 8.10801 2.19976

C 1.90022 9.19288 1.30461

C 3.23334 9.71983 1.26182

C 4.21399 9.16929 2.12908

C 3.90471 8.12226 2.95762

C 2.59056 7.56697 2.98203

C 0.926337 9.76909 0.443738

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H 5.62005 2.54844 5.1495

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I3 regioisomer

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Au -2.52471 0.41237 1.21365

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Au 2.21426 1.97136 -1.43183

Au 1.55278 -0.954461 -1.33326

Au 2.49794 -2.28606 1.03002

Au 4.31974 -0.358679 2.54915

Au -0.111217 0.728869 -3.02099

Au -0.105101 -2.22288 -3.29701

Au 2.79942 2.09452 3.37676

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Au -4.16418 -0.865976 -0.787028

Au 4.39236 2.07414 0.735462

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Au 1.69788 -0.667652 3.73789

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Au -2.20235 -3.59434 -5.16092

Au -1.13416 -2.76549 4.10675

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Au 3.86615 -2.93069 4.16775

Au 5.63081 1.87599 -2.1473

Au -0.18801 -5.54595 -2.95099

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S 7.72829 1.09201 -1.42416

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S -2.84265 -3.92211 2.97312

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S 4.71857 -1.94571 6.13317

S 3.22717 2.48286 5.73322

S 2.50178 6.17327 3.77386

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S 5.37063 -1.86659 -2.199

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C -4.57939 7.44093 -2.98903

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H -6.13762 7.89006 -4.38748

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H -2.33716 9.78204 -5.14903

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S -2.50429 3.95622 -1.82798

I4 regioisomer

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Au -0.44224 1.47944 3.05814

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Au 4.22951 -0.36639 0.299395

Au -2.69012 0.466432 1.33636

Au 1.8663 0.539912 1.65306

Au -0.419172 -1.20815 1.9609

Au -2.69381 -2.61188 0.96804

Au -2.7075 1.59199 -1.50182

Au 2.43981 1.81377 -0.812114

Au 1.63496 -0.940799 -0.81558

Au 2.26629 -2.29207 1.66153

Au 3.97115 -0.606294 3.2839

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Au 0.171908 -2.11261 -2.97078

Au 2.43822 1.80238 4.05564

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C 4.94978 7.01493 6.11262

C 4.78393 6.8558 4.70575

C 5.90487 6.8303 3.86672

C 5.77229 6.74401 2.37471

C 5.82545 7.95294 1.60143

C 5.76563 7.89029 0.167473

C 5.65919 6.62083 -0.457736

C 5.60146 5.47247 0.292909

C 5.65262 5.52038 1.71059

C 5.92439 9.2363 2.21008

C 5.96535 10.386 1.44747

C 5.9128 10.3181 0.03555

C 5.81377 9.09163 -0.587943

H 8.75481 7.29633 7.50826

H 10.7791 7.20882 6.07156

H 10.5385 6.9429 3.5974

H 8.30243 6.77147 2.56987

H 6.30651 7.25618 7.75483

H 4.05162 7.03883 6.73081

H 5.96194 9.30354 3.29803

H 6.0375 11.3573 1.9397

H 5.94849 11.2346 -0.555914

H 5.76879 9.02406 -1.67769

H 5.61853 6.564 -1.54799

H 5.51499 4.49869 -0.194044

H 2.58361 6.50983 -0.134706

C 1.6786 6.12408 -0.620821

H 1.16637 6.93196 -1.15658

H 1.93956 5.31125 -1.30641

S 0.566698 5.53153 0.725256

Au -1.28423 4.56773 -0.342175

S -3.28541 3.95696 -1.42502

H -4.60223 5.18126 0.204886

C -4.5781 4.13384 -0.118062

H -4.37579 3.47717 0.735366

H -5.53855 3.86955 -0.578207