Supplementary Information

A computational study of two promising tweezers

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Table S1a: Energy difference between angular and planar geometry, ΔE(kJ/mol), for optimized structures for both tweezers with or without sodium cation at B3LYP, CAM-B3LYP, M062X, MN12L, MN12SX, and ωB97X-D with 6-31G(d,p) level of theory.

	DFT functional	ΔE(kJ/mol)
tw1	B3LYP	-19.40
	CAM-B3LYP	-34.28
	M062X	-38.52
	MN12L	-13.16
	MN12SX	-21.60
	ωB97X-D	-46.10
tw2	B3LYP	-63.69
	CAM-B3LYP	-87.82
	M062X	-97.84
	MN12L	-59.65
	MN12SX	-72.12
	ωB97X-D	-107.39
tw1+Na	B3LYP	-30.08
	CAM-B3LYP	-54.42
	M062X	-66.36
	MN12L	-35.08
	MN12SX	-44.20
	ωB97X-D	-83.86
tw2+Na	B3LYP	-163.90
	CAM-B3LYP	-182.70
	M062X	-213.15
	MN12L	-194.70
	MN12SX	-201.13
	ωB97X-D	-247.41

Table S1b: Energy difference between angular and planar geometry, ΔE(kJ/mol), for optimized structures for both tweezers with or without sodium cation at B3LYP, CAM-B3LYP, M062X, MN12L, MN12SX, and ωB97X-D with 6-31G(2d,2p) level of theory.

	DFT functional	ΔE(kJ/mol)
tw1	B3LYP	-20.02
	CAM-B3LYP	-34.91
	M062X	-37.98
	MN12L	-10.67
	MN12SX	-20.20
	ωB97X-D	-46.01
tw2	B3LYP	-65.82
	CAM-B3LYP	-90.04
	M062X	-97.94
	MN12L	-54.92
	MN12SX	-69.60
	ωB97X-D	-108.24
tw1+Na	B3LYP	-15.60
	CAM-B3LYP	-32.72
	M062X	-45.11
	MN12L	-32.50
	MN12SX	-42.33
	ωB97X-D	-84.15
tw2+Na	B3LYP	-164.78
	CAM-B3LYP	-208.18
	M062X	-235.20
	MN12L	-189.41
	MN12SX	-197.95
	ωB97X-D	-273.23

Table S2: Calculation excitations with oscilator strenght no zero (the first is always showm) at CAM-B3LYP/6-31G/d,p) level.

Structure	Excited State	λ(nm)	Oscillator strength	Main CI coefficient	
tw1					
	1	361.1	0.000	139 ->142	0.33
				140 ->141	0.63
	2	357,7	0.089	139 ->141	0.40
				140 ->142	0.57
	3	335.2	0.097	139 ->144	0.20
				140 ->143	0.40
	4	331.5	0.021	139 ->143	0.29
				140 ->144	0.26
	5	286.6	3.141	138 ->141	0.54
				140 ->143	0.23
tw2					
	1	286.6	0.002	87 -> 88	0.87
	5	240.9	0.146	84 -> 90	0.19
				87 -> 92	0.21
	6	237.1	1.216	86 -> 88	0.34
				87 -> 89	0.43
	7	218.5	0.034	83 -> 88	0.24
				86 -> 89	0.37
	9	211.2	0.059	83 -> 88	0.19
				86 -> 89	0.47
	10	209.1	0.558	85 -> 89	0.44
				87 -> 91	0.21
tw1+Na					
	1	306.1	0.000	144 ->146	0.55
				145 ->147	0.42
	2	358.8	0.092	144 ->147	0.37
				145 ->146	0.60
	13	268.1	2.618	141 ->147	0.33
				145 ->149	0.24
	14	250.0	1.096	141 ->146	0.50
tw2+Na					
	1	243.3	0.010	92 -> 93	0.28
				92 -> 96	0.25
	6	219.1	0.344	91 -> 94	0.45
				92 -> 96	0.32
	8	211.4	0.042	92 -> 93	0.46
	10	207.4	0.202	90 -> 93	0.19
				91 -> 95	0.93
	14	202.3	0.097	91 -> 93	0.19
				92 -> 98	0.56
	16	200.7	0.032	88 -> 94	0.53
	17	199.6	0.142	90 -> 93	0.20
				90 -> 96	0.40
				92 -> 97	0.20

Table S3a: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer one (tw1) planar at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
BCP	**C27-H54**	0.286	-1.060	-0.340	0.037	-0.302
BCP	**C16-C26**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**C18-C27**	0.294	-0.777	-0.356	0.081	-0.275
BCP	**N40-C28**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C28-O42**	0.418	0.140	-1.470	0.752	-0.718
BCP	**C8-N40**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C24-C29**	0.326	-0.908	-0.450	0.112	-0.339
BCP	**H58-C36**	0.287	-1.030	-0.347	0.045	-0.303
BCP	**C24-H51**	0.285	-1.032	-0.342	0.042	-0.300
BCP	**H46-C5**	0.285	-1.032	-0.342	0.042	-0.300
BCP	**C29-C30**	0.274	-0.692	-0.309	0.068	-0.241
BCP	**H57-C34**	0.287	-1.030	-0.347	0.045	-0.303
BCP	**C32-C31**	0.274	-0.692	-0.309	0.068	-0.241
BCP	**C34-C36**	0.336	-0.952	-0.497	0.129	-0.367
BCP	**H44-C3**	0.284	-1.029	-0.339	0.041	-0.298
BCP	**H47-C6**	0.284	-1.029	-0.339	0.041	-0.298
BCP	**C23-H50**	0.284	-1.029	-0.339	0.041	-0.298
BCP	**C26-H53**	0.284	-1.029	-0.339	0.041	-0.298
BCP	**C15-C6**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**H48-C7**	0.286	-1.060	-0.340	0.037	-0.302
BCP	**O41-C8**	0.418	0.140	-1.470	0.752	-0.718
BCP	**C17-C7**	0.294	-0.777	-0.356	0.081	-0.275
BCP	**C1-C9**	0.273	-0.704	-0.304	0.064	-0.240
BCP	**C9-C2**	0.336	-0.969	-0.481	0.119	-0.362
BCP	**C11-C3**	0.315	-0.870	-0.415	0.099	-0.316
BCP	**C17-C18**	0.289	-0.747	-0.347	0.080	-0.267
BCP	**H59-N37**	0.340	-1.839	-0.555	0.048	-0.508
BCP	**C7-C19**	0.336	-0.969	-0.481	0.119	-0.362
BCP	**C19-C8**	0.273	-0.704	-0.304	0.064	-0.240
BCP	**C19-C20**	0.303	-0.813	-0.381	0.089	-0.292
BCP	**C20-C28**	0.273	-0.704	-0.304	0.064	-0.240
BCP	**C26-C18**	0.315	-0.870	-0.415	0.099	-0.316
BCP	**C1-N37**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C27-C20**	0.336	-0.969	-0.481	0.119	-0.362
BCP	**C22-C12**	0.294	-0.777	-0.356	0.081	-0.275
BCP	**N40-H60**	0.340	-1.839	-0.555	0.048	-0.508

BCP	**N37-C21**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C23-C14**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**C14-C24**	0.302	-0.819	-0.374	0.085	-0.289
BCP	**C22-H49**	0.286	-1.060	-0.340	0.037	-0.302
BCP	**C31-C25**	0.326	-0.908	-0.450	0.112	-0.339
BCP	**C21-O39**	0.418	0.140	-1.470	0.752	-0.718
BCP	**C32-H56**	0.287	-1.030	-0.347	0.045	-0.303
BCP	**C25-H52**	0.285	-1.032	-0.342	0.042	-0.300
BCP	**C25-C16**	0.302	-0.819	-0.374	0.085	-0.289
BCP	**C30-H55**	0.287	-1.030	-0.347	0.045	-0.303
BCP	**C30-C32**	0.336	-0.952	-0.497	0.129	-0.367
BCP	**C4-C33**	0.326	-0.908	-0.450	0.112	-0.339
BCP	**C33-C34**	0.274	-0.692	-0.309	0.068	-0.241
BCP	**C36-C35**	0.274	-0.692	-0.309	0.068	-0.241
BCP	**H45-C4**	0.285	-1.032	-0.342	0.042	-0.300
BCP	**C35-C5**	0.326	-0.908	-0.450	0.112	-0.339
BCP	**C2-C11**	0.294	-0.777	-0.356	0.081	-0.275
BCP	**C3-C13**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**H43-C2**	0.286	-1.060	-0.340	0.037	-0.302
BCP	**O38-C1**	0.418	0.140	-1.470	0.752	-0.718
BCP	**C33-C29**	0.284	-0.727	-0.333	0.075	-0.257
BCP	**C13-C4**	0.302	-0.819	-0.374	0.085	-0.289
BCP	**C11-C12**	0.289	-0.747	-0.347	0.080	-0.267
BCP	**C35-C31**	0.284	-0.727	-0.333	0.075	-0.257
BCP	**C5-C15**	0.302	-0.819	-0.374	0.085	-0.289
BCP	**C9-C10**	0.303	-0.813	-0.381	0.089	-0.292
BCP	**C21-C10**	0.273	-0.704	-0.304	0.064	-0.240
BCP	**C13-C14**	0.300	-0.806	-0.371	0.085	-0.286
BCP	**C12-C23**	0.315	-0.870	-0.415	0.099	-0.316
BCP	**C10-C22**	0.336	-0.969	-0.481	0.119	-0.362
BCP	**C6-C17**	0.315	-0.870	-0.415	0.099	-0.316
BCP	**C15-C16**	0.300	-0.806	-0.371	0.085	-0.286
RCP	**C5-C15-C16-C25-C31-C35**	0.020	0.153	-0.021	0.030	0.008
RCP	**C2-C9-C10-C22-C12-C11**	0.020	0.155	-0.022	0.030	0.009
RCP	**C6-C15-C16-C26-C18-C17**	0.020	0.154	-0.021	0.030	0.009
RCP	**C7-C17-C18-C27-C20-C19**	0.020	0.155	-0.022	0.030	0.009
RCP	**C8-C19-C20-C28-N40**	0.041	0.328	-0.058	0.070	0.012
RCP	**C29-C30-C32-C31-C35-C36-C34**	0.004	0.020	-0.003	0.004	0.001
RCP	**C4-C13-C14-C24-C29-C33**	0.020	0.153	-0.021	0.030	0.008
RCP	**C1-C9-C10-C21-N37**	0.041	0.328	-0.058	0.070	0.012
RCP	**C3-C11-C12-C23-C14-C13**	0.020	0.154	-0.021	0.030	0.009

Table S3b: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer one with sodium (tw1+Na) planar at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
BCP	**N40-C28**	0.307	-1.002	-0.646	0.198	-0.448
BCP	**C8-N40**	0.307	-1.002	-0.646	0.198	-0.448
BCP	**C24-C29**	0.323	-0.894	-0.443	0.110	-0.333
BCP	**C24-H51**	0.287	-1.051	-0.342	0.040	-0.303
BCP	**C29-C30**	0.270	-0.666	-0.305	0.069	-0.236
BCP	**C32-C31**	0.270	-0.666	-0.305	0.069	-0.236
BCP	**C31-C25**	0.323	-0.894	-0.443	0.110	-0.333
BCP	**O38-C1**	0.420	0.164	-1.486	0.764	-0.723
BCP	**C32-H56**	0.289	-1.053	-0.348	0.043	-0.306
BCP	**C21-O39**	0.420	0.164	-1.486	0.764	-0.723
BCP	**C25-H52**	0.287	-1.051	-0.342	0.040	-0.303
BCP	**O41-C8**	0.420	0.164	-1.486	0.764	-0.723
BCP	**C30-H55**	0.289	-1.053	-0.348	0.043	-0.306
BCP	**C28-O42**	0.420	0.164	-1.486	0.764	-0.723
BCP	**H44-C3**	0.285	-1.043	-0.340	0.040	-0.300
BCP	**H47-C6**	0.285	-1.043	-0.340	0.040	-0.300
BCP	**C23-H50**	0.285	-1.043	-0.340	0.040	-0.300
BCP	**C26-H53**	0.285	-1.043	-0.340	0.040	-0.300
BCP	**C15-C6**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**H48-C7**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C17-C7**	0.294	-0.776	-0.356	0.081	-0.275
BCP	**C1-C9**	0.271	-0.695	-0.297	0.062	-0.236
BCP	**C9-C2**	0.337	-0.977	-0.484	0.120	-0.364
BCP	**C11-C3**	0.315	-0.874	-0.415	0.098	-0.317
BCP	**C17-C18**	0.289	-0.747	-0.345	0.079	-0.266
BCP	**H59-N37**	0.339	-1.841	-0.552	0.046	-0.506
BCP	**C7-C19**	0.337	-0.977	-0.484	0.120	-0.364
BCP	**C19-C8**	0.271	-0.695	-0.297	0.062	-0.236
BCP	**C19-C20**	0.305	-0.827	-0.386	0.090	-0.296
BCP	**C26-C18**	0.315	-0.874	-0.415	0.098	-0.317
BCP	**C1-N37**	0.307	-1.002	-0.646	0.198	-0.448
BCP	**C27-C20**	0.337	-0.977	-0.484	0.120	-0.364
BCP	**C22-C12**	0.294	-0.776	-0.356	0.081	-0.275
BCP	**N40-H60**	0.339	-1.841	-0.552	0.046	-0.506
BCP	**N37-C21**	0.307	-1.002	-0.646	0.198	-0.448
BCP	**C20-C28**	0.271	-0.695	-0.297	0.062	-0.236

BCP	**C23-C14**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**C14-C24**	0.303	-0.826	-0.377	0.085	-0.292
BCP	**C22-H49**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C25-C16**	0.303	-0.826	-0.377	0.085	-0.292
BCP	**C30-C32**	0.328	-0.901	-0.476	0.125	-0.350
BCP	**C27-H54**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C4-C33**	0.323	-0.894	-0.443	0.110	-0.333
BCP	**C16-C26**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**C33-C34**	0.270	-0.666	-0.305	0.069	-0.236
BCP	**C18-C27**	0.294	-0.776	-0.356	0.081	-0.275
BCP	**H45-C4**	0.287	-1.051	-0.342	0.040	-0.303
BCP	**C36-C35**	0.270	-0.666	-0.305	0.069	-0.236
BCP	**C35-C5**	0.323	-0.894	-0.443	0.110	-0.333
BCP	**H58-C36**	0.289	-1.053	-0.348	0.043	-0.306
BCP	**Na61-C30**	0.013	0.059	-0.010	0.012	0.002
BCP	**H46-C5**	0.287	-1.051	-0.342	0.040	-0.303
BCP	**Na61-C34**	0.013	0.059	-0.010	0.012	0.002
BCP	**H57-C34**	0.289	-1.053	-0.348	0.043	-0.306
BCP	**C34-C36**	0.328	-0.901	-0.476	0.125	-0.350
BCP	**C2-C11**	0.294	-0.776	-0.356	0.081	-0.275
BCP	**C3-C13**	0.314	-0.869	-0.413	0.098	-0.315
BCP	**H43-C2**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C33-C29**	0.281	-0.707	-0.331	0.077	-0.254
BCP	**C11-C12**	0.289	-0.747	-0.345	0.079	-0.266
BCP	**C13-C4**	0.303	-0.826	-0.377	0.085	-0.292
BCP	**C35-C31**	0.281	-0.707	-0.331	0.077	-0.254
BCP	**C9-C10**	0.305	-0.827	-0.386	0.090	-0.296
BCP	**C5-C15**	0.303	-0.826	-0.377	0.085	-0.292
BCP	**C21-C10**	0.271	-0.695	-0.297	0.062	-0.236
BCP	**C13-C14**	0.298	-0.797	-0.367	0.084	-0.283
BCP	**C12-C23**	0.315	-0.874	-0.415	0.098	-0.317
BCP	**C10-C22**	0.337	-0.977	-0.484	0.120	-0.364
BCP	**C6-C17**	0.315	-0.874	-0.415	0.098	-0.317
BCP	**C15-C16**	0.298	-0.797	-0.367	0.084	-0.283
RCP	**C29-C30-Na61-C34-C33**	0.008	0.039	-0.007	0.008	0.002
RCP	**C29-C30-Na61-C34-C33**	0.008	0.039	-0.007	0.008	0.002
RCP	**C30-C32-C31-C35-C36-C34-Na61**	0.020	0.152	-0.021	0.030	0.008
RCP	**C5-C15-C16-C25-C31-C35**	0.020	0.156	-0.022	0.030	0.009
RCP	**C2-C9-C10-C22-C12-C11**	0.020	0.156	-0.022	0.030	0.009
RCP	**C7-C17-C18-C27-C20-C19**	0.040	0.327	-0.058	0.070	0.012
RCP	**C1-C9-C10-C21-N37**	0.040	0.327	-0.058	0.070	0.012

RCP	**C8-C19-C20-C28-N40**	0.020	0.152	-0.021	0.030	0.008
RCP	**C3-C11-C12-C23-C14-C13**	0.020	0.153	-0.021	0.030	0.009
RCP	**C6-C15-C16-C26-C18-C17**	0.020	0.153	-0.021	0.030	0.009

Table S3c: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer one (tw1) angular at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(\mathbf{r})$	V(r)	G(r)	H(r)
BCP	**C2-C1**	0.288	-0.739	-0.347	0.081	-0.266
BCP	**C3-C1**	0.328	-0.924	-0.460	0.115	-0.346
BCP	**C4-C3**	0.300	-0.805	-0.371	0.085	-0.286
BCP	**C5-C4**	0.297	-0.789	-0.365	0.084	-0.281
BCP	**C6-C2**	0.328	-0.924	-0.460	0.115	-0.346
BCP	**C5-C6**	0.300	-0.805	-0.371	0.085	-0.286
BCP	**C7-C4**	0.313	-0.862	-0.409	0.097	-0.312
BCP	**C8-C7**	0.316	-0.876	-0.419	0.100	-0.319
BCP	**C10-C5**	0.313	-0.862	-0.409	0.097	-0.312
BCP	**C9-C8**	0.289	-0.745	-0.345	0.080	-0.266
BCP	**C9-C10**	0.316	-0.876	-0.419	0.100	-0.319
BCP	**C11-C8**	0.293	-0.773	-0.354	0.080	-0.274
BCP	**C12-C11**	0.336	-0.972	-0.483	0.120	-0.363
BCP	**C14-C9**	0.293	-0.773	-0.354	0.080	-0.274
BCP	**C13-C12**	0.302	-0.808	-0.379	0.088	-0.290
BCP	**C13-C14**	0.336	-0.972	-0.483	0.120	-0.363
BCP	**C2-C15**	0.270	-0.683	-0.296	0.063	-0.233
BCP	**C15-C16**	0.346	-1.005	-0.526	0.137	-0.388
BCP	**H49-C15**	0.283	-1.016	-0.338	0.042	-0.296
BCP	**C16-C17**	0.270	-0.683	-0.296	0.063	-0.233
BCP	**C20-H52**	0.283	-1.016	-0.338	0.042	-0.296
BCP	**C17-C18**	0.288	-0.739	-0.347	0.081	-0.266
BCP	**C20-C19**	0.346	-1.005	-0.526	0.137	-0.388
BCP	**C19-C18**	0.270	-0.683	-0.296	0.063	-0.233
BCP	**C1-C20**	0.270	-0.683	-0.296	0.063	-0.233
BCP	**H50-C16**	0.283	-1.016	-0.338	0.042	-0.296
BCP	**C17-C21**	0.328	-0.924	-0.460	0.115	-0.346
BCP	**C21-C22**	0.300	-0.805	-0.371	0.085	-0.286
BCP	**C18-C24**	0.328	-0.924	-0.460	0.115	-0.346
BCP	**C22-C23**	0.297	-0.789	-0.365	0.084	-0.281
BCP	**C19-H51**	0.283	-1.016	-0.338	0.042	-0.296

BCP	**C24-C23**	0.300	-0.806	-0.371	0.085	-0.286
BCP	**C22-C25**	0.313	-0.862	-0.409	0.097	-0.312
BCP	**C25-C26**	0.316	-0.876	-0.419	0.100	-0.319
BCP	**C23-C28**	0.313	-0.862	-0.409	0.097	-0.312
BCP	**C26-C27**	0.289	-0.745	-0.345	0.080	-0.266
BCP	**C28-C27**	0.316	-0.876	-0.419	0.100	-0.319
BCP	**C26-C29**	0.293	-0.773	-0.354	0.080	-0.274
BCP	**C29-C30**	0.336	-0.972	-0.483	0.120	-0.363
BCP	**C27-C32**	0.293	-0.773	-0.354	0.080	-0.274
BCP	**C30-C31**	0.302	-0.808	-0.379	0.088	-0.290
BCP	**C32-C31**	0.336	-0.972	-0.483	0.120	-0.363
BCP	**C30-C33**	0.274	-0.705	-0.304	0.064	-0.240
BCP	**C31-C35**	0.274	-0.705	-0.304	0.064	-0.240
BCP	**C33-N34**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**N34-C35**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C36-C12**	0.274	-0.705	-0.304	0.064	-0.240
BCP	**C38-C13**	0.274	-0.705	-0.304	0.064	-0.240
BCP	**N37-C36**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C38-N37**	0.305	-0.993	-0.640	0.196	-0.444
BCP	**C35-O39**	0.418	0.138	-1.469	0.752	-0.717
BCP	**O40-C33**	0.418	0.138	-1.469	0.752	-0.717
BCP	**O41-C38**	0.418	0.138	-1.469	0.752	-0.717
BCP	**C36-O42**	0.418	0.138	-1.469	0.752	-0.717
BCP	**C3-H43**	0.284	-1.025	-0.339	0.041	-0.298
BCP	**H44-C6**	0.284	-1.025	-0.339	0.041	-0.298
BCP	**C7-H45**	0.284	-1.027	-0.339	0.041	-0.298
BCP	**H46-C10**	0.284	-1.027	-0.339	0.041	-0.298
BCP	**C11-H47**	0.286	-1.059	-0.340	0.038	-0.302
BCP	**H48-C14**	0.286	-1.059	-0.340	0.038	-0.302
BCP	**H53-C21**	0.284	-1.025	-0.339	0.041	-0.298
BCP	**C24-H54**	0.284	-1.025	-0.339	0.041	-0.298
BCP	**H55-C25**	0.284	-1.027	-0.339	0.041	-0.298
BCP	**C28-H56**	0.284	-1.027	-0.339	0.041	-0.298
BCP	**H57-C29**	0.286	-1.059	-0.340	0.038	-0.302
BCP	**C32-H58**	0.286	-1.059	-0.340	0.038	-0.302
BCP	**N34-H59**	0.340	-1.839	-0.555	0.048	-0.508
BCP	**H60-N37**	0.340	-1.839	-0.555	0.048	-0.508
RCP	**C1-C2-C6-C5-C4-C3**	0.020	0.153	-0.021	0.030	0.009
RCP	**C4-C5-C10-C9-C8-C7**	0.020	0.153	-0.021	0.030	0.009
RCP	**C8-C9-C14-C13-C12-C11**	0.020	0.155	-0.022	0.030	0.009
RCP	**C12-C13-C38-N37-C36**	0.041	0.328	-0.058	0.070	0.012

RCP	**C1-C2-C15-C16-C17-C18-C19-C20**	0.009	0.031	-0.005	0.006	0.002
RCP	**C17-C18-C24-C23-C22-C21**	0.020	0.153	-0.021	0.030	0.009
RCP	**C22-C23-C28-C27-C26-C25**	0.020	0.153	-0.021	0.030	0.009
RCP	**C26-C27-C32-C31-C30-C29**	0.020	0.155	-0.022	0.030	0.009
RCP	**C30-C31-C35-N34-C33**	0.041	0.328	-0.058	0.070	0.012

Table S3d: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer one with sodium (tw1+Na) angular at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
BCP	**C28-C27**	0.316	-0.877	-0.418	0.099	-0.319
BCP	**C26-C29**	0.293	-0.773	-0.354	0.080	-0.273
BCP	**C29-C30**	0.337	-0.979	-0.486	0.121	-0.365
BCP	**C27-C32**	0.293	-0.773	-0.354	0.080	-0.273
BCP	**C31-C30**	0.304	-0.820	-0.382	0.089	-0.294
BCP	**C32-C31**	0.337	-0.979	-0.486	0.121	-0.365
BCP	**C30-C33**	0.271	-0.696	-0.297	0.062	-0.236
BCP	**H43-C3**	0.285	-1.046	-0.339	0.039	-0.300
BCP	**C6-H44**	0.285	-1.046	-0.339	0.039	-0.300
BCP	**C31-C35**	0.271	-0.696	-0.297	0.062	-0.236
BCP	**H45-C7**	0.285	-1.041	-0.339	0.040	-0.300
BCP	**N34-C33**	0.306	-1.001	-0.643	0.196	-0.447
BCP	**C10-H46**	0.285	-1.041	-0.339	0.040	-0.300
BCP	**H47-C11**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C14-H48**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C21-H53**	0.285	-1.046	-0.339	0.039	-0.300
BCP	**H54-C24**	0.285	-1.046	-0.339	0.039	-0.300
BCP	**C25-H55**	0.285	-1.041	-0.339	0.040	-0.300
BCP	**H56-C28**	0.285	-1.041	-0.339	0.040	-0.300
BCP	**C4-C7**	0.312	-0.856	-0.407	0.096	-0.311
BCP	**C7-C8**	0.316	-0.877	-0.418	0.099	-0.319
BCP	**C5-C10**	0.312	-0.856	-0.407	0.096	-0.311
BCP	**C8-C9**	0.289	-0.745	-0.344	0.079	-0.265
BCP	**C10-C9**	0.316	-0.877	-0.418	0.099	-0.319
BCP	**C16-C17**	0.267	-0.670	-0.291	0.062	-0.229
BCP	**C8-C11**	0.293	-0.773	-0.354	0.080	-0.273
BCP	**H52-C20**	0.284	-1.041	-0.338	0.039	-0.299
BCP	**C11-C12**	0.337	-0.979	-0.486	0.121	-0.365
BCP	**C18-C17**	0.283	-0.709	-0.339	0.081	-0.258

BCP	**C9-C14**	0.293	-0.773	-0.354	0.080	-0.273
BCP	**C19-C20**	0.347	-1.009	-0.531	0.139	-0.392
BCP	**C20-C1**	0.267	-0.670	-0.291	0.062	-0.229
BCP	**C19-C18**	0.267	-0.670	-0.291	0.062	-0.229
BCP	**H50-C16**	0.284	-1.041	-0.338	0.039	-0.299
BCP	**C18-C24**	0.325	-0.902	-0.453	0.114	-0.339
BCP	**C17-C21**	0.325	-0.902	-0.453	0.114	-0.339
BCP	**C23-C22**	0.294	-0.772	-0.360	0.083	-0.276
BCP	**H51-C19**	0.284	-1.041	-0.338	0.039	-0.299
BCP	**C21-C22**	0.296	-0.783	-0.362	0.083	-0.279
BCP	**C24-C23**	0.296	-0.783	-0.362	0.083	-0.279
BCP	**C22-C25**	0.312	-0.856	-0.407	0.096	-0.311
BCP	**C25-C26**	0.316	-0.877	-0.418	0.099	-0.319
BCP	**C35-N34**	0.306	-1.001	-0.643	0.196	-0.447
BCP	**C23-C28**	0.312	-0.856	-0.407	0.096	-0.311
BCP	**C12-C36**	0.271	-0.696	-0.297	0.062	-0.236
BCP	**C27-C26**	0.289	-0.745	-0.344	0.079	-0.265
BCP	**C13-C38**	0.271	-0.696	-0.297	0.062	-0.236
BCP	**C36-N37**	0.306	-1.001	-0.643	0.196	-0.447
BCP	**N37-C38**	0.306	-1.001	-0.643	0.196	-0.447
BCP	**O39-C35**	0.421	0.168	-1.489	0.766	-0.724
BCP	**C29-H57**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C33-O40**	0.421	0.168	-1.489	0.766	-0.724
BCP	**H58-C32**	0.287	-1.070	-0.341	0.037	-0.304
BCP	**C38-O41**	0.421	0.168	-1.489	0.766	-0.724
BCP	**N34-H59**	0.339	-1.841	-0.552	0.046	-0.506
BCP	**O42-C36**	0.421	0.168	-1.489	0.766	-0.724
BCP	**N37-H60**	0.339	-1.841	-0.552	0.046	-0.506
BCP	**C1-Na61**	0.012	0.054	-0.009	0.011	0.002
BCP	**C1-C2**	0.283	-0.709	-0.339	0.081	-0.258
BCP	**C1-C3**	0.325	-0.902	-0.453	0.114	-0.339
BCP	**C3-C4**	0.296	-0.783	-0.362	0.083	-0.279
BCP	**C12-C13**	0.304	-0.820	-0.382	0.089	-0.294
BCP	**C4-C5**	0.294	-0.772	-0.360	0.083	-0.276
BCP	**C14-C13**	0.337	-0.979	-0.486	0.121	-0.365
BCP	**C2-C6**	0.325	-0.902	-0.453	0.114	-0.339
BCP	**C6-C5**	0.296	-0.783	-0.362	0.083	-0.279
BCP	**C15-C2**	0.267	-0.670	-0.291	0.062	-0.229
BCP	**C16-C15**	0.347	-1.009	-0.531	0.139	-0.392
BCP	**H49-C15**	0.284	-1.041	-0.338	0.039	-0.299
BCP	**C17-Na61**	0.012	0.054	-0.009	0.011	0.002

CCP	**C1-C2-C15-C16-C17-C18-C19-C20**	0.008	0.042	-0.006	0.008	0.002
RCP	**C30-C31-C35-N34-C33**	0.040	0.327	-0.058	0.070	0.012
RCP	**C4-C5-C10-C9-C8-C7**	0.020	0.152	-0.021	0.030	0.008
RCP	**C8-C9-C14-C13-C12-C11**	0.020	0.155	-0.022	0.030	0.009
RCP	**C17-C18-C24-C23-C22-C21**	0.020	0.151	-0.021	0.030	0.008
RCP	**C22-C23-C28-C27-C26-C25**	0.020	0.152	-0.021	0.030	0.008
RCP	**C26-C27-C32-C31-C30-C29**	0.020	0.155	-0.022	0.030	0.009
RCP	**C12-C13-C38-N37-C36**	0.040	0.327	-0.058	0.070	0.012
RCP	**C1-C2-C6-C5-C4-C3**	0.020	0.151	-0.021	0.030	0.008
RCP	**C1-C2-C15-C16-C17-C18-C19-C20**	0.010	0.035	-0.005	0.007	0.002
RCP	**C1-C2-C15-C16-C17-C18-C19-C20**	0.009	0.031	-0.005	0.006	0.001
RCP	**C1-C2-C15-C16-C17-C18-C19-C20-Na61**	0.008	0.025	-0.005	0.006	0.000

Table S3e: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer two (tw2) planar at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(\mathbf{r})$	V(r)	G(r)	H(r)
BCP	**C4-C5**	0.320	-0.902	-0.431	0.103	-0.328
BCP	**C36-C3**	0.311	-0.842	-0.406	0.098	-0.308
BCP	**C6-H16**	0.285	-1.035	-0.340	0.041	-0.300
BCP	**C3-C6**	0.319	-0.896	-0.426	0.101	-0.325
BCP	**C6-C7**	0.320	-0.902	-0.431	0.103	-0.328
BCP	**C9-H19**	0.287	-1.033	-0.344	0.043	-0.301
BCP	**C27-C21**	0.302	-0.800	-0.382	0.091	-0.291
BCP	**C10-H20**	0.286	-1.032	-0.342	0.042	-0.300
BCP	**C8-C21**	0.311	-0.842	-0.406	0.098	-0.308
BCP	**C21-C22**	0.270	-0.678	-0.301	0.066	-0.235
BCP	**H15-C5**	0.285	-1.035	-0.340	0.041	-0.300
BCP	**C27-C28**	0.270	-0.678	-0.301	0.066	-0.235
BCP	**C24-C9**	0.314	-0.860	-0.412	0.098	-0.313
BCP	**C25-C24**	0.272	-0.687	-0.304	0.066	-0.238
BCP	**C25-H26**	0.286	-1.024	-0.346	0.045	-0.301
BCP	**C33-C34**	0.272	-0.687	-0.304	0.066	-0.238
BCP	**C22-H23**	0.287	-1.026	-0.347	0.045	-0.302
BCP	**C34-C37**	0.338	-0.961	-0.502	0.131	-0.371
BCP	**C22-C25**	0.338	-0.961	-0.502	0.131	-0.371
BCP	**H38-C37**	0.287	-1.026	-0.347	0.045	-0.302
BCP	**C30-C24**	0.307	-0.829	-0.394	0.094	-0.301
BCP	**C40-C39**	0.270	-0.678	-0.301	0.066	-0.235

BCP	**C42-C43**	0.272	-0.687	-0.304	0.066	-0.238
BCP	**C43-H44**	0.286	-1.024	-0.346	0.045	-0.301
BCP	**C40-H41**	0.287	-1.026	-0.347	0.045	-0.302
BCP	**C43-C40**	0.338	-0.961	-0.502	0.131	-0.371
BCP	**C1-C27**	0.311	-0.842	-0.406	0.098	-0.308
BCP	**C5-C8**	0.319	-0.896	-0.426	0.101	-0.325
BCP	**H14-C4**	0.285	-1.035	-0.340	0.041	-0.300
BCP	**C4-C1**	0.319	-0.896	-0.426	0.101	-0.325
BCP	**C36-C39**	0.302	-0.800	-0.382	0.091	-0.291
BCP	**C39-C10**	0.311	-0.842	-0.406	0.098	-0.308
BCP	**C7-H17**	0.285	-1.035	-0.340	0.041	-0.300
BCP	**C10-C7**	0.319	-0.896	-0.426	0.101	-0.325
BCP	**H11-C1**	0.286	-1.032	-0.342	0.042	-0.300
BCP	**C30-C2**	0.314	-0.860	-0.412	0.098	-0.313
BCP	**H12-C2**	0.287	-1.033	-0.344	0.043	-0.301
BCP	**C31-C30**	0.272	-0.687	-0.304	0.066	-0.238
BCP	**H13-C3**	0.286	-1.032	-0.342	0.042	-0.300
BCP	**H32-C31**	0.286	-1.024	-0.346	0.045	-0.301
BCP	**C8-H18**	0.286	-1.032	-0.342	0.042	-0.300
BCP	**H29-C28**	0.287	-1.026	-0.347	0.045	-0.302
BCP	**C28-C31**	0.338	-0.961	-0.502	0.131	-0.371
BCP	**C2-C33**	0.314	-0.860	-0.412	0.098	-0.313
BCP	**C33-C42**	0.307	-0.829	-0.394	0.094	-0.301
BCP	**C9-C42**	0.314	-0.860	-0.412	0.098	-0.313
BCP	**H35-C34**	0.286	-1.024	-0.346	0.045	-0.301
BCP	**C37-C36**	0.270	-0.678	-0.301	0.066	-0.235
RCP	**C33-C34-C37-C36-C39-C40-C43-C42**	0.004	0.020	-0.003	0.004	0.001
RCP	**C3-C6-C7-C10-C39-C36**	0.021	0.164	-0.023	0.032	0.009
RCP	**C21-C22-C25-C24-C30-C31-C28-C27**	0.004	0.020	-0.003	0.004	0.001
RCP	**C2-C30-C24-C9-C42-C33**	0.021	0.163	-0.023	0.032	0.009
RCP	**C1-C4-C5-C8-C21-C27**	0.021	0.164	-0.023	0.032	0.009

Table S3f: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer two with sodium (tw2+Na) planar at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(\mathbf{r})$	V(r)	G(r)	H(r)
BCP	**C4-C5**	0.322	-0.915	-0.436	0.103	-0.332
BCP	**C36-C3**	0.312	-0.849	-0.409	0.098	-0.311
BCP	**C6-H16**	0.287	-1.063	-0.342	0.038	-0.304
BCP	**C3-C6**	0.318	-0.896	-0.423	0.099	-0.323
BCP	**C8-H18**	0.287	-1.049	-0.343	0.040	-0.303
BCP	**C6-C7**	0.322	-0.915	-0.436	0.103	-0.332
BCP	**C9-H19**	0.288	-1.058	-0.345	0.040	-0.305
BCP	**C27-C21**	0.301	-0.798	-0.381	0.091	-0.290
BCP	**C10-H20**	0.287	-1.049	-0.343	0.040	-0.303
BCP	**C8-C21**	0.312	-0.849	-0.409	0.098	-0.311
BCP	**C21-C22**	0.272	-0.688	-0.305	0.067	-0.239
BCP	**C27-C28**	0.272	-0.688	-0.305	0.067	-0.239
BCP	**C24-C9**	0.301	-0.786	-0.384	0.094	-0.290
BCP	**C25-C24**	0.271	-0.681	-0.306	0.068	-0.238
BCP	**C37-C36**	0.272	-0.688	-0.305	0.067	-0.239
BCP	**C25-H26**	0.287	-1.027	-0.347	0.045	-0.302
BCP	**C33-C34**	0.271	-0.681	-0.306	0.068	-0.238
BCP	**C22-H23**	0.289	-1.059	-0.349	0.042	-0.307
BCP	**C34-C37**	0.337	-0.956	-0.498	0.130	-0.368
BCP	**C22-C25**	0.337	-0.956	-0.498	0.130	-0.368
BCP	**H38-C37**	0.289	-1.059	-0.349	0.042	-0.307
BCP	**C40-C39**	0.272	-0.688	-0.305	0.067	-0.239
BCP	**C42-C43**	0.271	-0.681	-0.306	0.068	-0.238
BCP	**C43-H44**	0.287	-1.027	-0.347	0.045	-0.302
BCP	**Na45-C9**	0.021	0.116	-0.020	0.024	0.005
BCP	**C40-H41**	0.289	-1.059	-0.349	0.042	-0.307
BCP	**C43-C40**	0.337	-0.956	-0.498	0.130	-0.368
BCP	**Na45-C2**	0.021	0.116	-0.020	0.024	0.005
BCP	**H15-C5**	0.287	-1.063	-0.342	0.038	-0.304
BCP	**C1-C27**	0.312	-0.849	-0.409	0.098	-0.311
BCP	**C5-C8**	0.318	-0.896	-0.423	0.099	-0.323
BCP	**H14-C4**	0.287	-1.063	-0.342	0.038	-0.304
BCP	**C4-C1**	0.318	-0.896	-0.423	0.099	-0.323
BCP	**C36-C39**	0.301	-0.798	-0.381	0.091	-0.290
BCP	**C39-C10**	0.312	-0.849	-0.409	0.098	-0.311
BCP	**C7-H17**	0.287	-1.063	-0.342	0.038	-0.304

BCP	**C10-C7**	0.318	-0.896	-0.423	0.099	-0.323
BCP	**C30-C24**	0.296	-0.766	-0.369	0.089	-0.280
BCP	**H11-C1**	0.287	-1.049	-0.343	0.040	-0.303
BCP	**C30-C2**	0.301	-0.786	-0.384	0.094	-0.290
BCP	**H12-C2**	0.288	-1.058	-0.345	0.040	-0.305
BCP	**C31-C30**	0.271	-0.681	-0.306	0.068	-0.238
BCP	**H13-C3**	0.287	-1.049	-0.343	0.040	-0.303
BCP	**H32-C31**	0.287	-1.027	-0.347	0.045	-0.302
BCP	**H29-C28**	0.289	-1.059	-0.349	0.042	-0.307
BCP	**C28-C31**	0.337	-0.956	-0.498	0.130	-0.368
BCP	**C2-C33**	0.301	-0.786	-0.384	0.094	-0.290
BCP	**C33-C42**	0.296	-0.766	-0.369	0.089	-0.280
BCP	**C9-C42**	0.301	-0.786	-0.384	0.094	-0.290
BCP	**H35-C34**	0.287	-1.027	-0.347	0.045	-0.302
CCP	**C2-C9-C24-C30-C33-C42-Na45**	0.014	0.076	-0.014	0.016	0.003
RCP	**C1-C4-C5-C8-C21-C27**	0.021	0.164	-0.023	0.032	0.009
RCP	**C33-C34-C37-C36-C39-C40-C43-C42**	0.004	0.020	-0.003	0.004	0.001
RCP	**C3-C6-C7-C10-C39-C36**	0.021	0.164	-0.023	0.032	0.009
RCP	**C2-C30-C24-C9-Na45**	0.018	0.102	-0.017	0.021	0.004
RCP	**C2-C33-C42-C9-Na45**	0.018	0.102	-0.017	0.021	0.004
RCP	**C21-C22-C25-C24-C30-C31-C28-C27**	0.004	0.020	-0.003	0.004	0.001
RCP	**C2-C30-C24-C9-C42-C33**	0.021	0.154	-0.023	0.031	0.008

Table S3g: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer two (tw2) angular at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(r)$	V(r)	G(r)	H(r)
BCP	**C6-C7**	0.316	-0.877	-0.419	0.100	-0.319
BCP	**C5-C8**	0.319	-0.891	-0.429	0.103	-0.326
BCP	**C7-C10**	0.319	-0.891	-0.429	0.103	-0.326
BCP	**H11-C1**	0.284	-1.025	-0.339	0.042	-0.298
BCP	**H12-C2**	0.284	-1.020	-0.339	0.042	-0.297
BCP	**H13-C3**	0.284	-1.025	-0.339	0.042	-0.298
BCP	**C24-C9**	0.314	-0.861	-0.416	0.100	-0.316
BCP	**H14-C4**	0.285	-1.030	-0.340	0.041	-0.299
BCP	**C30-C2**	0.314	-0.861	-0.416	0.100	-0.316
BCP	**H15-C5**	0.285	-1.030	-0.340	0.041	-0.299
BCP	**C30-C24**	0.308	-0.825	-0.400	0.097	-0.303
BCP	**H16-C6**	0.285	-1.030	-0.340	0.041	-0.299

BCP	**C25-C24**	0.270	-0.684	-0.297	0.063	-0.234
BCP	**C25-H26**	0.282	-1.007	-0.337	0.043	-0.294
BCP	**C27-C28**	0.270	-0.683	-0.296	0.062	-0.233
BCP	**C36-C39**	0.308	-0.823	-0.401	0.098	-0.303
BCP	**C28-C31**	0.346	-1.007	-0.526	0.137	-0.389
BCP	**C37-H38**	0.282	-1.007	-0.337	0.043	-0.295
BCP	**H29-C28**	0.282	-1.007	-0.337	0.043	-0.295
BCP	**C31-C30**	0.270	-0.684	-0.297	0.063	-0.234
BCP	**C39-C40**	0.270	-0.683	-0.296	0.062	-0.233
BCP	**C43-C40**	0.346	-1.007	-0.526	0.137	-0.389
BCP	**C40-H41**	0.282	-1.007	-0.337	0.043	-0.295
BCP	**C42-C43**	0.270	-0.684	-0.297	0.063	-0.234
BCP	**C43-H44**	0.282	-1.007	-0.337	0.043	-0.294
BCP	**C4-C1**	0.319	-0.891	-0.429	0.103	-0.326
BCP	**H17-C7**	0.285	-1.030	-0.340	0.041	-0.299
BCP	**C4-C5**	0.316	-0.877	-0.419	0.100	-0.319
BCP	**C8-H18**	0.284	-1.025	-0.339	0.042	-0.298
BCP	**C6-C3**	0.319	-0.891	-0.429	0.103	-0.326
BCP	**C9-H19**	0.284	-1.020	-0.339	0.042	-0.297
BCP	**C10-H20**	0.284	-1.025	-0.339	0.042	-0.298
BCP	**C8-C21**	0.311	-0.846	-0.407	0.098	-0.309
BCP	**C1-C27**	0.311	-0.846	-0.407	0.098	-0.309
BCP	**C27-C21**	0.308	-0.823	-0.401	0.098	-0.303
BCP	**C31-H32**	0.282	-1.007	-0.337	0.043	-0.294
BCP	**C21-C22**	0.270	-0.683	-0.296	0.062	-0.233
BCP	**C2-C33**	0.314	-0.861	-0.416	0.100	-0.316
BCP	**C22-C25**	0.346	-1.007	-0.526	0.137	-0.389
BCP	**C9-C42**	0.314	-0.861	-0.416	0.100	-0.316
BCP	**H23-C22**	0.282	-1.007	-0.337	0.043	-0.295
BCP	**C33-C42**	0.308	-0.825	-0.400	0.097	-0.303
BCP	**C33-C34**	0.270	-0.684	-0.297	0.063	-0.234
BCP	**C34-H35**	0.282	-1.007	-0.337	0.043	-0.294
BCP	**C3-C36**	0.311	-0.846	-0.407	0.098	-0.309
BCP	**C10-C39**	0.311	-0.846	-0.407	0.098	-0.309
BCP	**C36-C37**	0.270	-0.683	-0.296	0.062	-0.233
BCP	**C34-C37**	0.346	-1.007	-0.526	0.137	-0.389
RCP	**C2-C30-C24-C9-C42-C33**	0.021	0.162	-0.023	0.032	0.009
RCP	**C21-C22-C25-C24-C30-C31-C28-C27**	0.009	0.031	-0.005	0.006	0.002
RCP	**C33-C34-C37-C36-C39-C40-C43-C42**	0.009	0.031	-0.005	0.006	0.002
RCP	**C1-C4-C5-C8-C21-C27**	0.021	0.165	-0.023	0.032	0.009
RCP	**C3-C6-C7-C10-C39-C36**	0.021	0.165	-0.023	0.032	0.009

Table S3h: Electron density $\rho(\mathbf{r})$, Laplacian of the electron density $\nabla^2\rho(\mathbf{r})$ gradient kinetic density G(r), virial field V(r), and electronic energy density H(r) evaluated at bond critical points (BCPs), ring critical points (RCPs), and cage critical points (CCPs) for tweezer two with sodium (tw2+Na) angular at CAM-B3LYP/6-31G(d,p) level of theory. All values are in au.

Type	BONDING	ρ(r)	$\nabla^2\rho(\mathbf{r})$	V(r)	G(r)	H(r)
BCP	**C40-H41**	0.284	-1.037	-0.338	0.039	-0.299
BCP	**C40-C43**	0.347	-1.008	-0.531	0.139	-0.392
BCP	**C42-C43**	0.268	-0.677	-0.293	0.062	-0.231
BCP	**C43-H44**	0.284	-1.039	-0.338	0.039	-0.299
BCP	**Na45-C36**	0.008	0.033	-0.006	0.007	0.001
BCP	**C6-C3**	0.315	-0.873	-0.419	0.100	-0.319
BCP	**C6-C7**	0.314	-0.867	-0.414	0.099	-0.315
BCP	**C5-C8**	0.315	-0.873	-0.419	0.100	-0.319
BCP	**C9-H19**	0.286	-1.048	-0.340	0.039	-0.301
BCP	**C7-C10**	0.315	-0.873	-0.419	0.100	-0.319
BCP	**C10-H20**	0.286	-1.054	-0.340	0.038	-0.302
BCP	**H11-C1**	0.286	-1.054	-0.340	0.038	-0.302
BCP	**C8-C21**	0.309	-0.835	-0.404	0.097	-0.306
BCP	**Na45-C30**	0.006	0.025	-0.005	0.005	0.001
BCP	**C1-C27**	0.309	-0.835	-0.404	0.097	-0.306
BCP	**C27-C21**	0.304	-0.801	-0.393	0.096	-0.297
BCP	**C28-C31**	0.347	-1.008	-0.531	0.139	-0.392
BCP	**C21-C22**	0.268	-0.674	-0.292	0.062	-0.230
BCP	**C31-C30**	0.268	-0.677	-0.293	0.062	-0.231
BCP	**H23-C22**	0.284	-1.037	-0.338	0.039	-0.299
BCP	**C31-H32**	0.284	-1.039	-0.338	0.039	-0.299
BCP	**C24-C9**	0.312	-0.849	-0.412	0.100	-0.312
BCP	**C2-C33**	0.312	-0.849	-0.412	0.100	-0.312
BCP	**Na45-C42**	0.006	0.025	-0.005	0.005	0.001
BCP	**C9-C42**	0.312	-0.849	-0.412	0.100	-0.312
BCP	**C3-C36**	0.309	-0.835	-0.404	0.097	-0.306
BCP	**C33-C42**	0.306	-0.812	-0.398	0.097	-0.300
BCP	**C10-C39**	0.309	-0.835	-0.404	0.097	-0.306
BCP	**C33-C34**	0.268	-0.677	-0.293	0.062	-0.231
BCP	**C34-H35**	0.284	-1.039	-0.338	0.039	-0.299
BCP	**C37-C34**	0.347	-1.008	-0.531	0.139	-0.392
BCP	**C36-C39**	0.304	-0.801	-0.393	0.096	-0.297
BCP	**C36-C37**	0.268	-0.674	-0.292	0.062	-0.230
BCP	**C37-H38**	0.284	-1.037	-0.338	0.039	-0.299
BCP	**C39-C40**	0.268	-0.674	-0.292	0.062	-0.230
BCP	**C27-Na45**	0.008	0.033	-0.006	0.007	0.001

BCP	**H12-C2**	0.286	-1.048	-0.340	0.039	-0.301
BCP	**C4-C1**	0.315	-0.873	-0.419	0.100	-0.319
BCP	**H13-C3**	0.286	-1.054	-0.340	0.038	-0.302
BCP	**H14-C4**	0.287	-1.060	-0.341	0.038	-0.303
BCP	**C4-C5**	0.314	-0.867	-0.414	0.099	-0.315
BCP	**H15-C5**	0.287	-1.060	-0.341	0.038	-0.303
BCP	**H16-C6**	0.287	-1.060	-0.341	0.038	-0.303
BCP	**H17-C7**	0.287	-1.060	-0.341	0.038	-0.303
BCP	**C30-C2**	0.312	-0.849	-0.412	0.100	-0.312
BCP	**C8-H18**	0.286	-1.054	-0.340	0.038	-0.302
BCP	**C22-C25**	0.347	-1.008	-0.531	0.139	-0.392
BCP	**C30-C24**	0.306	-0.812	-0.398	0.097	-0.300
BCP	**C25-C24**	0.268	-0.677	-0.293	0.062	-0.231
BCP	**C25-H26**	0.284	-1.039	-0.338	0.039	-0.299
BCP	**C27-C28**	0.268	-0.674	-0.292	0.062	-0.230
BCP	**H29-C28**	0.284	-1.037	-0.338	0.039	-0.299
CCP	**C1-C4-C5-C8-C21-C27**	0.006	0.027	-0.005	0.006	0.001
CCP	**C3-C6-C7-C10-C36-C39**	0.006	0.027	-0.005	0.006	0.001
CCP	**C2-C9-C24-C30-C33-C42-Na45**	0.005	0.024	-0.005	0.005	0.001
CCP	**C33-C34-C36-C37-C39-C40-C42-C43**	0.009	0.044	-0.006	0.009	0.002
CCP	**C21-C22-C24-C25-C27-C28-C30-C31**	0.009	0.044	-0.006	0.009	0.002
RCP	**C3-C6-C7-C10-C39-C36**	0.021	0.163	-0.023	0.032	0.009
RCP	**C2-C30-C24-C9-C42-C33**	0.021	0.162	-0.023	0.032	0.009
RCP	**C2-C30-Na45-C42-C33**	0.006	0.025	-0.005	0.005	0.001
RCP	**C21-C22-C25-C24-C30-C31-C28-C27-Na45**	0.006	0.019	-0.004	0.004	0.000
RCP	**C33-C34-C37-C36-C39-C40-C43-C42-Na45**	0.006	0.019	-0.004	0.004	0.000
RCP	**C33-C34-C37-C36-C39-C40-C43-C42**	0.010	0.035	-0.005	0.007	0.002
RCP	**C33-C34-C37-C36-C39-C40-C43-C42**	0.010	0.036	-0.005	0.007	0.002
RCP	**C1-C4-C5-C8-C21-C27**	0.021	0.163	-0.023	0.032	0.009
RCP	**C1-C4-C5-C8-C21-C27**	0.006	0.027	-0.005	0.006	0.001
RCP	**C3-C6-C7-C10-C39-C36**	0.006	0.027	-0.005	0.006	0.001
RCP	**C21-C22-C25-C24-C30-C31-C28-C27**	0.010	0.035	-0.005	0.007	0.002
RCP	**C9-C24-C30-Na45-C42**	0.006	0.025	-0.005	0.005	0.001
RCP	**C21-C22-C25-C24-C30-C31-C28-C27**	0.010	0.036	-0.005	0.007	0.002

Figure S1: Comparation of UV-vis spectrum for tw2 at different level of theory.

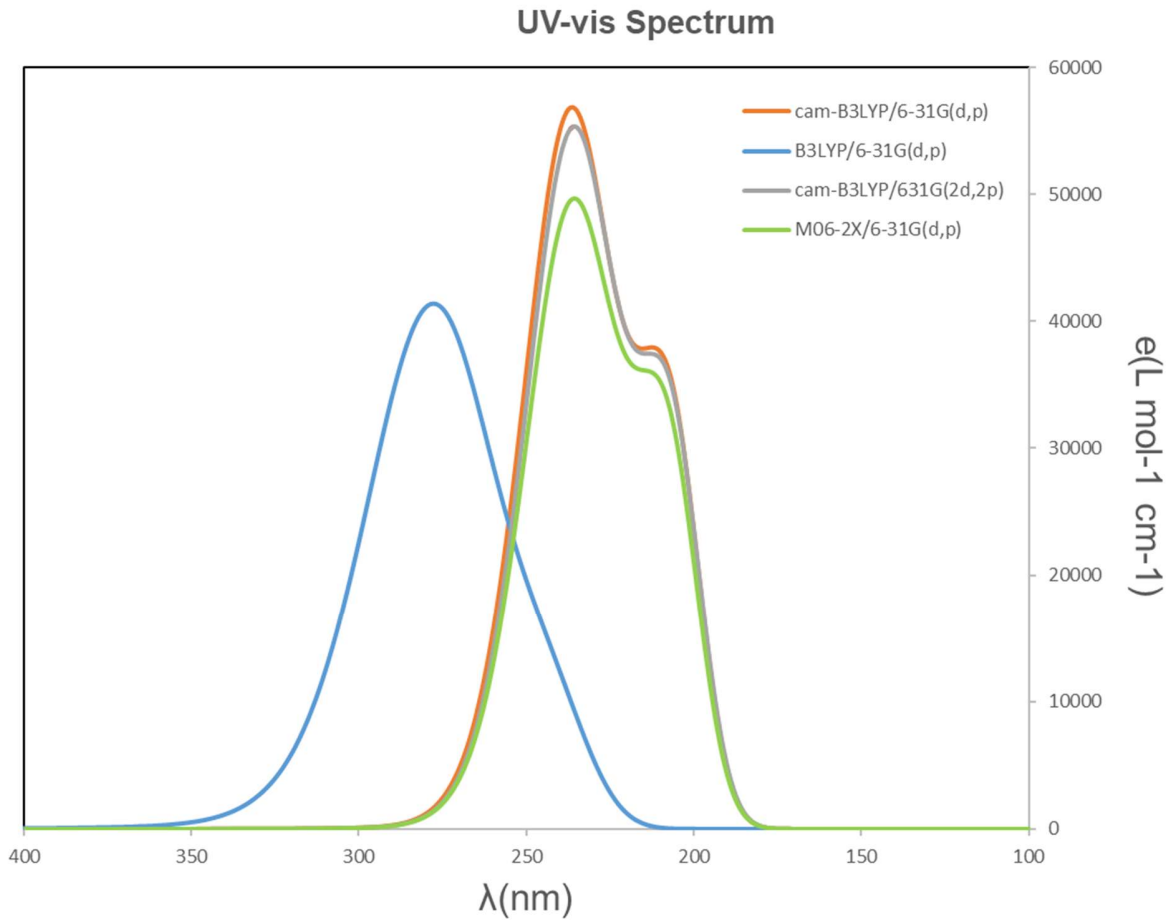

Figure S2a: Molecular orbitals involved in main electronic transitions for tw1 at CAM-B3LYP/6-31G(d,p) level.

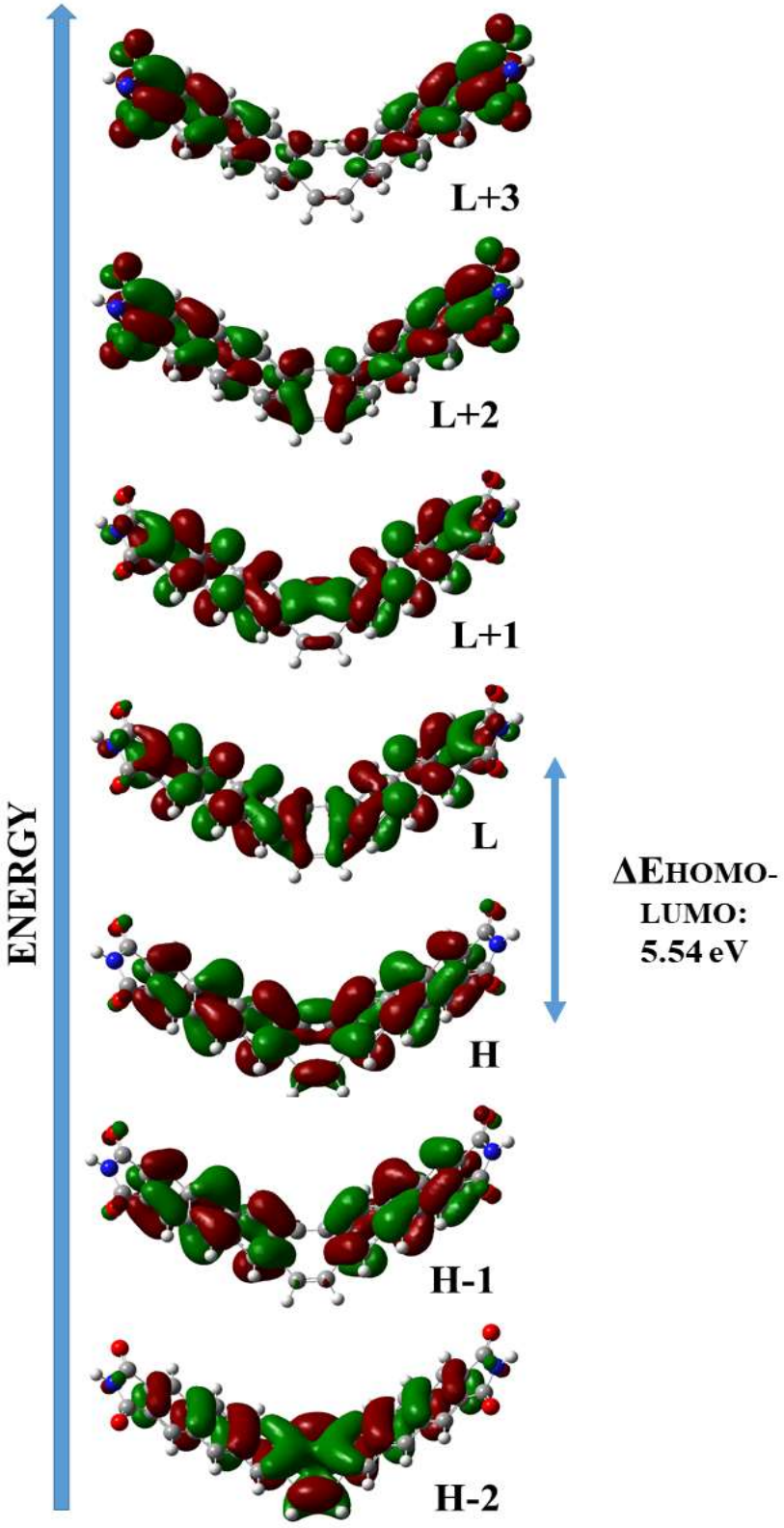

Figure S2b: Molecular orbitals involved in main electronic transitions for tw2 at CAM-B3LYP/6-31G(d,p) level.