Supplementary Information

Influence of End-Capped Modifications in Nonlinear Optical Amplitude of Non-Fullerene Based D-π-A Architecture Chromophores: A DFT/TDDFT Study

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Table S1: Calculated DFT values of selected bond lengths and bond angles of **CC10R** by using M06/6-311G(d,p)

Bond length		**Bond angle**	
C1-C2	1.378	C2-C1-C4	111.3
C1-C4	1.4	C2-C1-H39	111.2
C1-C39	1.517	C1-C2-S8	114.7
C2-S8	1.731	C1-C2-C9	108.7
C2-C9	1.431	C4-C1-H39	137.4
C3-C4	1.402	C1-C4-C3	112.6
C3-C5	1.392	C1-C4-S7	136
C3-S8	1.749	C1-H39-C10	99.8
C4-S7	1.723	C1-H39-C40	107.9
C5-C6	1.382	C1-H39-C46	111.6
C6-S7	1.763	S8-C2-C9	136.6
C6-C61	1.416	C2-S8-C3	89.1

C9-C10	1.37	C2-C9-C10	109.3
C9-S13	1.732	C2-C9-S13	136
C10-C11	1.421	C4-C3-C5	114.1
C10-C39	1.523	C4-C3-S8	112.3
C11-C12	1.431	C3-C4-S7	111.2
C11-C14	1.396	C5-C3-S8	133.5
C12-S13	1.763	C3-C5-C6	112
C12-C17	1.374	C4-S7-C6	90.8
C14-C15	1.381	C5-C6-S7	111.9
C15-C16	1.421	C5-C6-C61	129.1
C15-S20	1.742	S7-C6-C61	118.9
C16-C17	1.401	C6-C61-C27	130.7
C16-C18	1.414	C10-C9-S13	114.7
C18-C19	1.369	C9-C10-C11	112.9
C19-S20	1.762	C9-C10-H39	111
C19-C52	1.423	C9-S13-C12	89.3
C21-C22	1.398	C11-C10-H39	136.1
C21-C26	1.377	C10-C11-C12	110.5
C21-C64	1.478	C10-C11-C14	130.1
C22-C23	1.387	C10-H39-C40	113.7
C22-C62	1.477	C10-H39-C46	108.6
C23-C24	1.391	C12-C11-C14	119.3
C24-C25	1.401	C11-C12-S13	112.4
C24-Cl36	1.727	C11-C12-C17	122.5
C25-C26	1.387	C11-C14-C15	118.2
C25-Cl35	1.727	S13-C12-C17	125.1
C27-C61	1.363	C12-C17-C16	118
C27-C62	1.451	C14-C15-C16	122.3
C27-C64	1.491	C14-C15-S20	126.4
C28-C29	1.398	C16-C15-S20	111.3
C28-C33	1.377	C15-C16-C17	119.7
C28-C59	1.477	C15-C16-C18	112
C29-C30	1.388	C15-S20-C19	91
C29-C53	1.476	C17-C16-C18	128.3
C30-C31	1.39	C16-C18-C19	113.8
C31-C32	1.402	C18-C19-S20	111.9
C31-H38	1.727	C18-C19-C52	129.3
C32-C33	1.387	S20-C19-C52	118.6
C32-H37	1.727	C19-C52-C34	131.6
C34-C52	1.358	C22-C21-C26	122.4
C34-C53	1.454	C22-C21-C64	109.7
C34-C59	1.496	C21-C22-C23	119.3
Cl39-C40	1.527	C21-C22-C62	108.9
Cl39-C46	1.532	C26-C21-C64	127.9
C40-C41	1.395	C21-C26-C25	118.3
C40-C42	1.392	C21-C64-C27	105.4
C41-C43	1.386	C21-C64-O65	127.2
C42-C44	1.388	C23-C22-C62	131.8
C43-C45	1.388	C22-C23-C24	118.7
C44-C45	1.386	C22-C62-C27	106.8

C46-C47	1.394	C22-C62-C63	124.7
C46-C48	1.393	C23-C24-C25	121.3
C47-C49	1.387	C23-C24-Cl36	118.2
C48-C50	1.387	C25-C24-Cl36	120.6
C49-C51	1.387	C24-C25-C26	119.9
C50-C51	1.386	C24-C25-Cl35	121.1
C53-C54	1.369	C26-C25-Cl35	119
C54-C55	1.423	C61-C27-C62	134.7
C54-C57	1.421	C61-C27-C64	117.5
C55-N56	1.155	C62-C27-C64	107.7
C57-N58	1.155	C27-C62-C63	127.6
C59-O60	1.205	C27-C64-O65	127.3
C62-C63	1.372	C29-C28-C33	122.4
C63-C66	1.422	C29-C28-C59	109.7
C63-C68	1.421	C28-C29-C30	119.4
C64-O65	1.206	C28-C29-C53	108.9
C66-N67	1.155	C33-C28-C59	127.9
C68-N69	1.155	C28-C33-C32	118.3

Table S1: **(**continue…) Calculated DFT values of selected bond angles of **CC10R** by using M06/6-311G(d,p)

Bond angle	
C28-C59-C34	105.4
C28-C59-O60	127.3
C30-C29-C53	131.7
C29-C30-C31	118.7
C29-C53-C34	106.8
C29-C53-C54	125
C30-C31-C32	121.3
C30-C31-H38	118.2
C32-C31-H38	120.5
C31-C32-C33	120
C31-C32-H37	121.1
C33-C32-H37	119
C52-C34-C53	135.3
C52-C34-C59	117
C53-C34-C59	107.4
C34-C53-C54	127.4
C34-C59-O60	127.2
C40-Cl39-C46	114.3
Cl39-C40-C41	120.1
Cl39-C40-C42	121.2
Cl39-C46-C47	120.8
Cl39-C46-C48	120.6
C41-C40-C42	118.6

C40-C41-C43	120.7
C40-C42-C44	120.6
C41-C43-C45	120.2
C42-C44-C45	120.3
C43-C45-C44	119.5
C47-C46-C48	118.5
C46-C47-C49	120.8
C46-C48-C50	120.7
C47-C49-C51	120.2
C48-C50-C51	120.3
C49-C51-C50	119.5
C53-C54-C55	122.4
C53-C54-C57	122.8
C55-C54-C57	114.6
C54-C55-N56	178.8
C54-C57-N58	178.5
C62-C63-C66	122.5
C62-C63-C68	123.1
C66-C63-C68	114.2
C63-C66-N67	178.8
C63-C68-N69	178

Table S2: Calculated DFT values of selected bond lengths and bond angles of **CC10D1** by using M06/6-311G(d,p)

Bond length		**Bond angle**	
C1-C2	1.378	C2-C1-C4	111.3
C1-C4	1.399	C2-C1-C27	111.2
C1-C27	1.517	C1-C2-S8	114.5
C2-S8	1.731	C1-C2-C9	108.6
C2-C9	1.433	C4-C1-C27	137.2
C3-C4	1.4	C1-C4-C3	113
C3-C5	1.396	C1-C4-S7	135.7
C3-S8	1.75	C1-C27-C10	99.8
C4-S7	1.726	C1-C27-C28	107.9
C5-C6	1.382	C1-C27-C34	111.5
C6-S7	1.762	S8-C2-C9	136.7
C6-C64	1.42	C2-S8-C3	89.3
C9-C10	1.368	C2-C9-C10	109.3
C9-S13	1.734	C2-C9-S13	136.2
C10-C11	1.424	C4-C3-C5	113.9
C10-C27	1.523	C4-C3-S8	112
C11-C12	1.426	C3-C4-S7	111.3
C11-C14	1.397	C5-C3-S8	134.2
C12-S13	1.763	C3-C5-C6	112
C12-C17	1.379	C4-S7-C6	90.7

C14-C15	1.381	C5-C6-S7	111.9
C15-C16	1.419	C5-C6-C64	125.3
C15-S18	1.749	S7-C6-C64	122.7
C16-C17	1.395	C6-C64-C23	131.2
C16-C63	1.428	C10-C9-S13	114.4
S18-C65	1.767	C9-C10-C11	113.1
C19-C20	1.369	C9-C10-C27	111
C19-C44	1.458	C9-S13-C12	89.5
C19-S60	1.733	C11-C10-C27	135.9
C20-C21	1.417	C10-C11-C12	110.6
C20-C42	1.469	C10-C11-C14	130.3
C21-C22	1.409	C10-C27-C28	113.5
C21-C56	1.396	C10-C27-C34	109.3
C22-C57	1.387	C12-C11-C14	119.1
C22-S60	1.759	C11-C12-S13	112.4
C23-C42	1.497	C11-C12-C17	122.5
C23-C44	1.457	C11-C14-C15	118.2
C23-C64	1.358	S13-C12-C17	125.1
C24-C25	1.443	C12-C17-C16	118.2
C24-C26	1.391	C14-C15-C16	122.5
C24-C40	1.407	C14-C15-S18	126
C25-C41	1.407	C16-C15-S18	111.5
C25-C53	1.392	C15-C16-C17	119.4
C26-C51	1.384	C15-C16-C63	112
C27-C28	1.528	C15-S18-C65	90.3
C27-C34	1.532	C17-C16-C63	128.5
C28-C29	1.395	C16-C63-C65	113.1
C28-C30	1.392	S18-C65-N55	119.8
C29-C31	1.386	S18-C65-C63	113.1
C30-C32	1.389	C20-C19-C44	110.9
C31-C33	1.388	C20-C19-S60	113.2
C32-C33	1.386	C19-C20-C21	114
C34-C35	1.394	C19-C20-C42	109.6
C34-C36	1.393	C44-C19-S60	135.6
C35-C37	1.387	C19-C44-C23	105.6
C36-C38	1.387	C19-C44-C45	124.4
C37-C39	1.387	C19-S60-C22	89.7
C38-C39	1.386	C21-C20-C42	136.3
C40-C50	1.388	C20-C21-C22	110.3
C40-N55	1.396	C20-C21-C56	129.9
C41-N55	1.398	C20-C42-C23	104.9
C41-C67	1.387	C20-C42-O43	127.8
C42-O43	1.207	C22-C21-C56	119.8
C44-C45	1.371	C21-C22-C57	121.1
C45-C46	1.421	C21-C22-S60	112.7
C45-C48	1.421	C21-C56-C58	119.1
C46-N47	1.156	C57-C22-S60	126.2
C48-N49	1.155	C22-C57-C59	118.4
C50-C52	1.385	C42-C23-C44	107.6
C51-C52	1.397	C42-C23-C64	118.6
C53-C54	1.384	C23-C42-O43	127.3

C54-C66	1.397	C44-C23-C64	133.6
N55-C65	1.389	C23-C44-C45	129
C56-C58	1.377	C25-C24-C26	133.6
C57-C59	1.382	C25-C24-C40	107
C58-C59	1.409	C24-C25-C41	107
C58-Cl61	1.732	C24-C25-C53	133.7
C59-Cl62	1.731	C26-C24-C40	119.4
C63-C65	1.353	C24-C26-C51	119
C66-C67	1.385	C24-C40-C50	122

Table S2: **(**continue…) Calculated DFT values of selected bond angles of **CC10D1** compound by using M06/6-311G(d,p)

Bond angle	
C24-C40-N55	108.8
C41-C25-C53	119.3
C25-C41-N55	108.8
C25-C41-C67	122.1
C25-C53-C54	119
C26-C51-C52	120.7
C28-C27-C34	114
C27-C28-C29	119.9
C27-C28-C30	121.4
C27-C34-C35	121
C27-C34-C36	120.5
C29-C28-C30	118.6
C28-C29-C31	120.8
C28-C30-C32	120.6
C29-C31-C33	120.2
C30-C32-C33	120.4
C31-C33-C32	119.5
C35-C34-C36	118.5
C34-C35-C37	120.8
C34-C36-C38	120.7
C35-C37-C39	120.2
C36-C38-C39	120.3
C37-C39-C38	119.4
C50-C40-N55	129.2
C40-C50-C52	117.4
C40-N55-C41	108.4
C40-N55-C65	126.3
N55-C41-C67	129.1
C41-N55-C65	125.3
C41-C67-C66	117.4
C44-C45-C46	120.6
C44-C45-C48	123.4
C46-C45-C48	115.8
C45-C46-N47	178.9
C45-C48-N49	176.9
C50-C52-C51	121.5
C53-C54-C66	120.7

C54-C66-C67	121.4
N55-C65-C63	127
C56-C58-C59	120.6
C56-C58-Cl61	118.9
C57-C59-C58	121
C57-C59-Cl62	118.5
C59-C58-Cl61	120.6
C58-C59-Cl62	120.6

Table S3: Calculated DFT values of selected bond lengths and bond angles of **CC10D2** by using M06/6-311g(d,p)

Bond length		**Bond angle**	
C1-C2	1.38	C2-C1-C4	111.3
C1-C4	1.395	C2-C1-C27	111.2
C1-C27	1.517	C1-C2-S8	114.5
C2-S8	1.731	C1-C2-C9	108.6
C2-C9	1.431	C4-C1-C27	137.2
C3-C4	1.402	C1-C4-C3	113.1
C3-C5	1.393	C1-C4-S7	135.2
C3-S8	1.751	C1-C27-C10	99.8
C4-S7	1.725	C1-C27-C28	107.6
C5-C6	1.385	C1-C27-C34	111.8
C6-S7	1.763	S8-C2-C9	136.7
C6-C62	1.415	C2-S8-C3	89.3
C9-C10	1.37	C2-C9-C10	109.3
C9-S13	1.734	C2-C9-S13	136.3
C10-C11	1.423	C4-C3-C5	113.9
C10-C27	1.522	C4-C3-S8	111.8
C11-C12	1.426	C3-C4-S7	111.4
C11-C14	1.397	C5-C3-S8	134.2
C12-S13	1.763	C3-C5-C6	112
C12-C17	1.379	C4-S7-C6	90.6
C14-C15	1.381	C5-C6-S7	111.9
C15-C16	1.419	C5-C6-C62	125.8
C15-S18	1.749	S7-C6-C62	122.2
C16-C17	1.395	C6-C62-C23	130
C16-C61	1.427	C10-C9-S13	114.4
S18-C63	1.768	C9-C10-C11	113
C19-C20	1.367	C9-C10-C27	111.1
C19-C44	1.462	C9-S13-C12	89.5
C19-S60	1.731	C11-C10-C27	135.9
C20-C21	1.415	C10-C11-C12	110.6
C20-C42	1.473	C10-C11-C14	130.2
C21-C22	1.411	C10-C27-C28	113.1
C21-C56	1.399	C10-C27-C34	110.2
C22-C57	1.39	C12-C11-C14	119.2
C22-S60	1.755	C11-C12-S13	112.4
C23-C42	1.494	C11-C12-C17	122.4
C23-C44	1.454	C11-C14-C15	118.2
C23-C62	1.363	S13-C12-C17	125.1

C24-C25	1.443	C12-C17-C16	118.2
C24-C26	1.391	C14-C15-C16	122.5
C24-C40	1.407	C14-C15-S18	126.1
C25-C41	1.407	C16-C15-S18	111.5
C25-C53	1.392	C15-C16-C17	119.5
C26-C51	1.384	C15-C16-C61	112.1
C27-C28	1.53	C15-S18-C63	90.3
C27-C34	1.532	C17-C16-C61	128.4
C28-C29	1.395	C16-C61-C63	113.1
C28-C30	1.391	S18-C63-N55)	119.8
C29-C31	1.385	S18-C63-C61	113
C30-C32	1.389	C20-C19-C44	110.8
C31-C33	1.389	C20-C19-S60	113.4
C32-C33	1.385	C19-C20-C21	113.8
C34-C35	1.394	C19-C20-C42	109.6
C34-C36	1.394	C44-C19-S60	135.5
C35-C37	1.387	C19-C44-C23	105.6
C36-C38	1.388	C19-C44-C45	123.8
C37-C39	1.387	C19-S60-C22	89.7
C38-C39	1.386	C21-C20-C42	136.5
C40-C50	1.388	C20-C21-C22	110.3
C40-N55	1.397	C20-C21-C56	129.9
C41-N55	1.399	C20-C42-C23	104.9
C41-C65	1.387	C20-C42-O43	127.5
C42-C43	1.207	C22-C21-C56	119.8
C44-C45	1.372	C21-C22-C57	121.2
C45-C46	1.421	C21-C22-S60	112.8
C45-C48	1.421	C21-C56-C58	118.5
C46-N47	1.156	C57-C22-S60	126
C48-N49	1.155	C22-C57-C59	117.9
C50-C52	1.386	C42-C23-C44	107.8
C51-C52	1.397	C42-C23-C62	119
C53-C54	1.384	C23-C42-O43	127.5
C54-C64	1.397	C44-C23-C62	133.1
N55-C63	1.388	C23-C44-C45	129.4
C56-C58	1.371	C25-C24-C26	133.5
C57-C59	1.375	C25-C24-C40	107
C58-C59	1.403	C24-C25-C41	107
C58-N69	1.478	C24-C25-C53	133.6
C59-N66	1.477	C26-C24-C40	119.4
C61-C63	1.354	C24-C26-C51	119
C64-C65	1.386	C24-C40-C50	122
N66-O67	1.208	C24-C40-N55	108.8
N66-O68	1.209	C41-C25-C53	119.4
N69-O70	1.208	C25-C41-N55	108.7
N69-O71	1.208	C25-C41-C65	122.1

Table S3: (continue…) Calculated DFT values of selected bond lengths and bond angles of **CC10D2** by using M06/6-311G(d,p)

Bond angle

C25-C53-C54	119
C26-C51-C52	120.7
C28-C27-C34	113.5
C27-C28-C29	119.5
C27-C28-C30	121.8
C27-C34-C35	120.6
C27-C34-C36	120.9
C29-C28-C30	118.5
C28-C29-C31	120.9
C28-C30-C32	120.6
C29-C31-C33	120.2
C30-C32-C33	120.4
C31-C33-C32	119.4
C35-C34-C36	118.5
C34-C35-C37	120.9
C34-C36-C38	120.6
C35-C37-C39	120.2
C36-C38-C39	120.4
C37-C39-C38	119.4
C50-C40-N55	129.2
C40-C50-C52	117.4
C40-N55-C41	108.4
C40-N55-C63	126.4
N55-C41-C65	129.2
C41-N55-C63	125.2
C41-C65-C64	117.4
C44-C45-C46	120.6
C44-C45-C48	123.4
C46-C45-C48	115.8
C45-C46-N47	178.7
C45-C48-N49	176.7
C50-C52-C51	121.4
C53-C54-C64	120.7
C54-C64-C65	121.4
N55-C63-C61	127.1
C56-C58-C59	121.2
C56-C58-N69	116.9
C57-C59-C58	121.3
C57-C59-N66	116.7
C59-C58-N69	121.6
C58-C59-N66	121.6
C58-N69-O70	116.3
C58-N69-O71	116.8
C59-N66-O67	116.5
C59-N66-O68	116.8
O67-N66-O68	126.6
O70-N69-O71	126.8

Table S4: DFT values of selected bond lengths and bond angles of **CC10D3** of by using M06/6-311G(d,p)

Bond length		Bond angle	
C1-C2	1.379	C2-C1-C4	111.3
C1-C4	1.396	C2-C1-C27	111.3
C1-C27	1.517	C1-C2-S8	114.5
C2-S8	1.731	C1-C2-C9	108.6
C2-C9	1.432	C4-C1-C27	137.2
C3-C4	1.401	C1-C4-C3	113.1
C3-C5	1.395	C1-C4-S7	135.3
C3-S8	1.750	C1-C27-C10	99.8
C4-S7	1.725	C1-C27-C28	107.7
C5-C6	1.383	C1-C27-C34	111.8
C6-S7	1.763	S8-C2-C9	136.7
C6-C62	1.418	C2-S8-C3	89.3
C9-C10	1.369	C2-C9-C10	109.3
C9-S13	1.734	C2-C9-S13	136.2
C10-C11	1.423	C4-C3-C5	113.9
C10-C27	1.523	C4-C3-S8	111.8
C11-C12	1.426	C3-C4-S7	111.4
C11-C14	1.397	C5-C3-S8	134.2
C12-S13	1.763	C3-C5-C6	112.0
C12-C17	1.380	C4-S7-C6	90.6
C14-C15	1.381	C5-C6-S7	112.0
C15-C16	1.419	C5-C6-C62	125.8
C15-S18	1.749	S7-C6-C62	122.3
C16-C17	1.395	S6-C62-C23	130.3
C16-C61	1.427	C10-C9-S13	114.5
S18-C63	1.768	C9-C10-C11	113.0
C19-C20	1.368	C9-C10-C27	111.0
C19-C44	1.461	C9-S13-C12	89.5
C19-S60	1.733	C11-C10-C27	136.0
C20-C21	1.416	C10-C11-C12	110.6
C20-C42	1.471	C10-C11-C14	130.2
C21-C22	1.405	C10-C27-C28	113.1
C21-C56	1.396	C10-C27-C34	110.3
C22-C57	1.388	C12-C11-C14	119.2
C22-S60	1.757	C11-C12-S13	112.4
C23-C42	1.496	C11-C12-C17	122.4
C23-C44	1.456	C11-C14-C15	118.2
C23-C62	1.360	S13-C12-C17	125.2
C24-C25	1.443	C12-C17-C16	118.2
C24-C26	1.391	C14-C15-C16	122.4
C24-C40	1.407	C14-C15-S18	126.1
C25-C41	1.407	C16-C15-S18	111.5
C25-C53	1.392	C15-C16-C17	119.5
C26-C51	1.384	C15-C16-C61	112.1
C27-C28	1.530	C15-S18-C63	90.3
C27-C34	1.532	C17-C16-C61	128.4
C28-C29	1.395	C16-C61-C63	113.1
C28-C30	1.391	S18-C63-N55	119.9
C29-C31	1.385	S18-C63-C61	113.0
C30-C32	1.389	C20-C19-C44	110.8

C31-C33	1.389	C20-C19-S60	113.3
C32-C33	1.385	C19-C20-C21	113.8
C34-C35	1.394	C19-C20-C42	109.7
C34-C36	1.394	C44-C19-S60	135.6
C35-C37	1.386	C19-C44-C23	105.6
C36-C38	1.388	C19-C44-C45	124.1
C37-C39	1.387	C19-S60-C22	89.7
C38-C39	1.386	C21-C20-C42	136.5
C40-C50	1.388	C20-C21-C22	110.5
C40-N55	1.397	C20-C21-C56	130.1
C41-N55	1.398	C20-C42-C23	104.9
C41-C65	1.387	C20-C42-O43	127.7
C42-O43	1.207	C22-C21-C56	119.4
C44-C45	1.371	C21-C22-C57	120.8
C45-C46	1.421	C21-C22-S60	112.8
C45-C48	1.421	C21-C56-C58	120.2
C46-N47	1.156	C57-C22-S60	126.4
C48-N49	1.155	C22-C57-C59	119.5
C50-C52	1.385	C42-C23-C44	107.7
C51-C52	1.397	C42-C23-C62	118.9
C53-C54	1.384	C23-C42-C43	127.4
C54-C64	1.397	C44-C23-C62	133.3
N55-C63	1.388	C23-C44-C45	129.2
C56-C58	1.379	C25-C24-C26	133.6
C57-C59	1.383	C25-C24-C40	107.0
C58-C59	1.418	C24-C25-C41	107.0
C58-C67	1.511	C24-C25-C53	133.6
C59-C66	1.512	C26-C24-C40	119.4
C61-C63	1.354	C24-C26-C51	119.0
C64-C65	1.386	C24-C40-C50	122.0
C66-F68	1.332	C24-C40-N55	108.8
C66-F69	1.329	C41-C25-C53	119.4
C66-F70	1.338	C25-C41-N55	108.8
C67-F71	1.330	C25-C41-C65	122.0
C67-F72	1.335	C25-C53-C54	119.0
C67-F73	1.333	C26-C51-C52	120.7

Table S4: **(**continue…) DFT values of selected bond angles of **CC10D3** of by using M06/6-311G(d,p)

Bond angle	
C28-C27-C34	113.4
C27-C28-C29	119.6
C27-C28-C30	121.8
C27-C34-C35	120.6
C27-C34-C36	120.9
C29-C28-C30	118.5
C28-C29-C31	120.9
C28-C30-C32	120.6
C29-C31-C33	120.2
C30-C32-C33	120.4

C31-C33-C32	119.4
C35-C34-C36	118.5
C34-C35-C37	120.9
C34-C36-C38	120.6
C35-C37-C39	120.2
C36-C38-C39	120.4
C37-C39-C38	119.4
C50-C40-N55	129.2
C40-C50-C52	117.4
C40-N55-C41	108.4
C40-N55-C63	126.4
N55-C41-C65	129.2
C41-N55-C63	125.2
C41-C65-C64	117.4
C44-C45-C46	120.7
C44-C45-C48	123.4
C46-C45-C48	115.7
C45-C46-N47	178.8
C45-C48-N49	176.6
C50-C52-C51	121.4
C53-C54-C64	120.7
C54-C64-C65	121.4
N55-C63-C61	127.0
C56-C58-C59	119.9
C56-C58-C67	116.5
C57-C59-C58	120.2
C57-C59-C66	116.3
C59-C58-C67	123.5
C58-C59-C66	123.4
C58-C67-F71	112.4
C58-C67-F72	111.0
C58-C67-F73	111.5
C59-C66-F68	111.5
C59-C66-F69	112.4
C59-C66-F70	110.9
F68-C66-F69	108.2
F68-C66-F70	106.7
F69-C66-F70	106.9
F71-C67-F72	106.9
F71-C67-F73	108.1
F72-C67-F73	106.8

Table S5: DFT values of selected bond lengths and bond angles of **CC10D4** of by using M06/6-311G(d,p)

Bond length		**Bond angle**	
C1-C2	1.380	C2-C1-C4	111.3
C1-C4	1.395	C2-C1-C27	111.3
C1-C27	1.516	C1-C2-S8	114.5
C2-S8	1.731	C1-C2-C9	108.6
C2-C9	1.431	C4-C1-C27	137.1

C3-C4	1.403	C1-C4-C3	113.1
C3-C5	1.393	C1-C4-S7	135.2
C3-S8	1.751	C1-C27-C10	99.8
C4-S7	1.725	C1-C27-C28	107.8
C5-C6	1.385	C1-C27-C34	111.5
C6-S7	1.763	S8-C2-C9	136.7
C6-C62	1.414	C2-S8-C3	89.3
C9-C10	1.370	C2-C9-C10	109.3
C9-S13	1.734	C2-C9-S13	136.2
C10-C11	1.423	C4-C3-C5	113.9
C10-C27	1.522	C4-C3-S8	111.8
C11-C12	1.426	C3-C4-S7	111.5
C11-C14	1.397	C5-C3-S8	134.2
C12-S13	1.763	C3-C5-C6	112.0
C12-C17	1.380	C4-S7-C6	90.6
C14-C15	1.381	C5-C6-S7	111.9
C15-C16	1.419	C5-C6-C62	125.6
C15-S18	1.749	S7-C6-C62	122.5
C16-C17	1.395	S6-C62-C23	130.3
C16-C61	1.427	C10-C9-S13	114.5
S18-C63	1.768	C9-C10-C11	113.0
C19-C20	1.367	C9-C10-C27	111.1
C19-C44	1.463	C9-S13-C12	89.5
C19-S60	1.732	C11-C10-C27	135.9
C20-C21	1.415	C10-C11-C12	110.7
C20-C42	1.473	C10-C11-C14	130.1
C21-C22	1.408	C10-C27-C28	113.2
C21-C56	1.399	C10-C27-C34	110.2
C22-C57	1.391	C12-C11-C14	119.2
C22-S60	1.754	C11-C12-S13	112.4
C23-C42	1.494	C11-C12-C17	122.4
C23-C44	1.453	C11-C14-C15	118.2
C23-C62	1.363	S13-C12-C17	125.2
C24-C25	1.443	C12-C17-C16	118.2
C24-C26	1.391	C14-C15-C16	122.4
C24-C40	1.407	C14-C15-S18	126.1
C25-C41	1.406	C16-C15-S18	111.5
C25-C53	1.391	C15-C16-C17	119.5
C26-C51	1.384	C15-C16-C61	112.1
C27-C28	1.529	C15-S18-C63	90.3
C27-C34	1.532	C17-C16-C61	128.4
C28-C29	1.395	C16-C61-C63	113.1
C28-C30	1.391	S18-C63-N55	119.8
C29-C31	1.385	S18-C63-C61	113.0
C30-C32	1.389	C20-C19-C44	110.8
C31-C33	1.389	C20-C19-S60	113.4
C32-C33	1.385	C19-C20-C21	113.8
C34-C35	1.394	C19-C20-C42	109.6
C34-C36	1.393	C44-C19-S60	135.5
C35-C37	1.386	C19-C44-C23	105.6
C36-C38	1.388	C19-C44-C45	123.6

C37-C39	1.388	C19-S60-C22	89.7
C38-C39	1.386	C21-C20-C42	136.6
C40-C50	1.388	C20-C21-C22	110.4
C40-N55	1.397	C20-C21-C56	129.9
C41-N55	1.399	C20-C42-C23	104.9
C41-C65	1.387	C20-C42-O43	127.5
C42-O43	1.206	C22-C21-C56	119.7
C44-C45	1.372	C21-C22-C57	121.2
C45-C46	1.421	C21-C22-S60	112.8
C45-C48	1.421	C21-C56-C58	119.2
C46-N47	1.156	C57-C22-S60	126.0
C48-N49	1.155	C22-C57-C59	118.6
C50-C52	1.386	C42-C23-C44	107.8
C51-C52	1.397	C42-C23-C62	118.8
C53-C54	1.384	C23-C42-C43	127.5
C54-C64	1.397	C44-C23-C62	133.3
N55-C63	1.388	C23-C44-C45	129.7
C56-C58	1.376	C25-C24-C26	133.5
C57-C59	1.379	C25-C24-C40	107.0
C58-C59	1.417	C24-C25-C41	107.1
C58-O67	1.794	C24-C25-C53	133.5
C59-S66	1.794	C26-C24-C40	119.4
C61-C63	1.354	C24-C26-C51	119.0
C64-C65	1.386	C24-C40-C50	122.0
S66-O67	1.453	C24-C40-N55	108.8
S66-O68	1.431	C41-C25-C53	119.4
S66-O72	1.581	C25-C41-N55	108.7
S69-O70	1.454	C25-C41-C65	122.0
S69-O71	1.430	C25-C53-C54	119.0
S69-O73	1.582	C26-C51-C52	120.7

Table S5: **(**continue…) DFT values of selected bond lengths and bond angles of **CC10D4** of by using M06/6-311G(d,p)

Bond angle	
C28-C27-C34	113.4
C27-C28-C29	119.6
C27-C28-C30	121.7
C27-C34-C35	120.6
C27-C34-C36	120.9
C29-C28-C30	118.5
C28-C29-C31	120.8
C28-C30-C32	120.6
C29-C31-C33	120.2
C30-C32-C33	120.4
C31-C33-C32	119.4
C35-C34-C36	118.5
C34-C35-C37	120.8
C34-C36-C38	120.7
C35-C37-C39	120.2
C36-C38-C39	120.3

C37-C39-C38	119.4
C50-C40-N55	129.2
C40-C50-C52	117.4
C40-N55-C41	108.4
C40-N55-C63	126.4
N55-C41-C65	129.2
C41-N55-C63	125.2
C41-C65-C64	117.4
C44-C45-C46	120.4
C44-C45-C48	123.7
C46-C45-C48	115.6
C45-C46-N47	178.6
C45-C48-N49	176.4
C50-C52-C51	121.4
C53-C54-C64	120.7
C54-C64-C65	121.4
N55-C63-C61	127.1
C56-C58-C59	120.6
C56-C58-S69	115.5
C57-C59-C58	120.8
C57-C59-S66	115.1
C59-C58-S69	123.9
C58-C59-S66	124.1
C58-S69-O70	106.8
C58-S69-O71	108.7
C58-S69-O73	103.7
C59-S66-O67	106.9
C59-S66-O68	108.5
C59-S66-O72	103.9
O67-S66-O68	120.4
O67-S66-O72	109.3
O68-S66-O72	106.7
O70-S69-O71	120.5
O70-S69-O73	109.2
O71-S69-O73	106.7

Table S6: Calculated DFT values of selected bond lengths and bond angles of **CC10D5** of by using M06/6-311G (d, p)

Bond length		**Bond angle**	
C1-C2	1.378	C2-C1-C4	135.9
C1-C4	1.397	C1-C2-S8	112.4
C3-C4	1.4	C1-C2-C9	119.2
C3-C5	1.397	C2-C1-C27	122.4
C5-C6	1.381	C1-C4-C3	89.5
C4-S7	1.725	C1-C4-C7	125.2
C6-S7	1.762	C4-C1-C27	118.2
C3-S8	1.75	C4-C3-C5	122.5
C2-S8	1.732	C3-C4-S7	126.1

C2-C9	1.433	C4-C3-S8	119.5
C9-C10	1.369	C3-C5-C6	111.5
C10-C11	1.423	C5-C3-S8	112.1
C11-C12	1.425	C5-C6-S7	118.2
C12-S13	1.763	C5-C6-C62	128.4
C9-S13	1.735	C4-S7-C6	90.3
C11-C14	1.396	C7-C6-C62	114
C14-C15	1.381	C3-S8-C2	109.5
C15-C16	1.419	S8-C2-C9	111
C12-C17	1.38	C2-C9-C16	113.2
C16-C17	1.395	C2-C9-S13	110.3
C15-S18	1.749	C9-C10-C11	136.5
C19-C20	1.37	C10-C9-S13	130.2
C20-21	1.417	C9-C10-C27	119.6
C21-C22	1.409	C10-C11-C12	121.2
C24-C25	1.443	C10-C11-C14	112.8
C24-C26	1.391	C25-C24-C26	133.6
C1-C27	1.517	C25-C24-C40	107
C10-C27	1.522	C24-C25-C41	107
C27-C28	1.529	C24-C25-C53	133.5
C28-C29	1.395	C26-C24-C40	119.4
C28-C30	1.391	C24-C26-C51	119
C29-C31	1.385	C1-C27-C10	99.8
C30-C32	1.389	C1-C27-C28	107.7
C31-C33	1.389	C1-C27-C34	111.7
C32-C33	1.385	C10-C27-C28	113.2
C27-C34	1.532	C10-C27-C34	110.1
C34-C35	1.394	C27-C28-C29	119.6
C34-C36	1.394	C27-C28-C30	121.8
C35-C37	1.387	C28-C27-C34	113.5
C36-C38	1.388	C29-C28-C30	118.5
C38-C39	1.386	C28-C29-C31	120.9
C37-C39	1.387	C28-C30-C32	120.6
C24-C40	1.407	C29-C31-C33	120.2
C25-C41	1.407	C30-C32-C33	120.4
C20-C42	1.47	C31-C33-C35	119.4
C23-C42	1.498	C27-C34-C35	120.6
C42-O43	1.207	C27-C34-C36	120.9
C19-C44	1.458	C35-C34-C36	118.5
C23-C44	1.458	C34-C35-C37	120.9
C44-C45	1.371	C34-C36-C38	120.6
C45-C46	1.421	C35-C37-C39	120.2
C46-N47	1.156	C36-C38-C39	120.4
C45-C48	1.421	C38-C39-C37	119.4
C48-N49	1.155	C24-C40-C50	122
C40-C50	1.388	C24-C40-N55	108.8
C26-C51	1.384	C41-C25-C53	119.4
C50-C52	1.386	C25-C41-N55	108.7
C51-C52	1.397	C25-C41-C65	122
C25-C53	1.391	C20-C42-C23	104.9

C53-C54	1.384	C20-C42-C43	128
C41-N55	1.398	C23-C42-C43	127.1
C40-N55	1.396	C42-C23-C44	107.6
C21-C56	1.399	C42-C23-C62	118.9
C22-C57	1.39	C19-C44-C23	105.6
C56-C58	1.379	C19-C44-C45	124.3
C57-C59	1.383	C44-C19-S60	135.5
C58-C59	1.413	C23-C44-C45	129.1
C22-S60	1.758	C44-C23-C62	133.3
C19-S60	1.731	C44-C45-C46	120.7
C16-C61	1.428	C44-C45-C48	123.6
C23-C62	1.358	C45-C46-C47	178.9
C6-C62	1.421	C46-C45-C48	115.5
S18-C63	1.768	C45-C48-C49	176.5
N55-C63	1.389	C40-C50-C52	117.4
C61-C63	1.353	C50-C40-C55	129.2
C54-C64	1.397	C26-C51-C52	120.7
C64-C65	1.386	C50-C52-C51	121.4
C41-C66	1.387	C25-C53-C54	119
C59-C66	1.492	C53-C54-C64	120.7
C66-O67	1.198	C41-C55-C40	108.4
C66-O68	1.338	C41-C55-C63	125.2
C58-C69	1.491	C55-C41-C65	129.2
C69-O70	1.199	C40-C55-C63	126.3
C69-O71	1.336	C21-C56-C58	119.4
O68-C72	1.425	C22-C57-C59	118.7
O71-C73	1.425	C57-C22-S60	126.1

Table S6: **(**continue…) Calculated DFT values of selected bond angles of **CC10D5** of by using M06/6-311G (d, p)

Bond Angle	
C56-C58-C59	120.4
C56-C58-C69	119.3
C57-C59-C58	120.7
C57-C59-C66	118.7
C58-C59-C66	120.1
C59-C58-C69	119.8
C22-S60-C19	89.8
C16-C61-C63	113.1
C23-C62-C6	130.1
S18-C63-N55	119.8
C18-C63-C61	113
N55-C63-C61	127.1
C54-C64-C65	121.4
C64-C65-C41	117.4
C59-C66-O67	124.1
C59-C66-O68	111.4

O67-C66-O68	124.4
C66-O68-C72)	114.9
C58-C69-O70)	124
C58-C69-O71)	111.5
O70-C69-O71)	124.4
C69-O71-C73)	115

Table S7: Calculated DFT values of selected bond lengths and bond angles of **CC10D6** of by using M06/6-311G (d, p)

Bond length		**Bond angle**	
C1-C2	1.379	C2-C1-C4	111.3
C1-C4	1.397	C2-C1-C27	111.2
C1-C27	1.517	C1-C2-S8	114.6
C2-S8	1.731	C1-C2-C9	108.7
C2-C9	1.432	C4-C1-C27	137.3
C3-C4	1.403	C1-C4-C3	113
C3-C5	1.393	C1-C4-S7	135.6
C3-S8	1.75	C1-C27-C10	99.8
C4-S7	1.725	C1-C27-C28	107.9
C5-C6	1.385	C1-C27-C34	111.4
C6-S7	1.764	S8-C2-C9	136.6
C6-C62	1.415	C2-S8-C3	89.2
C9-C10	1.369	C2-C9-C10	109.3
C9-S13	1.734	C2-C9-S13	136.3
C10-C11	1.423	C4-C3-C5	113.9
C10-C27	1.523	C4-C3-S8	111.9
C11-C12	1.426	C3-C4-S7	111.4
C11-C14	1.397	C5-C3-S8	134.2
C12-S13	1.763	C3-C5-C6	112.1
C12-C17	1.379	C4-S7-C6	90.7
C14-C15	1.381	C5-C6-S7	111.9
C15-C16	1.419	C5-C6-C62	125.1
C15-S18	1.749	S7-C6-C62	123
C16-C17	1.395	C6-62-C23	131.2
C16-C61	1.427	C10-C9-S13	114.5
S18-C63	1.767	C9-C10-C11	113
C19-C20	1.367	C9-C10-C27	111.1
C19-C44	1.462	C9-S13-C12	89.5
C19-S60	1.732	C11-10-C27	135.9
C20-C21	1.416	C10-C11-C12	110.6
C20-C42	1.472	C10-C11-C14	130.3
C21-C22	1.412	C10-C27-C28	113.5
C21-C56	1.396	C10-C27-C34	109.3
C22-C57	1.387	C12-C11-C14	119.1
C22-S60	1.756	C11-C12-S13	112.5
C23-C42	1.494	C11-C12-C17	122.5
C23-C44	1.454	C11-C14-C15	118.2

C23-C62	1.362	S13-C12-C17	125
C24-C25	1.443	C12-C17-C16	118.2
C24-C26	1.391	C14-C15-C16	122.5
C24-C40	1.407	C14-C15-C18	126
C25-C41	1.407	C16-C15-C18	111.5
C25-C53	1.392	C15-C16-C17	119.5
C26-C51	1.384	C15-C16-C61	112.1
C27-C28	1.528	C15-C18-C63	90.3
C27-C34	1.532	C17-C16-C61	128.5
C28-C29	1.395	C16-C61-C63	113.1
C28-C30	1.392	C18-C63-N55	119.8
C29-C31	1.385	C18-C63-C61	113.1
C30-C32	1.389	C20-C19-C44	110.8
C31-C33	1.388	C20-C19-S60	113.3
C32-C33	1.386	C19-C20-C21	113.9
C34-C35	1.394	C19-C20-C42	109.6
C34-C36	1.393	C44-C19-S60	135.6
C35-C37	1.387	C19-C44-C23	105.7
C36-C38	1.387	C19-C44-C45	124
C37-C39	1.387	C19-S60-C22	89.7
C38-C39	1.386	C21-C20-C42	136.4
C40-C50	1.388	C20-C21-C22	110.3
C40-N55	1.396	C20-C21-C56	129.8
C41-N55	1.398	C20-C42-C23	104.9
C41-C65	1.387	C20-C42-C43	127.5
C42-O43	1.207	C22-C21-C56	119.9
C44-C45	1.371	C21-C22-C57	121.2
C45-C46	1.421	C21-C22-S60	112.7
C45-C48	1.421	C21-C56-C58	119.1
C46-C47	1.156	C57-C22-S60	126
C48-N49	1.155	C22-C57-C59	118.5
C50-C52	1.386	C42-C23-C44	107.7
C51-C52	1.397	C42-C23-C62	118.6
C53-C54	1.384	C23-C42-C43	127.6
C54-C64	1.397	C44-C23-C62	133.5
N55-C63	1.388	C23-C44-C45	129.3
C56-C58	1.383	C25-C24-C26	133.5
C57-C59	1.387	C25-C24-C40	107
C58-C59	1.419	C24-C25-C41	107
C58-C68	1.427	C24-C25-C53	133.6
C59-C66	1.426	C26-C24-C40	119.4
C61-C63	1.353	C24-C26-C51	119
C64-C65	1.385	C24-C40-C50	122
C66-N67	1.153	C24-C40-N55	108.8
C68-N69	1.153	C41-C25-C53	119.3

Table S7: **(**continue…) Calculated DFT values of selected bond angles of **CC10D6** of by using M06/6-311G (d, p)

Bond angle	
C25-C41-N55	108.8

C25-C41-C65	122.1
C25-C53-C54	119
C26-C51-C52	120.7
C28-C27-C34	114
C27-C28-C29	119.8
C27-C28-C30	121.4
C27-C34-C35	121
C27-C34-C36	120.4
C29-C28-C30	118.6
C28-C29-C31	120.8
C28-C30-C32	120.6
C29-C31-C33	120.2
C30-C32-C33	120.4
C31-C33-C32	119.5
C35-C34-C36	118.5
C34-C35-C37	120.8
C34-C36-C38	120.8
C35-C37-C39	120.2
C36-C38-C39	120.3
C37-C39-C38	119.4
C50-C40-N55	129.2
C40-C50-C52	117.4
C40-N55-C41	108.4
C40-N55-C63	126.3
N55-C41-C65	129.1
C41-N55-C63	125.3
C41-C65-C64	117.4
C44-C45-C46	120.5
C44-C45-C48	123.2
C46-C45-C48	116.1
C45-C46-C47	178.6
C45-C48-N49	177
C50-C52-C51	121.5
C53-C54-C64	120.7
C54-C64-C65	121.4
C55-C63-C61	127
C56-C58-C59	120.4
C56-C58-C68	119.5
C57-C59-C58	120.7
C57-C59-C66	118.9
C59-C58-C68	120.1

C58-C59-C66	120.4
C58-C68-N69	179.3
C59-C66-N67	178.8

Table S8: Calculated DFT values of selected bond lengths and bond angles of **CC10D7** by using M06/6-311G(d,p)

Bond length		**Bond angle**	
C1-C2	1.377	C2-C1-C4	111.4
C1-C4	1.398	C2-C1-C27	111.4
C1-C27	1.517	C1-C2-S8	114.3
C2-S8	1.733	C1-C2-C9	108.5
C2-C9	1.433	C4-C1-C27	136.9
C3-C4	1.398	C1-C4-C3	113.2
C3-C5	1.399	C1-C4-S7	135.1
C3-S8	1.75	C1-C27-C10	99.8
C4-S7	1.725	C1-C27-C28	107.7
C5-C6	1.38	C1-C27-C38	111.4
C5-H80	1.084	S8-C2-C9	136.9
C6-S7	1.761	C2-S8-C3	89.4
C6-C76	1.424	C2-C9-C10	109.4
C9-C10	1.369	C2-C9-S13	136.1
C9-S13	1.734	C4-C3-C5	113.8
C10-C11	1.424	C4-C3-S8	111.8
C10-C27	1.522	C3-C4-S7	111.4
C11-C12	1.426	C5-C3-S8	134.2
C11-C14	1.397	C3-C5-C6	111.9
C12-S13	1.763	C3-C5-H80	125.7
C12-C17	1.379	C4-S7-C6	90.7
C14-C15	1.382	C6-C5-H80	122.3
C14-H48	1.085	C5-C6-S7	112.1
C15-C16	1.419	C5-C6-C76	126.5
C15-C18	1.75	S7-C6-C76	121.5
C16-C17	1.395	C6-C76-C23	129.7
C16-C75	1.428	C6-C76-H77	116.2
C17-H49	1.086	C10-C9-S13	114.5
S18-C78	1.767	C9-C10-C11	113
C19-C20	1.378	C9-C10-C27	111
C19-C54	1.453	C9-S13-C12	89.5
C19-S68	1.72	C11-C10-C27	136
C20-C21	1.406	C10-C11-C12	110.7
C20-C52	1.475	C10-C11-C14	130.2
C21-C22	1.364	C10-C27-C28	113.2
C21-H86	1.082	C10-C27-C38	110.6
C22-S68	1.735	C12-C11-C14	119.1
C22-H85	1.082	C11-C12-S13	112.4
C23-C52	1.501	C11-C12-C17	122.4
C23-C54	1.461	C11-C14-C15	118.3
C23-C76	1.356	C11-C14-H48	120.5

C24-C25	1.443	S13-C12-C17	125.2
C24-C26	1.391	C12-C17-C16	118.3
C24-C50	1.407	C12-C17-H49	121.4
C25-C51	1.407	C15-C14-H48	121.2
C25-C65	1.392	C14-C15-16	122.4
C26-C63	1.384	C14-C15-S18	126.1
C26-H72	1.086	C16-C15-S18	111.4
C27-C28	1.529	C15-C16-C17	119.5
C27-C38	1.532	C15-C16-C75	112.1
C28-C29	1.395	C15-S18-C78	90.3
C28-C30	1.391	C17-C16-C75	128.4
C29-C31	1.385	C16-C17-H49	120.3
C29-C32	1.087	C16-C75-C78	113.1
C30-C33	1.389	C16-C75-H79	124.4
C30-H34	1.086	S18-C78-N67	119.6
C31-C35	1.389	S18-C78-C75	113.1
C31-H36	1.086	C20-C19-C54	111.4
C33-C35	1.385	C20-C19-S68	111.6
C33-H37	1.086	C19-C20-C21	114
C35-H60	1.085	C19-C20-C52	109.1
C38-C39	1.394	C54-C19-S68	136.7
C38-C40	1.394	C19-C54-C23	105.4
C39-C41	1.387	C19-C54-N55	124.6
C39-H42	1.087	C19-S68-C22	90.2
C40-C43	1.388	C21-C20-C52	136.9
C40-C44	1.087	C20-C21-C22	110.6
C41-C45	1.388	C20-C21-H86	124.8
C41-H46	1.086	C20-C52-C23	104.8
C43-C45	1.386	C20-C52-O53	128.3
C43-H47	1.087	C22-C21-H86	124.6
C45-H61	1.085	C21-C22-S68	113.6
C50-C62	1.388	C21-C22-H85	128
C50-N67	1.396	S68-C22-H85	118.4
C51-N67	1.397	C52-C23-C54	107.7
C51-C83	1.387	C52-C23-C76	118.9
C52-O53	1.205	C23-C52-O53	126.8
C54-C55	1.371	C54-C23-C76	133.1
C55-C56	1.421	C23-C54-C55	129
C55-C58	1.421	C23-C76-H77	114
C56-N57	1.156	C25-C24-C26	133.7
C58-N59	1.155	C25-C24-C50	107
C62-C64	1.385	C24-C25-C51	107.1
C62-H69	1.085	C24-C25-C65	133.6
C63-C64	1.397	C26-C24-C50	119.4
C63-H71	1.085	C24-C26-C63	119
C64-H70	1.086	C24-C26-H72	120.4
C65-C66	1.384	C24-C50-C62	122.1
C65-H73	1.086	C24-C50-N67	108.8
C66-H74	1.085	C51-C25-C65	119.4
C66-C81	1.397	C25-C51-N67	108.7
N67-C78	1.389	C25-C51-C83	122

C75-C78	1.353	C25-C65-C66	119
C75-H79	1.085	C25-C65-H73	120.4
C76-H77	1.093	C63-C26-H72	120.6
C81-H82	1.086	C26-C63-C64	120.7
C81-C83	1.386	C26-C63-H71	119.8

Table S8: (continue…) Calculated DFT values of selected bond lengths and bond angles of **CC10D7** compound by using M06/6-311G(d,p)

Bond angle	
C28-C27-C38	113.3
C27-C28-C29	119.7
C27-C28-C30	121.7
C27-C38-C39	120.7
C27-C38-C40	121
C29-C28-C30	118.5
C28-C29-C31	120.8
C28-C29-C32	119.6
C28-C30-C33	120.7
C28-C30-H34	119.8
C31-C29-C32	119.5
C29-C31-C35	120.2
C29-C31-H36	119.6
C33-C30-H34	119.5
C30-C33-C35	120.4
C30-C33-H37	119.5
C35-C31-H36	120.2
C31-C35-C33	119.4
C31-C35-H60	120.2
C35-C33-H37	120.1
C33-C35-H60	120.3
C39-C38-C40	118.4
C38-C39-C41	120.8
C38-C39-H42	119.8
C38-C40-C43	120.8
C38-C40-C44	120.5
C41-C39-H42	119.3
C39-C41-C45	120.3
C39-C41-H46	119.6
C43-C40-C44	118.7
C40-C43-C45	120.3
C40-C43-H47	119.2
C45-C41-H46	120.1
C41-C45-C43	119.4
C41-C45-H61	120.3
C45-C43-H47	120.5
C43-C45-H61	120.3
C62-C50-N67	129.1

C50-C62-C64	117.4
C50-C62-H69	121.3
C50-N67-C51	108.4
C50-N67-C78	125.9
N67-C51-C83	129.2
C51-N67-C78	125.6
C51-C83-C81	117.4
C51-C83-H84	121.1
C54-C55-C56	120.6
C54-C55-C58	123.7
C56-C55-C58	115.5
C55-C56-N57	179
C55-C58-N59	176.1
C64-C62-H69	121.3
C62-C64-C63	121.4
C62-C64-H70	119.2
C64-C63-H71	119.5
C63-C64-H70	119.4
C66-C65-H73	120.6
C65-C66-H74	119.9
C65-C66-C81	120.7
H74-C66-C81	119.4
C66-C81-H82	119.4
C66-C81-C83	121.4
N67-C78-C75	127.2
C78-C75-H79	122.5
H82-C81-C83	119.2
C81-C83-H84	121.4

Table S9: Calculated DFT values of selected bond lengths and bond angles of **CC10D8** by using M06/6-311G(d,p)

Bond length		**Bond angle**	
C1-C2	1.377	C2-C1-C4	111.3
C1-C4	1.4	C2-C1-C27	111.1
C1-C27	1.519	C1-C2-S8	114.5
C2-S8	1.732	C1-C2-C9	108.7
C2-C9	1.433	C4-C1-C27	137.3
C3-C4	1.399	C1-C4-C3	113
C3-C5	1.397	C1-C4-S7	135.7
C3-S8	1.749	C1-C27-C10	99.8
C4-S7	1.726	C1-C27-C28	107.8
C5-C6	1.38	C1-C27-C38	111.5
C5-H80	1.084	S8-C2-C9	136.7

C6-S7	1.762	C2-C8-C3	89.3
C6-C76	1.423	C2-C9-C10	109.4
C9-C10	1.368	C2-C9-S13	136.1
C9-S13	1.734	C4-C3-C5	113.9
C10-C11	1.424	C4-C3-S8	112
C10-C27	1.523	C3-C4-S7	111.3
C11-C12	1.426	C5-C3-S8	134.1
C11-C14	1.397	C3-C5-C6	112
C12-S13	1.763	C3-C5-H80	125.7
C12-C17	1.379	C4-S7-C6	90.7
C14-C15	1.382	C6-C5-H80	122.2
C14-H48	1.085	C5-C6-S7	111.9
C15-C16	1.418	C5-C6-C76	125.5
C15-S18	1.75	S7-C6-C76	122.5
C16-C17	1.395	C6-C76-C23	131.1
C16-C75	1.428	C6-C76-H77	115.2
C17-H49	1.086	C10-C9-C13	114.5
S18-C78	1.768	C9-C10-C11	113
C19-C20	1.379	C9-C10-C27	111
C19-C54	1.451	C9-S13-C12	89.5
C19-S68	1.734	C11-C10-C27	136.1
C20-C21	1.401	C10-C11-C12	110.6
C20-C52	1.469	C10-C11-C14	130.3
C21-C22	1.391	C10-C27-C28	113.5
C21-S89	1.727	C10-C27-C38	109.7
C22-S68	1.747	C12-C11-C14	119.1
C22-C85	1.415	C11-C12-S13	112.4
C23-C52	1.497	C11-C12-C17	122.5
C23-C54	1.461	C11-C14-C15	118.3
C23-C76	1.356	C11-C14-H48	120.5
C24-C25	1.443	S13-C12-C17	125.1
C24-C26	1.391	C12-C17-C16	118.2
C24-C50	1.407	C12-C17-H49	121.4
C25-C51	1.407	C15-C14-H48	121.2
C25-C65	1.392	C14-C15-C16	122.5
C26-C63	1.384	C14-C15-S18	126.1
C26-H72	1.086	C16-C15-S18	111.4
C27-C28	1.528	C15-C16-C17	119.4
C27-C38	1.531	C15-C16-C75	112.1
C28-C29	1.395	C15-S18-C78	90.3
C28-C30	1.391	C17-C16-C75	128.4
C29-C31	1.385	C16-C17-H49	120.4
C29-H32	1.087	C16-C75-C78	113.1
C30-C33	1.389	C16-C75-H79	124.3
C30-H34	1.086	S18-C78-N67	119.8
C31-C35	1.388	S18-C78-C75	113.1
C31-H36	1.086	C20-C19-C54	110.9
C33-C35	1.385	C20-C19-S68	113.1
C33-H37	1.086	C19-C20-C21	112.6
C35-H60	1.085	C19-C20-C52	109.5

C38-C39	1.394	C54-C19-S68	135.7
C38-C40	1.393	C19-C54-C23	105.7
C39-C41	1.387	C19-C54-C55	124.9
C39-C42	1.087	C19-S68-C22	89.7
C40-C43	1.387	C21-C20-C52	137.8
C40-C44	1.086	C20-C21-C22	112.1
C41-C45	1.387	C20-C21-S89	136.4
C41-H46	1.086	C20-C52-C23	104.8
C43-C45	1.386	C20-C52-O53	127.7
C43-C47	1.085	C22-C21-S89	111.5
C45-H61	1.085	C21-C22-S68	112.4
C50-C62	1.388	C21-C22-C85	113.6
C50-N67	1.396	C21-S89-C87	90.1
C51-N67	1.398	S68-C22-C85	134
C51-C83	1.387	C22-C85-H86	125.5
C52-O53	1.207	C22-C85-C87	110.7
C54-C55	1.372	C52-C23-C54	107.7
C55-C56	1.421	C52-C23-C76	118.5
C55-C58	1.421	C23-C52-O53	127.5
C56-N57	1.156	C54-C23-C76	133.5
C58-N59	1.155	C23-C54-C55	128.5
C62-C64	1.386	C23-C76-H77	113.5
C62-H69	1.085	C25-C24-C26	133.6
C63-C64	1.397	C25-C24-C50	107
C63-H71	1.085	C24-C25-C51	107
C64-H70	1.086	C24-C25-C65	133.6
C65-C66	1.384	C26-C24-C50	119.4
C65-H73	1.086	C24-C26-C63	119
C66-H74	1.085	C24-C26-H72	120.4
C66-C81	1.397	C24-C50-C62	122
N67-C78	1.389	C24-C50-N67	108.8
C75-C78	1.353	C51-C25-C65	119.4
C75-H79	1.085	C25-C51-N67	108.8
C76-H77	1.093	C25-C51-C83	122.1
C81-H82	1.086	C25-C65-C66	119
C81-C83	1.385	C25-C65-H73	120.4
C83-H84	1.085	C63-C26-H72	120.6
C85-H86	1.082	C26-C63-C64	120.7
C85-C87	1.361	C26-C63-H71	119.9
C87-H88	1.082	C28-C27-C38	113.6

Table S9: (continue…) Calculated DFT values of selected bond angles of **CC10D8** compound by using M06/6-311G(d,p)

Bond angle	
C27-C28-C29	119.6
C27-C28-C30	121.7
C27-C38-C39	120.9
C27-C38-C40	120.5
C29-C28-C30	118.5
C28-C29-C31	120.8

C28-C29-H32	119.7
C28-C30-C33	120.6
C28-C30-C34	119.9
C31-C29-H32	119.5
C29-C31-C35	120.2
C29-C31-H36	119.6
C33-C30-C34	119.5
C30-C33-C35	120.4
C30-C33-H37	119.5
C35-C31-H36	120.2
C31-C35-C33	119.4
C31-C35-H60	120.3
C35-C33-H37	120.1
C33-C35-H60	120.3
C39-C38-C40	118.5
C38-C39-C41	120.8
C38-C39-H42	119.8
C38-C40-C43	120.8
C38-C40-C44	120
C41-C39-H42	119.4
C39-C41-C45	120.3
C39-C41-H46	119.6
C43-C40-C44	119.2
C40-C43-C45	120.2
C40-C43-H47	119.3
C45-C41-H46	120.1
C41-C45-C43	119.5
C41-C45-H61	120.2
C45-C43-H47	120.5
C43-C45-H61	120.3
C62-C50-N67	129.2
C50-C62-C64	117.4
C50-C62-H69	121.3
C50-N67-C51	108.4
C50-N67-C78	126.3
N67-C51-C83	129.1
C51-N67-C78	125.3
C51-C83-C81	117.4
C51-C83-H84	121.2
C54-C55-C56	120.4
C54-C55-C58	123.5
C56-C55-C58	115.8
C55-C56-N57	178.8
C55-C58-N59	176.9
C64-C62-H69	121.3
C62-C64-C63	121.5
C62-C64-H70	119.1
C64-C63-H71	119.5
C63-C64-H70	119.4
C66-C65-H73	120.6
C65-C66-H74	119.9

C65-C66-C81	120.7
74-C66-C81	119.5
C66-C81-H82	119.4
C66-C81-C83	121.4
N67-C78-C75	127
C78-C75-H79	122.6
H82-C81-C83	119.2
C81-C83-H84	121.4
H86-C85-C87	123.8
C85-C87-H88	127.2
C85-C87-S89	114.1
H88-C87-S89	118.6

Table S10: Percentages of donor moiety, π-spacer and acceptor moiety for HOMOs and LUMOs

Compounds	**LUMO**			**HOMO**		
	Donor	**π-spacer**	**Acceptor**	**Donor**	**π-spacer**	**Acceptor**
CC10R		27.7	72.3		83.1	16.9
CC10D1	0.1	18.0	81.9	9.8	81.7	8.6
CC10D2	0.1	13.8	86.1	12.0	79.2	8.9
CC10D3	0.1	15.3	84.6	11.3	80.2	8.5
CC10D4	0.1	16.4	83.5	12.0	79.3	8.7
CC10D5	0.1	14.4	85.5	10.3	81.4	8.3
CC10D6	0.1	14.9	85.0	11.2	79.7	9.1
CC10D7	0.1	19.5	80.4	8.8	83.3	7.9
CC10D8	0.1	16.5	83.4	9.3	82.2	8.5

Table S11: Wave length, excitation energy and oscillator strength of investigated compound **CC10R** at M06/6-311G (d, p) level of theory.

No.	**DFT** $\boldsymbol{\lambda}$ **(*nm*)**	**E (*eV*)**	$\boldsymbol{f_{os}}$	**MO contributions**
1	714.354	1.736	1.602	H→L (95%), H-1→L+1 (2%)

2	614.569	2.017	0.029	H→L+1 (94%), H-1→L (4%)
3	506.819	2.446	0.261	H-1→L (86%), H-1→L+1 (3%), H→L+1 (4%)
4	494.943	2.505	0.281	H→L+2 (87%), H-1→L (2%), H-1→L+3 (2%), H→L+3 (4%)
5	469.847	2.639	0.010	H→L+3 (79%), H-1→L+1 (6%), H-1→L+2 (2%), H→L+2 (5%)
6	457.926	2.708	0.011	H-1→L+1 (75%), H-2→L (6%), H-1→L (2%), H→L+3 (9%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S12: Wave length, excitation energy and oscillator strength of investigated compound **CC10D1** at M06/6-311G (d, p) level of theory.

No.	**DFT** λ **(*nm*)**	**E (*eV*)**	f_{os}	**MO contributions**
1	709.896	1.747	0.538	H→L (93%) H-2→L (2%), H-1→L (3%)
2	521.486	2.378	0.724	H→L+1 (92%)H-1→L+1 (2%)
3	498.005	2.489	0.099	H-2→L (35%), H-1→L (52%) H-5→L (2%), H→L (6%)
4	478.368	2.592	0.046	H-2→L (53%), H-1→L (43%)
5	436.592	2.839	0.008	H-4→L (84%) H-5→L (4%), H-3→L (2%), H-2→L (3%)
6	435.625	2.846	0.000	H-3→L (95%) H-4→L (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S13: Wave length, excitation energy and oscillator strength of investigated compound **CC10D2** at M06/6-311G (d, p) level of theory.

No.	**DFT** λ **(*nm*)**	**E (*eV*)**	f_{os}	**MO contributions**
1	782.674	1.584	0.489	H→L (93%) H-1→L (3%)
2	542.977	2.283	0.194	H-2→L (17%), H-1→L (58%), H→L+1 (10%) H-3→L (3%), H →L (5%), H→L+2 (3%)
3	542.478	2.286	0.590	H→L+1 (75%) H-2→L (3%), H-1→L (9%), H→L+2 (5%)
4	518.976	2.389	0.036	H-2→L (60%), H-1→L (27%) H-3→L (9%)
5	481.919	2.573	0.011	H→L+2 (88%) H→L+1 (7%)
6	473.816	2.616	0.0	H-3→L (87%), H-2→L (13%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S14: Wave length, excitation energy and oscillator strength of investigated compound **CC10D3** at M06/6-311G (d, p) level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	741.305	1.673	0.486	H→L (93%) H-2→L (2%), H-1→L (3%)
2	530.955	2.335	0.709	H→L+1 (92%) H-1→L+1 (2%)
3	515.824	2.404	0.065	H-2→L (30%), H-1→L (59%) H-6→L (3%), H→L (6%)
4	494.115	2.509	0.033	H-2→L (60%), H-1→L (36%)
5	449.541	2.758	0.000	H-3→L (98%)
6	448.111	2.767	0.021	H-4→L (88%) H-6→L (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S15: Wave length, excitation energy and oscillator strength of investigated compound **CC10D4** at M06/6-311G (d, p) level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	774.944	1.599	0.503	H→L (94%), H-1→L (3%)
2	541.247	2.291	0.724	H→L+1 (92%), H-1→L+1(3%)
3	537.585	2.306	0.058	H-2→L (21%), H-1→L (66%) H-6→L (2%), H-3→L (3%), H→L (5%)
4	514.988	2.408	0.039	H-2→L (60%), H-1→L (29%) H-3→L (9%)
5	469.438	2.641	0.0	H-3→L (87%), H-2→L (13%)
6	459.623	2.697	0.019	H-4→L (85%) H-6→L (5%), H-5→L (4%)

MO=molecular orbital, H=HOMO, L=LUMO, *f*= oscillator strength

Table S16: Wave length, excitation energy and oscillator strength of investigated compound **CC10D5** at **M06/6-311G (d, p)** level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	726.408	1.706	0.493	H→L (93%) H-2→L (2%), H-1→L (3%)
2	523.623	2.368	0.712	H→L+1 (92%)H-1→L+1 (2%)
3	504.879	2.456	0.073	H-2→L (36%), H-1→L (53%) HO→L (6%)
4	484.159	2.561	0.033	H-2→L (55%), H-1→L (42%)
5	442.972	2.799	0.027	H-4→L (89%) H-6→L (5%)
6	440.016	2.818	0.000	H-3→L (99%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S17: Wave length, excitation energy and oscillator strength of investigated compound **CC10D6** at M06/6-311G (d, p) level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	758.679	1.634	0.529	H→L (94%) H-1→L (3%)
2	537.376	2.307	0.746	H→L+1 (91%)H-1→L+1 (2%)
3	530.592	2.337	0.082	H-2→L (13%), H-1→L (67%) H-3→L (9%), H→L (5%)
4	509.214	2.434	0.054	H-3→L (28%), H-2→L (41%), H-1→L (27%)
5	465.735	2.662	0.000	H-3→L (59%), H-2→L (41%)
6	454.318	2.729	0.009	H-4→L (88%) H-6→L (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S18: Wave length, excitation energy and oscillator strength of investigated compound **CC10D7** at M06/6-311G (d, p) level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	665.539	1.863	0.509	H→L (94%) H-2→L (2%), H-1→L (2%)
2	498.526	2.487	0.551	H→L+1 (92%)
3	471.276	2.631	0.071	H-2→L (45%), H-1→L (44%) H-6→L (3%), H→L (5%)
4	455.486	2.722	0.025	H-2→L (45%), H-1→L (52%)
5	425.256	2.916	0.041	H-4→L (91%)
6	414.563	2.991	0.000	H-3→L (97%) H-2→L (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S19: Wave length, excitation energy and oscillator strength of investigated compound **CC10D8** at M06/6-311G (d, p) level of theory.

No.	DFT λ (*nm*)	E (*eV*)	f_{os}	MO contributions
1	666.685	1.859	0.585	H→L (93%), H-2→L (2%), H-1→L (3%)
2	511.884	2.422	0.631	H→L+1 (91%) H-1→L+1 (2%)
3	472.839	2.622	0.146	H-2→L (43%), H-1→L (43%), H→L (6%)

4	452.791	2.738	0.049	H-2→L (46%), H-1→L (51%)
5	420.896	2.946	0.291	H-5→L (31%), H-4→L (59%)
6	418.311	2.964	0.099	H-5→L (61%), H-4→L (27%), H-2→L (4%), H-2→L+1 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength

Table S20: Second order Perturbation theory analysis of Fock matrix in NBO (**CC10R**) at M06/6-311G(d,p)

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(j)E(i)[b](*a.u*)	F(i,j)[c](*a.u*)
C1-C2	σ	C1-C4	σ*	5.43	1.28	0.075
C72-C75	σ	C72-C73	σ*	2.6	1.25	0.051
C1-C2	σ	C1-C43	σ*	3.01	1.13	0.052
C1-C2	σ	C2-C9	σ*	5.18	1.23	0.072
C1-C2	σ	C4-S7	σ*	8.4	0.93	0.079
C1-C2	σ	C9-S13	σ*	7.6	0.92	0.075
C1-C2	π	C1-C2	π*	0.5	0.31	0.012
C1-C2	π	C3-C4	π*	17.17	0.28	0.067
C1-C2	π	C9-C10	π*	15.36	0.32	0.064
C1-C2	σ	C1-C2	σ*	4.44	1.29	0.068
C1-C2	σ	C1-C43	σ*	5.53	1.14	0.071
C1-C2	σ	C3-C4	σ*	5.47	1.25	0.074
C1-C2	σ	C4-S7	σ*	1.21	0.94	0.03
C3-C4	σ	C1-C4	σ*	6.46	1.29	0.082
C3-C4	σ	C1-C43	σ*	7.65	1.13	0.083
C3-C4	π	C1-C2	π*	18.07	0.31	0.068
C3-C4	π	C5-C6	π*	21.94	0.31	0.075
C3-S8	σ	C2-C9	σ*	5.29	1.2	0.071
C5-C6	σ	C3-S8	σ*	7.72	0.93	0.076
C5-C6	π	C3-C4	π*	15.12	0.28	0.062
C5-C6	π	C27-C80	π*	20.94	0.32	0.074
C6-S7	σ	C1-C4	σ*	5.33	1.23	0.072
C6-C80	σ	C27-C80	σ*	5.55	1.35	0.077
C9-C10	σ	C2-S8	σ*	7.64	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.53	1.24	0.074
C9-C10	π	C1-C2	π*	14.92	0.31	0.063
C9-C10	π	C11-C14	π*	19.47	0.32	0.074
C10-C11	σ	C11-C14	σ*	5.65	1.27	0.076
C11-C12	σ	C10-C43	σ*	6.67	1.11	0.077
C11-C14	σ	C10-C11	σ*	6.13	1.27	0.079
C11-C14	σ	C11-C12	σ*	5.04	1.23	0.07
C11-C14	π	C9-C10	π*	19.61	0.29	0.068
C11-C14	π	C12-C17	π*	17.44	0.29	0.064
C11-C14	π	C15-C16	π*	22.78	0.27	0.074
C12-S13	σ	C2-C9	σ*	5.66	1.18	0.073
C12-C17	π	C11-C14	π*	18.13	0.32	0.07
C12-C17	π	C15-C16	π*	17.94	0.3	0.07
C15-C16	π	C11-C14	π*	21.5	0.3	0.072
C15-C16	π	C12-C17	π*	19.56	0.29	0.069

C15-C16	π	C18-C19	π*	18.65	0.29	0.067
C16-C17	σ	C12-S13	σ*	5.67	0.91	0.064
C16-C17	σ	C15-C16	σ*	5.08	1.24	0.071
C18-C19	π	C15-C16	π*	14.04	0.3	0.063
C18-C19	π	C36-C69	π*	19.72	0.32	0.072
C18-H68	σ	C19-S20	σ*	5.94	0.74	0.059
C21-C22	σ	C21-C26	σ*	5.28	1.3	0.074
C21-C26	π	C22-C23	π*	21.88	0.3	0.073
C21-C26	π	C24-C25	π*	24.01	0.26	0.072
C21-C26	π	C83-O84	π*	17.8	0.31	0.069
C22-C23	π	C21-C26	π*	20.78	0.31	0.073
C22-C23	π	C24-C25	π*	24.58	0.26	0.073
C22-C23	π	C81-C82	π*	16.53	0.3	0.064
C24-C25	π	C21-C26	π*	19.46	0.34	0.073
C24-C25	π	C22-C23	π*	19.37	0.33	0.072
C27-C80	σ	C27-C81	σ*	6.33	1.25	0.079
C27-C80	π	C5-C6	π*	9.8	0.3	0.05
C27-C80	π	C81-C82	π*	22.06	0.3	0.073
C27-C80	π	C83-O84	π*	22.34	0.32	0.076
C27-C81	σ	C27-C80	σ*	6.33	1.3	0.081
C30-C31	σ	C30-C35	σ*	5.28	1.3	0.074
C30-C35	π	C31-C32	π*	21.98	0.3	0.073
C30-C35	π	C33-C34	π*	23.99	0.26	0.072
C30-C35	π	C77-O78	π*	17.93	0.31	0.07
C31-C32	π	C30-C35	π*	20.77	0.31	0.073
C31-C32	π	C33-C34	π*	24.67	0.26	0.073
C31-C32	π	C71-C72	π*	16.47	0.3	0.064
C33-C34	π	C30-C35	π*	19.56	0.34	0.073
C33-C34	π	C31-C32	π*	19.47	0.33	0.072
C36-C69	σ	C19-C69	σ*	5.58	1.3	0.076
C36-C69	σ	C36-C71	σ*	6.37	1.25	0.08
C36-C69	π	C18-C19	π*	9.92	0.32	0.051
C36-C69	π	C71-C72	π*	20.58	0.3	0.071
C36-C69	π	C77-O78	π*	21.47	0.32	0.075
C36-C71	σ	C36-C69	σ*	6.34	1.31	0.081
C44-C46	π	C45-C47	π*	21.06	0.3	0.071
C44-C46	π	C49-C51	π*	21.82	0.3	0.073
C45-C47	π	C44-C46	π*	22.82	0.3	0.074
C45-C47	π	C49-C51	π*	21.15	0.3	0.072
C49-C51	π	C44-C46	π*	22.43	0.3	0.073
C49-C51	π	C45-C47	π*	22.9	0.3	0.074
C54-C56	π	C55-C57	π*	21.48	0.3	0.072
C54-C56	π	C59-C61	π*	21.87	0.3	0.073
C55-C57	π	C54-C56	π*	22.93	0.3	0.074
C55-C57	π	C59-C61	π*	21.37	0.3	0.072
C59-C61	π	C54-C56	π*	22.75	0.3	0.073
C59-C61	π	C55-C57	π*	22.9	0.3	0.074
C71-C72	σ	C72-C73	σ*	5.83	1.27	0.077
C71-C72	σ	C72-C75	σ*	5.99	1.28	0.078
C71-C72	π	C31-C32	π*	9.35	0.33	0.051

C71-C72	π	C36-C69	π*	8.83	0.35	0.049
C72-C73	σ	C73-N74	σ*	8.22	1.61	0.103
C72-C75	σ	C71-C72	σ*	6.09	1.33	0.08
C72-C75	σ	C75-N76	σ*	8.29	1.62	0.104
C73-N74	σ	C72-C73	σ*	8.1	1.57	0.101
C75-N76	σ	C72-C75	σ*	8.17	1.57	0.102
C80-H89	σ	C27-C81	σ*	9.13	1.01	0.086
C80-H89	σ	C27-C83	σ*	0.82	0.95	0.025
C81-C82	σ	C82-C85	σ*	5.85	1.27	0.077
C81-C82	σ	C82-C87	σ*	5.99	1.28	0.078
C81-C82	π	C22-C23	π*	9.3	0.33	0.051
C81-C82	σ	C27-C80	π*	8.84	0.34	0.049
C82-C85	σ	C81-C82	σ*	5.92	1.33	0.079
C82-C85	σ	C85-N86	σ*	8.23	1.61	0.103
C82-C87	σ	C81-C82	σ*	6.09	1.33	0.08
C85-N86	σ	C82-C85	σ*	8.11	1.57	0.102
C87-N88	σ	C82-C87	σ*	8.12	1.57	0.102
S7	LP(1)	C3-C4	σ*	2.78	1.18	0.051
S7	LP(2)	C3-C4	π*	27.84	0.25	0.078
S7	LP(2)	C5-C6	π*	22.02	0.27	0.069
S8	LP(1)	C3-C5	σ*	0.66	1.23	0.025
S8	LP(2)	C1-C2	π*	26.75	0.28	0.077
S8	LP(2)	C3-C4	π*	24.03	0.25	0.072
S13	LP(2)	C9-C10	π*	25.71	0.28	0.076
S13	LP(2)	C12-C17	π*	21.77	0.28	0.07
S20	LP(2)	C15-C16	π*	21.9	0.26	0.072
S20	LP(2)	C18-C19	π*	22.11	0.27	0.07
Cl39	LP(1)	C24-C25	σ*	1.85	1.48	0.047
Cl39	LP(2)	C21-C26	σ*	0.53	0.93	0.02
Cl39	LP(2)	C24-C25	σ*	5.64	0.86	0.062
Cl39	LP(2)	C25-C26	σ*	4.49	0.89	0.057
Cl39	LP(3)	C24-C25	π*	16.36	0.31	0.071
Cl40	LP(2)	C24-C25	σ*	5.55	0.86	0.062
Cl40	LP(3)	C24-C25	π*	16.34	0.31	0.071
Cl41	LP(2)	C33-C34	σ*	5.65	0.86	0.063
Cl41	LP(3)	C33-C34	π*	16.42	0.31	0.071
Cl42	LP(2)	C33-C34	σ*	5.54	0.86	0.062
Cl42	LP(3)	C33-C34	π*	16.4	0.31	0.071
N74	LP(1)	C72-C73	σ*	12.59	1.04	0.102
N76	LP(1)	C72-C75	σ*	12.66	1.04	0.103
O78	LP(2)	C30-C77	σ*	21.48	0.75	0.115
O78	LP(2)	C36-C77	σ*	22.75	0.72	0.116
O84	LP(2)	C21-C83	σ*	21.51	0.74	0.115
O84	LP(2)	C27-C83	σ*	22.43	0.72	0.115
N86	LP(1)	C82-C85	σ*	12.59	1.04	0.102
N88	LP(1)	C82-C87	σ*	12.58	1.04	0.102

Table S21: Second order Perturbation theory analysis of Fock matrix in NBO (**CC10D1**) at M06/6-311G(d,p)

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(j)E(i)[b](*a.u*)	F(i,j)[c](*a.u*)
C1-C2	σ	C1-C4	σ*	5.53	1.28	0.076
C1-C2	σ	C1-C27	σ*	3.04	1.12	0.052
C1-C2	σ	C2-C9	σ*	5.13	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.57	0.93	0.08
C1-C2	σ	C9-S13	σ*	7.61	0.92	0.075
C1-C2	π	C3-C4	π*	17.88	0.28	0.068
C1-C2	π	C9-C10	π*	14.75	0.32	0.063
C1-C2	π	C27-C28	σ*	2.38	0.71	0.039
C1-C4	σ	C1-C2	σ*	4.53	1.29	0.068
C1-C4	σ	C1-C27	σ*	5.54	1.14	0.071
C1-C4	σ	C3-C4	σ*	5.52	1.25	0.074
C1-C27	σ	C27-C38	σ*	2.23	1.04	0.043
C3-C4	σ	C1-C4	σ*	6.54	1.29	0.082
C3-C4	σ	C1-C27	σ*	7.55	1.13	0.083
C3-C4	σ	C2-C9	σ*	0.51	1.24	0.023
C3-C4	π	C1-C2	π*	17.44	0.31	0.067
C3-C4	π	C5-C6	π*	21.79	0.31	0.075
C5-C6	σ	C3-S8	σ*	7.85	0.93	0.076
C5-C6	π	C3-C4	π*	14.67	0.28	0.062
C5-C6	π	C23-C83	π*	21.09	0.32	0.074
C5-H88	σ	C6-S7	σ*	6.06	0.73	0.06
C6-S7	σ	C1-C4	σ*	5.15	1.24	0.071
C6-C83	σ	C23-C83	σ*	5.93	1.35	0.08
C9-C10	σ	C2-S8	σ*	7.66	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.58	1.23	0.074
C9-C10	σ	C11-C14	σ*	5.08	1.29	0.073
C9-C10	π	C1-C2	π*	14.98	0.31	0.063
C9-C10	π	C11-C14	π*	18.08	0.32	0.072
C10-C27	σ	C1-C4	σ*	5.23	1.19	0.071
C11-C12	σ	C10-C27	σ*	6.62	1.11	0.076
C11-C14	σ	C10-C11	σ*	6.12	1.26	0.079
C11-C14	σ	C11-C12	σ*	5.22	1.23	0.072
C11-C14	σ	C15-S18	σ*	5.49	0.92	0.064
C11-C14	π	C9-C10	π*	20.2	0.29	0.069
C11-C14	π	C12-C17	π*	19.11	0.29	0.066
C11-C14	π	C15-C16	π*	21.62	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.63	1.18	0.073
C12-C17	π	C11-C14	π*	18.14	0.32	0.07
C12-C17	π	C15-C16	π*	19.16	0.3	0.072
C14-C15	σ	C15-C16	σ*	5.17	1.27	0.073
C15-C16	π	C11-C14	π*	22.83	0.3	0.075
C15-C16	π	C12-C17	π*	20.68	0.29	0.07
C15-C16	π	C82-C86	π*	15.14	0.29	0.061
C16-C17	σ	C12-S13	σ*	5.55	0.91	0.064
C16-C17	σ	C15-C16	σ*	5.22	1.25	0.072
C16-C82	σ	N67-C86	σ*	6.83	1.11	0.078
C17-H49	σ	C11-C12	σ*	5.12	1.05	0.066
C19-C20	π	C21-C22	π*	14.96	0.31	0.064
C19-C20	π	C52-O53	π*	20.11	0.33	0.074

C19-C20	π	C54-C55	π*	21.7	0.31	0.074
C20-C52	σ	C19-S73	σ*	5.15	0.87	0.06
C21-C22	σ	C20-C52	σ*	5.68	1.18	0.074
C21-C22	π	C19-C20	π*	18.49	0.3	0.067
C21-C22	π	C68-C71	π*	20.16	0.3	0.07
C21-C22	π	C70-C72	π*	23.81	0.29	0.075
C21-C68	σ	C20-C21	σ*	5.59	1.27	0.075
C21-C68	σ	C21-C22	σ*	5.56	1.25	0.075
C21-C68	σ	C22-S73	σ*	3.36	0.91	0.049
C23-C54	σ	C19-S73	σ*	6.86	0.89	0.07
C23-C54	σ	C23-C83	σ*	6.03	1.31	0.08
C23-C83	σ	C6-C83	σ*	5.16	1.3	0.073
C23-C83	π	C52-O53	π*	21.63	0.32	0.075
C23-C83	π	C54-C55	π*	20.84	0.3	0.072
C24-C25	σ	C25-C65	σ*	5.13	1.25	0.072
C24-C26	σ	C24-C25	σ*	5.84	1.24	0.076
C24-C26	σ	C24-C50	σ*	5.15	1.27	0.072
C24-C50	σ	C25-C65	σ*	5.13	1.27	0.072
C24-C50	σ	N67-C86	σ*	5.32	1.11	0.069
C24-C50	π	C25-C51	π*	18.84	0.29	0.067
C24-C50	π	C26-C63	π*	22.14	0.3	0.074
C24-C50	π	C62-C64	π*	19.88	0.3	0.07
C25-C51	σ	C24-C26	σ*	5.13	1.27	0.072
C25-C51	σ	N67-C86	σ*	5.17	1.11	0.068
C25-C51	π	C24-C50	π*	19.01	0.29	0.068
C25-C51	π	C65-C66	π*	22.19	0.3	0.074
C25-C51	π	C89-C91	π*	19.81	0.3	0.069
C25-C65	σ	C24-C25	σ*	5.85	1.24	0.076
C25-C65	σ	C25-C51	σ*	5.17	1.27	0.072
C26-C63	π	C24-C50	π*	19.77	0.29	0.071
C26-C63	π	C62-C64	π*	22.94	0.3	0.074
C28-C30	π	C29-C31	π*	21.03	0.3	0.071
C28-C30	π	C33-C35	π*	21.91	0.3	0.073
C29-C31	π	C28-C30	π*	22.73	0.3	0.074
C29-C31	π	C33-C35	π*	21.16	0.3	0.072
C33-C35	π	C28-C30	π*	22.2	0.3	0.073
C33-C35	π	C29-C31	π*	22.79	0.3	0.074
C38-C40	π	C39-C41	π*	21.66	0.3	0.072
C38-C40	π	C43-C45	π*	21.84	0.3	0.073
C39-C41	π	C38-C40	π*	22.81	0.3	0.074
C39-C41	π	C43-C45	π*	21.43	0.3	0.072
C43-C45	π	C38-C40	π*	22.73	0.3	0.073
C43-C45	π	C39-C41	π*	22.88	0.3	0.074
C54-C55	σ	C55-C56	σ*	5.54	1.27	0.075
C54-C55	σ	C55-C58	σ*	5.97	1.28	0.078
C54-C55	π	C19-C20	π*	9.32	0.32	0.051
C54-C55	π	C23-C83	π*	8.26	0.35	0.048
C55-C56	σ	C56-N57	σ*	8.21	1.61	0.103
C55-C58	σ	C54-C55	σ*	6.18	1.33	0.081
C55-C58	σ	C58-N59	σ*	8.31	1.62	0.104

C56-N57	σ	C55-C56	σ*	8.16	1.57	0.102
C58-N59	σ	C55-C58	σ*	8.25	1.57	0.102
C62-C64	σ	C50-N67	σ*	6.6	1.13	0.077
C62-C64	π	C24-C50	π*	22.9	0.3	0.077
C62-C64	π	C26-C63	π*	19.08	0.3	0.068
C65-C66	σ	C24-C25	σ*	5.17	1.24	0.072
C65-C66	π	C25-C51	π*	19.62	0.29	0.071
C65-C66	π	C89-C91	π*	22.83	0.3	0.074
C68-C71	σ	C71-C72	σ*	5.34	1.27	0.074
C68-C71	π	C21-C22	π*	19.01	0.3	0.072
C68-C71	π	C70-C72	π*	19.82	0.3	0.071
C70-C72	σ	C22-S73	σ*	5.24	0.94	0.063
C70-C72	σ	C71-C72	σ*	5.07	1.27	0.072
C70-C72	π	C21-C22	π*	17.49	0.3	0.068
C70-C72	π	C68-C71	π*	18.71	0.31	0.069
C82-C86	π	C15-C16	π*	13.24	0.32	0.065
C82-H87	σ	S18-C86	σ*	6.46	0.72	0.061
C83-H84	σ	C6-S7	σ*	6.79	0.71	0.062
C83-H84	σ	C23-C54	σ*	9.15	1	0.086
C89-C91	σ	C51-N67	σ*	6.63	1.13	0.078
C89-C91	π	C25-C51	π*	22.97	0.3	0.077
C89-C91	π	C65-C66	π*	19.08	0.3	0.068
S7	LP(2)	C3-C4	π*	27.7	0.25	0.078
S7	LP(2)	C5-C6	π*	21.35	0.27	0.069
S8	LP(1)	C1-C2	σ*	2.93	1.23	0.054
S8	LP(1)	C2-C9	σ*	0.91	1.18	0.029
S8	LP(1)	C3-C4	σ*	2.69	1.19	0.051
S8	LP(1)	C3-C5	σ*	0.66	1.22	0.025
S8	LP(2)	C1-C2	π*	26.65	0.28	0.077
S8	LP(2)	C3-C4	π*	23.56	0.25	0.072
S13	LP(1)	C2-C9	σ*	0.85	1.17	0.028
S13	LP(1)	C9-C10	σ*	2.75	1.24	0.052
S13	LP(1)	C11-C12	σ*	2.76	1.18	0.051
S13	LP(2)	C9-C10	π*	24.98	0.28	0.076
S13	LP(2)	C12-C17	π*	21.66	0.28	0.071
S18	LP(1)	C15-C16	σ*	2.58	1.2	0.05
S18	LP(1)	C82-C86	σ*	2.67	1.27	0.052
S18	LP(2)	C15-C16	π*	20.47	0.27	0.07
S18	LP(2)	C82-C86	π*	22.88	0.28	0.072
O53	LP(1)	C20-C52	σ*	2.54	1.17	0.049
O53	LP(1)	C23-C52	σ*	2.61	1.14	0.049
O53	LP(2)	C20-C52	σ*	21.58	0.75	0.115
O53	LP(2)	C23-C52	σ*	22.33	0.72	0.114
N57	LP(1)	C55-C56	σ*	12.52	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.66	1.04	0.103
N67	LP(1)	S18-C86	σ*	10.78	0.46	0.068
N67	LP(1)	C24-C50	π*	33.53	0.31	0.095
N67	LP(1)	C25-C51	π*	33.2	0.32	0.094
N67	LP(1)	C82-C86	σ*	4.29	0.89	0.06
N67	LP(1)	C82-C86	π*	10.45	0.3	0.051

S73	LP(1)	C19-C20	σ*	2.5	1.24	0.05
S73	LP(1)	C19-C54	σ*	1.01	1.14	0.03
S73	LP(1)	C21-C22	σ*	2.83	1.21	0.052
S73	LP(2)	C19-C20	π*	27.04	0.28	0.078
S73	LP(2)	C21-C22	π*	21.71	0.27	0.07
Cl74	LP(1)	C68-C71	σ*	1.74	1.52	0.046
Cl74	LP(1)	C71-C72	σ*	1.76	1.47	0.046
Cl74	LP(2)	C21-C68	σ*	0.57	0.9	0.02
Cl74	LP(2)	C68-C71	σ*	4.32	0.91	0.056
Cl74	LP(2)	C71-C72	σ*	5.52	0.86	0.062
Cl74	LP(3)	C68-C71	π*	14.46	0.34	0.067
Cl75	LP(1)	C70-C72	σ*	1.68	1.51	0.045
Cl75	LP(1)	C71-C72	σ*	1.8	1.47	0.046
Cl75	LP(2)	C22-C70	σ*	0.52	0.9	0.019
Cl75	LP(2)	C70-C72	σ*	4.47	0.9	0.057
Cl75	LP(2)	C71-C72	σ*	5.46	0.86	0.061
Cl75	LP(3)	C70-C72	π*	14.72	0.34	0.068

Table S22: Second order Perturbation theory analysis of Fock matrix in NBO (**CC10D2**) at M06/6-311G(d,p)

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(j)E(i)[b](*a.u*)**	**F(i,j)[c](*a.u*)**
C1-C2	σ	C1-C4	σ*	5.58	1.29	0.076
C1-C2	σ	C1-C27	σ*	3.06	1.12	0.052
C6-S7	σ	C3-C4	σ*	0.51	1.18	0.022
C1-C2	σ	C2-C9	σ*	5.11	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.63	0.93	0.08
C1-C2	σ	C9-S13	σ*	7.65	0.92	0.075
C1-C2	σ	C27-C38	σ*	1.08	1.13	0.031
C1-C2	π	C3-C4	π*	18.76	0.28	0.07
C1-C2	π	C9-C10	π*	14.79	0.32	0.063
C1-C2	π	C27-C28	σ*	2.44	0.71	0.039
C1-C4	σ	C1-C2	σ*	4.57	1.29	0.069
C1-C4	σ	C1-C27	σ*	5.63	1.14	0.072
C1-C4	σ	C3-C4	σ*	5.53	1.25	0.074
C3-C4	σ	C1-C4	σ*	6.56	1.3	0.082
C3-C4	σ	C1-C27	σ*	7.58	1.13	0.083
C3-C4	π	C1-C2	π*	17.58	0.31	0.067
C3-C4	π	C5-C6	π*	22.66	0.31	0.076
C3-S8	σ	C2-C9	σ*	5.21	1.2	0.071
C5-C6	σ	C3-S8	σ*	7.90	0.93	0.076
C5-C6	π	C3-C4	π*	14.65	0.28	0.061
C5-C6	π	C23-C81	π*	22.10	0.32	0.075
C5-H86	σ	C6-S7	σ*	6.06	0.73	0.06
C6-S7	σ	C1-C4	σ*	5.14	1.24	0.071
C9-C10	σ	C3-S8	σ*	7.70	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.58	1.23	0.074
C9-C10	σ	C 11-C14	σ*	5.09	1.29	0.073
C9-C10	π	C1-C2	π*	15.32	0.31	0.064
C9-C10	π	C 11-C14	π*	18.03	0.32	0.072

C10-C11	σ	C 11-C14	σ*	5.63	1.26	0.075
C11-C12	σ	C10-C27	σ*	6.62	1.11	0.076
C 11-C14	σ	C10-C11	σ*	6.10	1.26	0.078
C 11-C14	σ	C11-C12	σ*	5.24	1.23	0.072
C 11-C14	π	C9-C10	π*	20.50	0.29	0.069
C 11-C14	π	C12-C17	π*	19.18	0.29	0.066
C 11-C14	π	C15-C16	π*	21.49	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.62	1.18	0.073
C12-C17	π	C 11-C14	π*	18.14	0.31	0.07
C12-C17	π	C15-C16	π*	19.31	0.3	0.072
C15-C16	σ	C14-C15	σ*	5.00	1.29	0.072
C15-C16	π	C 11-C14	π*	23.14	0.3	0.075
C15-C16	π	C12-C17	π*	20.61	0.29	0.07
C15-C16	π	C80-C84	π*	15.03	0.29	0.061
C17-H49	σ	C11-C12	σ*	5.10	1.05	0.065
C19-C20	σ	C20-C21	σ*	5.41	1.29	0.074
C19-C20	σ	C21-C68	σ*	5.03	1.29	0.072
C19-C20	π	C21-C68	π*	18.74	0.32	0.072
C19-C20	π	C52-O53	π*	19.60	0.34	0.074
C19-C20	π	C54-C55	π*	20.12	0.32	0.072
C21-C22	σ	C20-C52	σ*	5.59	1.18	0.073
C21-C68	σ	C20-C21	σ*	5.37	1.27	0.074
C21-C68	σ	C21-C22	σ*	5.27	1.25	0.073
C21-C68	π	C19-C20	π*	20.66	0.29	0.071
C21-C68	π	C22-C70	π*	20.69	0.28	0.069
C21-C68	π	C71-C72	π*	27.82	0.26	0.077
C22-C70	π	C21-C68	π*	21.20	0.31	0.073
C22-C70	π	C71-C72	π*	22.54	0.28	0.074
C22-S73	σ	C19-C54	σ*	5.79	1.14	0.073
C23-C54	σ	C19-S73	σ*	6.80	0.88	0.069
C23-C54	σ	C23-C81	σ*	5.96	1.3	0.079
C23-C81	σ	C6-C81	σ*	5.02	1.3	0.072
C23-C81	σ	C23-C54	σ*	6.08	1.24	0.078
C23-C81	π	C5-C6	π*	9.26	0.3	0.049
C23-C81	π	C52-O53	π*	22.26	0.31	0.076
C23-C81	π	C54-C55	π*	22.24	0.3	0.073
C24-C26	σ	C24-C25	σ*	5.84	1.24	0.076
C24-C26	σ	C24-C50	σ*	5.16	1.27	0.072
C24-C26	π	C25-C65	π*	17.03	0.3	0.064
C24-C26	π	C50-C62	π*	23.41	0.29	0.074
C24-C26	π	C63-C64	π*	21.56	0.29	0.071
C24-C50	σ	C25-C65	σ*	5.12	1.27	0.072
C24-C50	σ	N67-C84	σ*	5.31	1.11	0.069
C25-C51	σ	C24-C26	σ*	5.12	1.27	0.072
C25-C65	σ	C24-C25	σ*	5.84	1.24	0.076
C25-C65	σ	C25-C51	σ*	5.18	1.27	0.072
C25-C65	π	C24-C26	π*	17.09	0.3	0.064
C25-C65	π	C51-C89	π*	23.46	0.29	0.074
C25-C65	π	C66-C87	π*	21.54	0.29	0.071
C28-C30	π	C29-C31	π*	20.85	0.3	0.071

C28-C30	π	C33-C35	π*	21.74	0.3	0.073
C29-C31	π	C28-C30	π*	22.55	0.3	0.074
C29-C31	π	C33-C35	π*	21.07	0.3	0.071
C33-C35	π	C28-C30	π*	22.16	0.3	0.073
C33-C35	π	C29-C31	π*	22.66	0.3	0.074
C38-C40	π	C39-C41	π*	21.64	0.3	0.072
C38-C40	π	C43-C45	π*	21.71	0.3	0.073
C39-C41	π	C38-C40	π*	22.77	0.3	0.074
C39-C41	π	C43-C45	π*	21.42	0.3	0.072
C43-C45	π	C38-C40	π*	22.70	0.3	0.073
C43-C45	π	C39-C41	π*	22.80	0.3	0.074
C50-C62	σ	C24-C50	σ*	5.84	1.28	0.077
C50-C62	π	C24-C26	π*	18.72	0.31	0.069
C50-C62	π	C63-C64	π*	23.75	0.3	0.076
C51-C89	σ	C25-C51	σ*	5.84	1.28	0.077
C51-C89	π	C25-C65	π*	18.77	0.31	0.069
C51-C89	π	C66-C87	π*	23.84	0.3	0.076
C54-C55	σ	C55-C56	σ*	5.53	1.28	0.075
C54-C55	σ	C55-C58	σ*	5.97	1.28	0.078
C54-C55	π	C19-C20	π*	9.72	0.32	0.051
C54-C55	π	C23-C81	π*	8.37	0.34	0.048
C55-C56	σ	C56-N57	σ*	8.23	1.61	0.103
C55-C58	σ	C54-C55	σ*	6.18	1.33	0.081
C55-C58	σ	C58-N59	σ*	8.34	1.62	0.104
C56-N57	σ	C55-C56	σ*	8.21	1.57	0.102
C62-C64	σ	C50-N67	σ*	6.61	1.13	0.078
C63-C64	π	C24-C26	π*	23.59	0.3	0.076
C63-C64	π	C50-C62	π*	20.46	0.29	0.069
C65-C66	σ	C24-C25	σ*	5.17	1.24	0.072
C66-C87	π	C25-C65	π*	23.66	0.3	0.076
C66-C87	π	C51-C89	π*	20.42	0.29	0.069
C70-C72	σ	C22-S73	σ*	5.41	0.94	0.064
C70-C72	σ	C71-C72	σ*	5.85	1.28	0.077
C71-C72	σ	C68-C71	σ*	5.43	1.33	0.076
C71-C72	σ	C70-C72	σ*	5.29	1.32	0.075
C71-C72	π	C21-C68	π*	21.86	0.32	0.075
C71-C72	π	C22-C70	π*	23.80	0.3	0.077
C71-C72	π	N91-O92	π*	14.91	0.19	0.05
C71-C72	π	N94-O95	π*	12.48	0.19	0.047
C80 - C84	π	C15-C16	π*	13.45	0.32	0.065
C80-H85	σ	S18-C84	σ*	6.43	0.72	0.061
C81-H82	σ	C6-S7	σ*	6.66	0.71	0.062
S7	LP(1)	C3-C4	σ*	2.82	1.19	0.052
O96	LP(2)	C71-C72	σ*	0.51	0.84	0.019
S7	LP(2)	C3-C4	π*	27.68	0.25	0.078
S7	LP(2)	C5-C6	π*	20.85	0.27	0.068
S73	LP(1)	C19-C54	σ*	1.01	1.14	0.03
S8	LP(2)	C1-C2	π*	26.83	0.28	0.078
S8	LP(2)	C3-C4	π*	23.36	0.25	0.071
S13	LP(2)	C9-C10	π*	24.95	0.28	0.075

S13	LP(2)	C12-C17	π*	21.75	0.28	0.071
S18	LP(2)	C15-C16	π*	20.41	0.27	0.07
S18	LP(2)	C80 - C84	π*	22.94	0.28	0.072
O53	LP(2)	C20-C52	σ*	22.12	0.74	0.116
O53	LP(2)	C23-C52	σ*	22.17	0.72	0.114
N57	LP(1)	C55-C56	σ*	12.57	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.70	1.04	0.103
N67	LP(1)	S18-C84	σ*	10.29	0.46	0.067
N67	LP(1)	C50-C62	π*	38.10	0.32	0.099
N67	LP(1)	C51-C89	π*	37.60	0.32	0.099
N67	LP(1)	C80-C84	σ*	4.05	0.88	0.058
N67	LP(1)	C80-C84	π*	12.04	0.3	0.055
S73	LP(2)	C19-C20	π*	27.14	0.28	0.079
S73	LP(2)	C22-C70	π*	23.84	0.27	0.071
O92	LP(1)	C72-N91	σ*	3.94	1.08	0.06
O92	LP(2)	C72-N91	σ*	16.06	0.58	0.086
O92	LP(2)	N91-O93	σ*	20.69	0.76	0.114
O93	LP(2)	C72-N91	σ*	16.11	0.57	0.086
O93	LP(2)	N91-O92	σ*	20.52	0.75	0.111
O95	LP(2)	C71-N94	σ*	16.04	0.57	0.086
O95	LP(2)	N94-O96	σ*	20.56	0.77	0.114
O96	LP(2)	C71-N94	σ*	16.05	0.57	0.086
O96	LP(2)	N94-O95	σ*	20.67	0.74	0.111

Table S23: Second order Perturbation theory analysis of Fock matrix in NBO (**CC10D3**) at M06/6-311G(d,p)

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(j)E(i)[b](*a.u*)**	**F(i,j)[c](*a.u*)**
C1-C2	σ	C1-C4	σ*	5.58	1.29	0.076
C1-C2	σ	C1-C27	σ*	3.06	1.12	0.052
C1-C2	σ	C2-C9	σ*	5.13	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.61	0.93	0.080
C1-C2	σ	C9-S13	σ*	7.65	0.93	0.075
C1-C2	π	C9-C10	π*	14.84	0.32	0.063
C1-C2	π	C3-C4	π*	18.39	0.28	0.069
C1-C4	σ	C1-C2	σ*	4.57	1.29	0.063
C1-C4	σ	C1-C27	σ*	5.59	1.14	0.072
C1-C4	σ	C3-C4	σ*	5.55	1.25	0.074
C2-S8	σ	C9-C10	σ*	1.12	1.28	0.034
C3-C4	σ	C1-C4	σ*	6.58	1.30	0.082
C3-C4	π	C1-C2	π*	17.56	0.31	0.068
C3-C4	π	C5-C6	π*	22.10	0.31	0.075
C3-C4	σ	C1-C27	σ*	7.56	1.13	0.083
C3-S8	σ	C2-C9	σ*	5.20	1.20	0.071
C5-C6	σ	C3-S8	σ*	7.87	0.93	0.076
C5-C6	π	C23-C81	π*	21.14	0.32	0.074
C5-H86	σ	C6-S7	σ*	6.08	0.73	0.060
C6-S7	σ	C1-C4	σ*	5.13	1.24	0.071
C6-C81	σ	C23-C81	σ*	5.78	1.35	0.079
C6-S7	σ	C5-C6	σ*	0.51	1.22	0.022
C9-C10	π	C1-C2	π*	15.09	0.31	0.064

C9-C10	π	C11-C14	π*	18.09	0.32	0.072
C11-C14	π	C9-C10	π*	20.33	0.29	0.069
C11-C14	π	C12-C17	π*	19.15	0.29	0.066
C11-C14	π	C15-C16	π*	21.52	0.28	0.072
C12-C17	π	C11-C14	π*	18.16	0.31	0.070
C12-C17	π	C15-C16	π*	19.27	0.30	0.072
C15-C16	π	C11-C14	π*	23.01	0.30	0.075
C15-C16	π	C12-C17	π*	20.67	0.29	0.070
C15-C16	π	C80-C84	π*	15.08	0.29	0.061
C19-C20	π	C21-C22	π*	15.57	0.31	0.065
C19-C20	π	C52-O53	π*	19.91	0.33	0.074
C19-C20	π	C54-C55	π*	20.90	0.32	0.073
C21-C22	π	C19-C20	π*	17.71	0.30	0.066
C21-C22	π	C68-C71	π*	18.81	0.31	0.070
C21-C22	π	C70-C72	π*	22.14	0.30	0.075
C62-C64	π	C24-C50	π*	22.85	0.30	0.077
C62-C64	π	C26-C63	π*	19.11	0.30	0.068
C24-C50	π	C25-C51	π*	18.82	0.29	0.067
C70-C72	π	C21-C22	π*	17.72	0.30	0.068
C70-C72	π	C68-C71	π*	19.48	0.31	0.070
C87-C89	π	C25-C51	π*	22.96	0.30	0.077
C87-C89	π	C65-C66	π*	19.14	0.30	0.069
F97	LP(2)	C21-C68	σ*	0.51	1.02	0.020
S7	LP(2)	C3-C4	π*	27.55	0.25	0.078
S7	LP(2)	C5-C6	π*	21.04	0.27	0.068
S8	LP(1)	C3-C4	σ*	2.66	1.19	0.050
S8	LP(2)	C1-C2	π*	26.66	0.28	0.077
S8	LP(2)	C3-C4	π*	23.45	0.25	0.072
S13	LP(2)	C9-C10	π*	24.97	0.28	0.076
S13	LP(2)	C12-C17	π*	21.74	0.28	0.071
S18	LP(2)	C15-C16	π*	20.38	0.27	0.070
S18	LP(2)	C80-C84	π*	22.89	0.28	0.072
N57	LP(1)	C55-C56	σ*	12.55	1.04	0.102
N67	LP(1)	C24-C50	π*	33.40	0.31	0.094
F93	LP(2)	C72-C91	σ*	6.65	0.81	0.066
F93	LP(3)	C91-F94	σ*	11.40	0.72	0.081
F94	LP(2)	C91-F93	σ*	5.27	0.72	0.056
F96	LP(3)	C92-F98	σ*	10.73	0.72	0.079
F95	LP(2)	C91-F94	σ*	3.86	0.72	0.048
F95	LP(3)	C91-F93	σ*	9.88	0.72	0.076
O53	LP(2)	C20-C52	σ*	21.80	0.75	0.115
O53	LP(2)	C23-C52	σ*	22.26	0.72	0.114
N57	LP(1)	C55-C56	σ*	12.55	1.04	0.102
N67	LP(1)	C25-C51	π*	33.04	0.32	0.094
F97	LP(3)	C92-F98	σ*	10.02	0.72	0.077
F98	LP(3)	C92-F96	σ*	11.45	0.72	0.081

Table S24: Second order Perturbation theory analysis of Fock matrix NBO (**CC10D4**) at M06/6-311G(d,p)

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](*a.u.*)	F(I,j)[c](*a.u.*)
C3-C4	σ	C2-C9	σ*	0.52	1.24	0.023
C10-C11	σ	C11-C14	σ*	5.65	1.26	0.076
C10-C11	σ	C12-C17	σ*	3.03	1.28	0.056
C1-C2	σ	C1-C4	σ*	5.58	1.29	0.076
C1-C2	σ	C2-C9	σ*	5.10	1.23	0.071
C1-C2	σ	C9-S13	σ*	7.65	0.92	0.075
C1-C2	σ	C27-C38	σ*	1.05	1.13	0.031
C1-C2	π	C3-C4	π*	18.78	0.28	0.070
C1-C2	π	C9-C10	π*	14.79	0.32	0.063
C1-C2	π	C27-C28	σ*	2.45	0.71	0.039
C1-C4	σ	C1-C27	σ*	5.63	1.14	0.072
C3-C4	σ	C1-C4	σ*	6.55	1.30	0.082
C3-C4	σ	C1-C27	σ*	7.56	1.13	0.083
C3-C4	π	C1-C2	π*	17.56	0.31	0.067
C3-C4	π	C5-C6	π*	22.73	0.31	0.076
C3-S8	σ	C2-C9	σ*	5.19	1.20	0.070
C5-C6	σ	C3-S8	σ*	7.92	0.93	0.076
C5-C6	π	C3-C4	π*	14.69	0.28	0.061
C5-C6	π	C23-C81	π*	22.48	0.32	0.076
C5-H86	σ	C6-S7	σ*	6.04	0.73	0.060
C6-H81	σ	C23-C81	σ*	5.76	1.35	0.079
C9-C10	σ	C2-S8	σ*	7.70	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.57	1.23	0.074
C9-C10	σ	C11-C14	σ*	5.10	1.29	0.073
C9-C10	π	C1-C2	π*	15.37	0.31	0.064
C9-C10	π	C11-C14	π*	18.05	0.32	0.072
C10-C27	σ	C1-C4	σ*	5.21	1.19	0.071
C10-C11	σ	C11-C12	σ*	4.05	1.22	0.063
C11-C12	σ	C10-C27	σ*	6.62	1.11	0.076
C11-C14	σ	C10-C11	σ*	6.11	1.26	0.079
C11-C14	σ	C11-C12	σ*	5.25	1.23	0.072
C11-C14	σ	C15-S18	σ*	5.52	0.92	0.064
C11-C14	π	C9-C10	π*	20.54	0.29	0.069
C11-C14	π	C12-C17	π*	19.19	0.29	0.066
C12-C17	π	C11-C14	π*	18.15	0.31	0.070
C14-C15	σ	C15-C16	σ*	5.18	1.27	0.073
C15-C16	σ	C14-C15	σ*	5.00	1.29	0.072
C16-C17	σ	C12-S13	σ*	5.56	0.91	0.064
C16-C80	σ	N67-C84	σ*	6.80	1.12	0.078
C17-H49	σ	C11-C12	σ*	5.09	1.05	0.065
C19-C20	σ	C20-C21	σ*	5.41	1.29	0.074
C19-C20	π	C21-C22	π*	16.38	0.31	0.067
C19-C20	π	C52-O53	π*	19.58	0.34	0.074
C19-C20	π	C54-C55	π*	20.02	0.32	0.072
C20-C21	σ	C21-C68	σ*	5.24	1.26	0.073
C20-C52	σ	C19-S73	σ*	5.23	0.87	0.060
C21-C22	σ	C20-C52	σ*	5.58	1.18	0.073
C21-C22	π	C19-C20	π*	16.98	0.30	0.065
C21-C22	π	C68-C71	π*	20.54	0.30	0.071

C21-C22	π	C70-C72	π*	24.66	0.30	0.077
C21-C68	σ	C20-C21	σ*	5.51	1.27	0.075
C21-C68	σ	C21-C22	σ*	5.40	1.25	0.074
C22-S73	σ	C19-C54	σ*	5.78	1.14	0.073
C23-C54	σ	C19-S73	σ*	6.77	0.88	0.069
C23-C54	σ	C23-C81	σ*	6.01	1.30	0.079
C23-C81	σ	C23-C54	σ*	6.13	1.24	0.078
C23-C81	π	C52-O53	π*	22.30	0.31	0.076
C23-C81	π	C54-C55	π*	22.51	0.30	0.074
C24-C26	σ	C24-C25	σ*	5.85	1.24	0.076
C24-C26	σ	C24-C50	σ*	5.16	1.27	0.072
C24-C50	σ	C25-C65	σ*	5.12	1.27	0.071
C24-C50	π	C25-C51	π*	18.82	0.29	0.067
C24-C50	π	C26-C63	π*	22.04	0.30	0.074
C24-C50	π	C62-C64	π*	19.89	0.30	0.070
C25-C51	σ	C51-C89	σ*	5.36	1.27	0.074
C25-C51	σ	N67-C84	σ*	5.14	1.11	0.067
C25-C51	π	C24-C50	π*	19.00	0.29	0.068
C25-C51	π	C65-C66	π*	22.11	0.30	0.074
C25-C51	π	C87-C89	π*	19.87	0.30	0.070
C25-C65	σ	C25-C51	σ*	5.19	1.27	0.072
C26-C63	π	C24-C50	π*	19.68	0.29	0.071
C26-C63	π	C62-C64	π*	22.95	0.30	0.074
C28-C30	π	C29-C31	π*	20.88	0.30	0.071
C28-C30	π	C33-C35	π*	21.77	0.30	0.073
C29-C31	π	C28-C30	π*	22.60	0.30	0.074
C29-C31	π	C33-C35	π*	21.08	0.30	0.071
C33-C35	π	C28-C30	π*	22.17	0.30	0.073
C33-C35	π	C29-C31	π*	22.69	0.30	0.074
C38-C40	π	C39-C41	π*	21.64	0.30	0.072
C38-C40	π	C43-C45	π*	21.64	0.30	0.072
C39-C41	π	C38-C40	π*	22.65	0.30	0.074
C39-C41	π	C43-C45	π*	21.38	0.30	0.072
C43-C45	π	C38-C40	π*	22.73	0.30	0.073
C43-C45	π	C39-C41	π*	22.76	0.30	0.074
C54-C55	π	C19-C20	π*	9.72	0.32	0.051
C54-C55	π	C23-C81	π*	8.41	0.34	0.048
C54-C55	π	C56-N57	π*	21.16	0.41	0.086
C54-C55	π	C58-N59	π*	20.86	0.41	0.086
C55-C56	σ	C56-N57	σ*	8.20	1.61	0.103
C55-C58	σ	C54-C55	σ*	6.23	1.33	0.081
C55-C58	σ	C58-N59	σ*	8.38	1.62	0.105
C58-N59	σ	C55-C58	σ*	8.34	1.57	0.103
C62-C64	σ	C50-N67	σ*	6.61	1.13	0.078
C62-C64	π	C24-C50	π*	22.85	0.30	0.077
C62-C64	π	C26-C63	π*	19.13	0.30	0.069
C65-C66	π	C25-C51	π*	19.72	0.29	0.071
C65-C66	π	C87-C89	π*	22.87	0.30	0.074
C68-C71	π	C21-C22	π*	16.80	0.31	0.068
C70-C72	π	C21-C22	π*	14.94	0.31	0.064

C70-C72	π	C68-C71	π*	18.35	0.32	0.068
C68-C71	π	C70-C72	π*	18.82	0.31	0.069
C70-H83	σ	C71-C72	σ*	5.53	1.05	0.068
C71-C72	σ	C68-C71	σ*	5.47	1.33	0.076
C71-C72	σ	C70-C72	σ*	5.27	1.32	0.075
C87-C89	σ	C51-N67	σ*	6.66	1.13	0.078
C87-C89	π	C25-C51	π*	22.96	0.30	0.077
C87-C89	π	C65-C66	π*	19.15	0.30	0.069
S7	LP(2)	C3-C4	π*	27.68	0.25	0.078
S7	LP(2)	C5-C6	π*	20.83	0.27	0.068
S8	LP(2)	C1-C2	π*	26.82	0.28	0.078
S8	LP(2)	C3-C4	π*	23.34	0.25	0.071
S13	LP(2)	C9-C10	π*	24.92	0.28	0.075
S13	LP(2)	C12-C17	π*	21.77	0.28	0.071
S18	LP(2)	C80-C84	π*	22.90	0.28	0.072
O53	LP(2)	C20-C52	σ*	22.14	0.74	0.116
O53	LP(2)	C23-C52	σ*	22.20	0.72	0.114
O95	LP(1)	O97-H98	σ*	6.95	1.26	0.081
N57	LP(1)	C55-C56	σ*	12.58	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.67	1.04	0.103
N67	LP(1)	S18-C84	σ*	10.30	0.46	0.067
N67	LP(1)	C24-C50	π*	33.30	0.32	0.094
N67	LP(1)	C25-C51	π*	32.95	0.32	0.094
N67	LP(1)	C80-C84	π*	12.10	0.30	0.055
S73	LP(2)	C19-C20	π*	27.05	0.28	0.079
S73	LP(2)	C21-C22	π*	23.71	0.27	0.072
O92	LP(2)	C72-S91	σ*	15.96	0.49	0.079
O92	LP(2)	S91-O93	σ*	6.72	0.66	0.060
O92	LP(2)	S91-O97	σ*	5.98	0.48	0.049
O92	LP(2)	O99-H100	σ*	6.02	0.74	0.062
O93	LP(2)	C72-S91	σ*	20.29	0.47	0.087
O93	LP(2)	S91-O92	σ*	12.17	0.62	0.078
O95	LP(2)	C71-S94	σ*	15.78	0.49	0.079
O95	LP(2)	S94-O96	σ*	6.90	0.66	0.061
O95	LP(2)	S96-O99	σ*	5.76	0.48	0.048
O96	LP(2)	O97-H98	σ*	6.17	0.74	0.063
O96	LP(2)	C71-S94	σ*	20.43	0.47	0.088
O96	LP(2)	S94-O95	σ*	12.13	0.62	0.078
O97	LP(2)	C72-S91	σ*	6.64	0.52	0.054
O97	LP(2)	S91-O92	σ*	6.08	0.66	0.058
O99	LP(2)	C71-S94	σ*	6.59	0.52	0.054
O99	LP(2)	S94-O95	σ*	6.02	0.66	0.058

Table S25: Second order Perturbation theory analysis of Fock matrix in NBO of **CC10D5** at M06/6-311G(d,p)

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)[b](*a.u.*)**	**F(I,j)[c](*a.u.*)**
C6-S7	σ	C3-C4	σ*	0.50	1.19	0.022
C1-C2	σ	C1-C4	σ*	5.58	1.28	0.076
C1-C2	σ	C1-C27	σ*	3.08	1.12	0.053

C1-C2	σ	C2-C9	σ*	5.13	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.57	0.93	0.080
C1-C2	σ	C9-S13	σ*	7.65	0.92	0.075
C1-C2	π	C3-C4	π*	18.05	0.28	0.069
C1-C2	π	C9-C10	π*	14.84	0.32	0.063
C3-C5	σ	C6-C81	σ*	4.54	1.27	0.068
C1-C4	σ	C1-C27	σ*	5.55	1.14	0.071
C1-C4	σ	C3-C4	σ*	5.58	1.25	0.075
C2-S8	σ	C2-C9	σ*	1.03	1.21	0.032
C2-S8	σ	C3-C5	σ*	4.38	1.25	0.066
C3-C4	σ	C1-C4	σ*	6.61	1.30	0.083
C3-C4	σ	C1-C27	σ*	7.53	1.14	0.083
C3-C4	π	C1-C2	π*	17.57	0.31	0.068
C3-C4	π	C5-C6	π*	21.55	0.31	0.074
C3-S8	σ	C2-C9	σ*	5.19	1.20	0.070
C5-C6	σ	C3-S8	σ*	7.82	0.93	0.076
C5-C6	π	C3-C4	π*	14.52	0.28	0.062
C5-C6	π	C23-C81	π*	19.86	0.32	0.072
C5-H86	σ	C6-S7	σ*	6.12	0.73	0.060
C6-S7	σ	C1-C4	σ*	5.13	1.24	0.071
C6-C81	σ	C23-C81	σ*	5.77	1.35	0.079
C9-C10	σ	C2-S8	σ*	7.67	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.55	1.23	0.074
C9-C10	σ	C11-C14	σ*	5.08	1.29	0.073
C9-C10	π	C1-C2	π*	14.87	0.31	0.063
C9-C10	π	C11-C14	π*	18.15	0.32	0.072
C10-C11	σ	C11-C12	σ*	4.04	1.22	0.063
C10-C11	σ	C11-C14	σ*	5.64	1.26	0.063
C10-C27	σ	C1-C4	σ*	5.21	1.19	0.071
C11-C12	σ	C10-C27	σ*	6.60	1.11	0.076
C11-C14	σ	C10-C11	σ*	6.11	1.26	0.078
C11-C14	σ	C15-S18	σ*	5.52	0.92	0.064
C11-C14	π	C9-C10	π*	20.21	0.29	0.069
C11-C14	π	C12-C17	π*	19.11	0.29	0.066
C11-C14	π	C15-C16	π*	21.58	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.60	1.18	0.073
C12-C17	π	C11-C14	π*	18.20	0.31	0.070
C12-C17	π	C15-C16	π*	19.21	0.30	0.072
C15-C16	σ	C14-C15	σ*	5.00	1.29	0.072
C15-C16	π	C11-C14	π*	22.86	0.30	0.075
C15-C16	π	C12-C17	π*	20.73	0.29	0.070
C15-C16	π	C20-C84	π*	15.12	0.29	0.061
C16-C17	σ	C15-C16	σ*	5.23	1.25	0.072
C16-C80	σ	N67-C84	σ*	6.83	1.11	0.078
C17-H49	σ	C11-C12	σ*	5.09	1.05	0.065
C19-C20	σ	C20-C21	σ*	5.37	1.29	0.074
C19-C20	π	C21-C22	π*	15.22	0.31	0.065
C19-C20	π	S2-O53	π*	20.03	0.33	0.074
C19-C20	π	C54-C55	π*	21.63	0.31	0.074
C20-C21	σ	C19-C20	σ*	5.19	1.27	0.073

C20-C21	σ	C19-C54	σ*	3.01	1.17	0.053
C20-C52	σ	C19-S73	σ*	5.14	0.87	0.060
C21-C22	σ	C20-C52	σ*	5.70	1.18	0.074
C21-C22	π	C19-C20	π*	18.41	0.29	0.066
C21-C22	π	C68-C71	π*	17.46	0.32	0.068
C21-C22	π	C70-C72	π*	20.39	0.31	0.073
C23-C54	σ	C19-S73	σ*	6.86	0.89	0.070
C23-C54	σ	C23-C81	σ*	5.95	1.31	0.079
C23-C81	σ	C6-C81	σ*	5.04	1.30	0.072
C23-C81	σ	C23-C54	σ*	6.04	1.24	0.077
C23-C81	π	C52-O53	π*	21.37	0.32	0.074
C23-C81	π	C54-C55	π*	20.74	0.30	0.072
C24-C25	σ	C24-C26	σ*	5.13	1.25	0.072
C24-C25	σ	C24-C50	σ*	3.01	1.22	0.054
C24-C25	σ	C25-C65	σ*	5.13	1.25	0.072
C24-C26	σ	C24-C25	σ*	5.85	1.25	0.076
C24-C26	σ	C24-C50	σ*	5.16	1.27	0.072
C24-C50	σ	C25-C65	σ*	5.13	1.27	0.072
C24-C50	σ	50-C62	σ*	5.39	1.27	0.074
C24-C50	σ	N67-C84	σ*	5.31	1.11	0.069
C24-C50	π	C25-C51	π*	18.85	0.29	0.067
C24-C50	π	C26-C63	π*	22.08	0.30	0.074
C24-C50	π	C62-C64	π*	19.87	0.30	0.070
C25-C51	σ	C51-C89	σ*	5.34	1.27	0.074
C25-C51	π	C24-C50	π*	19.03	0.29	0.068
C25-C51	π	C65-C66	π*	22.15	0.30	0.074
C25-C51	π	C87-C89	π*	19.85	0.30	0.070
C26-C63	π	C24-C50	π*	19.81	0.29	0.071
C26-C63	π	C62-C64	π*	22.93	0.30	0.074
C28-C30	π	C29-C31	π*	20.87	0.30	0.071
C28-C30	π	C33-C35	π*	21.82	0.30	0.073
C80-C84	π	C15-C16	π*	13.29	0.32	0.065
C81-H82	σ	C23-C54	σ*	9.05	1.00	0.085
C87-C89	σ	C51-N67	σ*	6.65	1.13	0.078
S7	LP(2)	C3-C4	π*	27.43	0.25	0.078
S7	LP(2)	C5-C6	π*	21.21	0.27	0.068
S8	LP(2)	C1-C2	π*	26.46	0.28	0.077
S8	LP(2)	C3-C4	π*	23.50	0.25	0.072
S13	LP(2)	C9-C10	π*	24.94	0.28	0.076
S13	LP(2)	C12-C17	π*	21.70	0.28	0.071
S18	LP(2)	C15-C16	π*	20.41	0.27	0.070
S18	LP(2)	C80-C84	π*	22.84	0.28	0.072
O53	LP(2)	C20-C53	σ*	21.68	0.75	0.115
O53	LP(2)	C23-C52	σ*	22.36	0.71	0.114
N57	LP(1)	C55-C56	σ*	12.55	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.68	1.04	0.103
N67	LP(1)	S18-C34	σ*	10.49	0.46	0.067
N69	LP(1)	C24-C50	π*	33.44	0.31	0.094
N67	LP(1)	C25-C51	π*	33.08	0.32	0.094
N67	LP(1)	C80-C84	π*	11.43	0.30	0.053

S73	LP(2)	C19-C20	π*	27.14	0.28	0.078
S73	LP(2)	C21-C22	π*	22.28	0.27	0.071
O92	LP(2)	C72-C91	σ*	19.45	0.71	0.107
O92	LP(2)	C91-O93	σ*	34.14	0.66	0.136
O93	LP(2)	C91-O92	π*	47.07	0.39	0.121
O95	LP(2)	C71-C94	σ*	19.33	0.71	0.107
O95	LP(2)	C94-O96	σ*	33.98	0.67	0.136
O96	LP(2)	C94-O96	π*	47.33	0.39	0.121

Table S26: Second order Perturbation theory analysis of Fock matrix in NBO **(CC10D6)** at M06/6-311G(d,p)

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)[b](*a.u.*)**	**F(I,j)[c](*a.u.*)**
C1-C2	σ	C2-C4	σ*	5.53	1.29	0.076
C1-C2	σ	C1-C27	σ*	3.03	1.12	0.052
C1-C2	σ	C2-C9	σ*	5.11	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.62	0.93	0.080
C1-C2	σ	C9-S13	σ*	7.61	0.92	0.075
C1-C2	σ	C27-C38	σ*	1.00	1.13	0.030
C1-C2	π	C3-C4	π*	18.49	0.28	0.069
C1-C2	π	C9-C10	π*	14.69	0.32	0.063
C1-C2	σ	C1-C27	σ*	5.61	1.14	0.072
C1-C4	σ	C3-C4	σ*	5.48	1.25	0.074
C3-C4	σ	C1-C4	σ*	6.50	1.30	0.082
C3-C4	σ	C1-C27	σ*	7.58	1.13	0.083
C2-S8	σ	C2-C9	σ*	24.97	1.22	0.032
C3-C4	π	C1-C2	π*	17.42	0.31	0.067
C3-C4	π	C5-C6	π*	22.76	0.31	0.076
C3-S8	σ	C2-C9	σ*	5.24	1.20	0.071
C5-C6	σ	C3-S8	σ*	7.91	0.93	0.076
C5-C6	π	C3-C4	π*	14.75	0.28	0.062
C5-C6	π	C23-C81	π*	23.11	0.32	0.077
C5-H86	σ	C6-S7	σ*	6.01	0.73	0.059
C6-S7	σ	C1-C4	σ*	5.15	1.24	0.071
C6-S7	σ	C3-C4	σ*	0.51	1.18	0.022
C6-C81	σ	C23-C81	σ*	5.89	1.35	0.080
C9-C10	σ	C2-S8	σ*	7.69	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.59	1.24	0.074
C9-C10	σ	C27-C29	σ*	1.03	1.13	0.031
C9-C10	π	C1-C2	π*	15.39	0.31	0.064
C9-C10	π	C11-C14	π*	17.99	0.32	0.072
C10-C11	σ	C11-C12	σ*	4.04	1.22	0.063
C10-C11	σ	C11-C14	σ*	5.65	1.26	0.076
C10-C11	σ	C12-C17	σ*	3.04	1.28	0.056
C10-C27	σ	C1-C4	σ*	5.24	1.19	0.071
C11-C14	σ	C10-C11	σ*	6.13	1.26	0.079
C11-C14	σ	C11-C12	σ*	5.22	1.23	0.072
C11-C14	π	C9-C10	π*	20.48	0.29	0.069
C11-C14	π	C12-C17	π*	19.18	0.29	0.066
C11-C14	π	C15-C16	π*	21.53	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.64	1.18	0.073

C12-C17	π	C11-C14	π*	18.11	0.31	0.070
C12-C17	π	C15-C16	π*	19.25	0.30	0.072
C15-C16	π	C11-C14	π*	23.07	0.30	0.075
C15-C16	π	C12-C17	π*	20.59	0.29	0.070
C15-C16	π	C80-C84	π*	15.06	0.29	0.061
C15-S18	σ	C16-C17	σ*	4.01	1.25	0.063
C16-C17	σ	C12-S13	σ*	5.55	0.91	0.063
C16-C17	σ	C15-C16	σ*	5.20	1.24	0.072
C17-H49	σ	C11-C12	σ*	5.12	1.05	0.066
C19-C20	σ	C20-C21	σ*	5.43	1.29	0.075
C19-C20	π	C21-C22	π*	16.02	0.31	0.066
C19-C20	π	C52-O53	π*	19.72	0.34	0.074
C19-C20	π	C54-C55	π*	20.25	0.32	0.072
C21-C22	π	C19-C20	π*	17.11	0.30	0.065
C21-C22	π	C68-C71	π*	19.18	0.31	0.070
C21-C22	π	C70-C72	π*	22.97	0.30	0.076
C23-C81	π	C52-O53	π*	22.32	0.31	0.076
C23-C81	π	C54-C55	π*	22.16	0.30	0.073
C24-C50	π	C25-C51	π*	18.83	0.29	0.067
C24-C50	π	C25-C63	π*	22.12	0.30	0.074
C24-C50	π	C62-C64	π*	19.90	0.30	0.070
C25-C51	π	C24-C50	π*	19.00	0.29	0.068
C25-C51	π	C65-C66	π*	22.16	0.30	0.074
C25-C51	π	C87-C89	π*	19.82	0.30	0.069
C72-C91	σ	C91-N92	σ*	8.93	1.62	0.108
C80-C84	π	C15-C16	π*	13.37	0.32	0.065
C87-C89	π	C25-C51	π*	22.97	0.30	0.077
C87-C89	π	C65-C66	π*	19.09	0.30	0.068
S7	LP(2)	C3-C4	π*	27.90	0.25	0.078
S7	LP(2)	C5-C6	π*	21.03	0.27	0.068
S8	LP(2)	C1-C2	π*	26.98	0.28	0.078
S8	LP(2)	C3-C4	π*	23.44	0.25	0.071
S13	LP(2)	C9-C10	π*	24.95	0.28	0.075
S13	LP(2)	C12-C17	π*	21.70	0.28	0.071
S18	LP(2)	C15-C16	π*	20.48	0.27	0.070
S18	LP(2)	C80-C84	π*	22.94	0.28	0.072
O53	LP(2)	C20-C52	σ*	21.97	0.74	0.116
O53	LP(2)	C23-C52	σ*	22.18	0.72	0.114
N57	LP(1)	C55-C56	σ*	12.55	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.67	1.04	0.103
N67	LP(1)	S18-C84	σ*	10.69	0.46	0.068
N67	LP(1)	C24-C50	π*	33.42	0.31	0.094
N67	LP(1)	C25-C51	π*	33.08	0.32	0.094
N67	LP(1)	C80-C84	π*	10.85	0.30	0.052
S73	LP(2)	C19-C20	π*	22.94	0.28	0.078
S73	LP(2)	C21-C22	π*	23.01	0.27	0.071
N92	LP(1)	C72-C91	σ*	12.28	1.05	0.101
N94	LP(1)	C71-C93	σ*	12.25	1.05	0.101

Table S27: Second order Perturbation theory analysis of Fock matrix in NBO **(CC10D7)** at M06/6-311G(d,p)

Donor(i)	Type	Acceptor(j)	Type	E(2)	E(J)E(i)[b](*a.u.*)	F(I,j)[c](*a.u.*)
C3-C4	σ	C2-C9	σ*	0.50	1.24	0.022
C1-C2	σ	C1-C4	σ*	5.58	1.28	0.076
C1-C2	σ	C2-C9	σ*	5.16	1.23	0.071
C1-C2	σ	C4-S7	σ*	8.52	0.93	0.080
C1-C2	σ	C9-S13	σ*	7.66	0.92	0.075
C1-C2	σ	C9-C38	σ*	1.04	1.13	0.031
C1-C2	π	C3-C4	π*	17.73	0.28	0.068
C1-C2	π	C9-C10	π*	14.95	0.32	0.063
C1-C4	σ	C1-C27	σ*	5.49	1.14	0.071
C1-C4	σ	C3-C4	σ*	5.61	1.26	0.075
C1-C27	σ	C28-C30	σ*	3.01	0.67	0.043
C2-S8	σ	C3-C5	σ*	4.36	1.25	0.066
C3-C4	σ	C1-C4	σ*	6.64	1.29	0.083
C3-C4	σ	C1-C27	σ*	7.47	1.14	0.082
C3-C4	π	C1-C2	π*	17.58	0.32	0.068
C3-C4	π	C5-C6	π*	21.00	0.31	0.074
C3-S8	σ	C2-C9	σ*	5.14	1.20	0.070
C5-C6	σ	C3-S8	σ*	7.78	0.93	0.076
C5-C6	π	C3-C4	π*	14.48	0.29	0.062
C5-C6	π	C23-C76	π*	18.74	0.32	0.070
C5-H80	σ	C6-S7	σ*	6.14	0.73	0.060
C6-S7	σ	C1-C4	σ*	5.12	1.24	0.071
C6-C76	σ	C23-C52	σ*	2.53	1.16	0.049
C6-C76	σ	C23-C76	σ*	5.73	1.35	0.079
C9-C10	σ	C11-C14	σ*	5.09	1.29	0.073
C9-C10	π	C1-C2	π*	14.63	0.31	0.063
C9-C10	π	C11-C14	π*	18.27	0.32	0.073
C10-C11	σ	C11-C14	σ*	5.62	1.26	0.075
C10-C27	σ	C1-C4	σ*	5.18	1.19	0.070
C11-C12	σ	C10-C27	σ*	6.59	1.11	0.076
C11-C14	σ	C10-C11	σ*	6.08	1.26	0.078
C11-C14	σ	C11-C12	σ*	5.22	1.23	0.072
C11-C14	σ	C15-S18	σ*	5.50	0.92	0.064
C11-C14	π	C9-C10	π*	20.01	0.29	0.069
C11-C14	π	C12-C17	π*	19.01	0.29	0.066
C11-C14	π	C15-C16	π*	21.65	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.59	1.17	0.072
C12-C17	π	C11-C14	π*	18.20	0.32	0.070
C12-C17	π	C15-C16	π*	19.10	0.30	0.072
C15-C16	π	C11-C14	π*	22.70	0.30	0.074
C15-C16	π	C12-C17	π*	20.78	0.29	0.070
C15-C16	π	C75-C78	π*	15.19	0.29	0.061
C16-C17	σ	C12-C13	σ*	5.56	0.91	0.064
C16-C75	σ	N67-C78	σ*	6.89	1.11	0.078
C19-C20	π	C21-C22	π*	16.18	0.31	0.064

C19-C20	π	C52-O53	π*	19.06	0.33	0.072
C19-C20	π	C54-C55	π*	23.65	0.31	0.077
C19-C20	π	C19-C20	π*	19.04	0.31	0.073
C21-C22	σ	C20-C52	σ*	6.34	1.21	0.079
C23-C54	σ	C19-S68	σ*	7.09	0.89	0.071
C23-C54	σ	C23-C76	σ*	5.89	1.31	0.079
C23-C76	π	C52-O53	π*	20.81	0.32	0.073
C23-C76	π	C54-C55	π*	19.88	0.30	0.071
C24-C26	σ	C24-C25	σ*	5.87	1.24	0.076
C24-C26	σ	C24-C50	σ*	5.16	1.27	0.072
C24-C50	σ	C25-C51	π*	18.91	0.29	0.067
C24-C50	π	C26-C63	π*	22.16	0.30	0.074
C24-C50	π	C62-C64	π*	19.83	0.30	0.069
C25-C51	π	C24-C50	π*	19.04	0.29	0.068
C25-C51	π	C65-C66	π*	22.22	0.30	0.074
C25-C51	π	C81-C83	π*	19.80	0.30	0.069
C25-C65	σ	C24-C25	σ*	5.85	1.24	0.076
C25-C65	σ	C25-C51	σ*	5.16	1.27	0.072
C26-C63	σ	C24-C25	σ*	5.18	1.25	0.072
C26-C63	π	C24-C50	π*	19.71	0.29	0.071
C26-C63	π	C62-C64	π*	22.91	0.30	0.074
C28-C30	π	C29-C31	π*	20.87	0.30	0.071
C28-C30	π	C33-C35	π*	21.87	0.30	0.073
C29-C31	π	C28-C30	π*	22.60	0.30	0.074
C29-C31	π	C33-C35	π*	21.11	0.30	0.071
C33-C35	π	C28-C30	π*	22.07	0.30	0.073
C33-C35	π	C29-C31	π*	22.69	0.30	0.074
C38-C40	π	C39-C41	π*	21.63	0.30	0.072
C38-C40	π	C43-C45	π*	21.72	0.30	0.073
C39-C41	π	C38-C40	π*	22.63	0.30	0.074
C39-C41	π	C43-C45	π*	21.41	0.30	0.072
C43-C45	π	C38-C40	π*	22.70	0.30	0.073
C43-C45	π	C39-C41	π*	22.80	0.30	0.074
C51-C83	σ	C25-C51	σ*	5.80	1.28	0.077
C54-C55	σ	C55-C56	σ*	5.62	1.28	0.076
C54-C55	σ	C55-C58	σ*	6.12	1.28	0.079
C54-C55	π	C56-N57	π*	22.04	0.41	0.087
C54-C55	π	C58-N59	π*	21.80	0.41	0.087
C55-C56	σ	C54-C55	σ*	5.79	1.33	0.078
C55-C56	σ	C56-N57	σ*	8.17	1.61	0.103
C58-N59	σ	C55-C58	σ*	8.23	1.58	1.102
C62-C64	σ	C50-N67	σ*	6.58	1.13	0.077
C62-C64	π	C24-C50	π*	22.88	0.30	0.077
C62-C64	π	C26-C63	π*	19.10	0.30	0.068
C65-C66	π	C25-C51	π*	19.59	0.29	0.071
C65-C66	π	C81-C83	π*	22.85	0.30	0.074
C75-C78	π	C15-C16	π*	13.13	0.32	0.065
C75-H79	σ	S18-C78	σ*	6.48	0.72	0.061
C76-H77	σ	C23-C54	σ*	9.02	1.00	0.085
C76-H77	σ	C6-S7	σ*	6.11	0.72	0.059

C81-C83	σ	C51-N67	σ*	6.63	1.13	0.078
C81-C83	π	C25-C51	π*	22.95	0.30	0.077
C81-C83	π	C65-C66	π*	19.09	0.30	0.068
S7	LP(2)	C3-C4	π*	27.33	0.25	0.077
S7	LP(2)	C5-C6	π*	21.41	0.27	0.069
S8	LP(2)	C1-C2	π*	26.20	0.28	0.077
S8	LP(2)	C3-C4	π*	23.54	0.25	0.072
S13	LP(2)	C9-C10	π*	25.07	0.28	0.076
S13	LP(2)	C12-C17	π*	21.67	0.28	0.071
S18	LP(2)	C15-C16	π*	20.45	0.27	0.070
S18	LP(2)	C75-C78	π*	22.75	0.28	0.072
O53	LP(2)	C20-C52	σ*	21.77	0.75	0.115
O53	LP(2)	C23-C52	σ*	22.62	0.71	0.115
N59	LP(1)	C55-C58	σ*	12.68	1.04	0.103
N67	LP(1)	S18-C78	σ*	10.95	0.46	0.069
N67	LP(1)	C24-C50	π*	33.57	0.31	0.095
N67	LP(1)	C25-C51	π*	33.34	0.32	0.094
S68	LP(2)	C19-C20	π*	27.60	0.27	0.078
S68	LP(2)	C21-C22	π*	23.21	0.28	0.075

Table S28: Second order Perturbation theory analysis of Fock matrix in NBO of **CC10D8** at M06/6-311G(d,p)

Donor(i)	**Type**	**Acceptor(j)**	**Type**	**E(2)**	**E(J)E(i)[b](*a.u.*)**	**F(I,j)[c](*a.u.*)**
C1-C2	π	C1-C2	π*	0.51	0.31	0.012
C1-C2	π	C3-C4	π*	17.51	0.28	0.068
C1-C2	π	C9-C10	π*	14.88	0.32	0.063
C1-C4	σ	C1-C27	σ*	5.45	1.14	0.071
C1-C27	σ	C27-C38	σ*	2.23	1.04	0.043
C1-C2	σ	C1-C4	σ*	5.51	1.28	0.075
C1-C2	σ	C1-C27	σ*	3.03	1.12	0.052
C1-C2	σ	C2-S8	σ*	0.60	0.92	0.021
C1-C2	σ	C2-C9	σ*	5.18	1.23	0.072
C1-C2	σ	C4-S7	σ*	8.57	0.93	0.080
C1-C2	σ	C9-S13	σ*	7.62	0.92	0.075
C1-C2	σ	C27-C38	σ*	1.01	1.13	0.030
C3-C4	σ	C1-C4	σ*	6.58	1.29	0.082
C3-C4	σ	C1-C27	σ*	7.56	1.13	0.083
C3-C4	π	C1-C2	π*	17.39	0.31	0.068
C3-C4	π	C5-C6	π*	21.21	0.31	0.074
C3-S8	σ	C2-C9	σ*	5.23	1.20	0.071
C5-C6	π	C3-C4	π*	14.68	0.28	0.062
C5-6	π	C23-C76	π*	19.80	0.32	0.072
C5-H80	σ	C6-S7	σ*	6.09	0.73	0.060
C6-S7	σ	C1-C4	σ*	5.15	1.23	0.071
C6-C76	σ	C23-C76	σ*	5.94	1.35	0.080
C9-C10	σ	C2-S8	σ*	7.65	0.92	0.075
C9-C10	σ	C2-C9	σ*	5.58	1.23	0.074
C9-C10	σ	C11-C14	σ*	5.11	1.29	0.073
C9-C10	π	C1-C2	π*	14.81	0.31	0.063

C9-C10	π	C11-C14	π*	18.21	0.32	0.073
C10-C11	σ	C11-C12	σ*	4.02	1.21	0.062
C10-C11	σ	C11-C14	σ*	5.64	1.26	0.075
C10-C27	σ	C1-C4	σ*	5.20	1.19	0.071
C11-C14	σ	C10-C27	σ*	6.62	1.11	0.076
C11-C14	σ	C10-C11	σ*	6.09	1.26	0.078
C11-C14	σ	C11-C12	σ*	5.21	1.23	0.072
C11-C14	π	C9-C10	π*	20.02	0.29	0.069
C11-C14	π	C12-C17	π*	19.06	0.29	0.066
C11-C14	π	C15-C16	π*	21.60	0.28	0.072
C12-S13	σ	C2-C9	σ*	5.61	1.18	0.073
C12-C17	π	C11-C14	π*	18.14	0.32	0.070
C12-C17	π	C15-C16	π*	19.14	0.30	0.072
C14-C15	σ	C15-C16	σ*	5.17	1.27	0.073
C15-C16	π	C11-C14	π*	22.73	0.30	0.074
C15-C16	π	C12-C17	π*	20.75	0.29	0.070
C15-C16	π	C75-C78	π*	15.17	0.29	0.061
C16-C17	σ	C12-S13	σ*	5.55	0.91	0.063
C16-C17	σ	C15-C16	σ*	5.24	1.25	0.072
C16-C75	σ	N67-C78	σ*	6.84	1.11	0.078
C17-H49	σ	C11-C12	σ*	5.12	1.05	0.066
C19-C20	σ	C20-C21	σ*	6.28	1.29	0.080
C19-C20	σ	C21-S89	σ*	7.71	0.94	0.076
C19-C20	π	C21-C22	π*	14.60	0.29	0.062
C19-C20	π	C52-O53	π*	19.50	0.33	0.073
C19-C20	π	C54-C55	π*	24.15	0.31	0.078
C20-C21	σ	C19-C20	σ*	5.24	1.28	0.073
C21-C22	σ	C20-C21	σ*	6.05	1.29	0.079
C21-C22	σ	C20-C52	σ*	6.67	1.19	0.080
C21-C22	π	C19-C20	π*	20.15	0.31	0.073
C21-C22	π	C85-C87	π*	15.92	0.32	0.064
C22-S68	σ	C19-C54	σ*	5.46	1.16	0.071
C23-C52	σ	C20-C21	σ*	5.07	1.21	0.070
C23-C54	σ	C19-S68	σ*	7.06	0.88	0.071
C23-C54	σ	C23-C76	σ*	5.96	1.31	0.079
C23-C76	σ	C23-C54	σ*	6.03	1.24	0.077
C23-C76	π	C52-O53	π*	21.52	0.32	0.074
C23-C76	π	C54-C55	π*	19.64	0.30	0.070
C24-C25	σ	C24-C26	σ*	5.13	1.25	0.072
C24-C26	σ	C24-C25	σ*	5.85	1.24	0.076
C24-C26	σ	C24-C50	σ*	5.15	1.27	0.072
C24-C50	π	C25-C51	π*	18.85	0.29	0.067
C24-C50	π	C26-C63	π*	22.14	0.30	0.074
C24-C50	π	C62-C64	π*	19.90	0.30	0.070
C25-C51	σ	C24-C26	σ*	5.13	1.27	0.072
C25-C51	π	C24-C50	π*	19.02	0.29	0.068
C25-C51	π	C65-C66	π*	22.18	0.30	0.074
C25-C51	π	C81-C83	π*	19.81	0.30	0.069
C26-C63	π	C24-C50	π*	19.79	0.29	0.071
C26-C63	π	C62-C64	π*	22.93	0.30	0.074

C28-C30	π	C29-C31	π*	20.90	0.30	0.071
C28-C30	π	C33-C35	π*	21.89	0.30	0.073
C29-C31	π	C28-C30	π*	22.60	0.30	0.074
C29-C31	π	C33-C35	π*	21.14	0.30	0.071
C33-C35	π	C28-C30	π*	22.10	0.30	0.073
C33-C35	π	C29-C31	π*	22.72	0.30	0.074
C38-C40	π	C39-C41	π*	21.57	0.30	0.072
C38-C40	π	C43-C45	π*	21.87	0.30	0.073
C39-C41	π	C38-C40	π*	22.79	0.30	0.074
C39-C41	π	C43-C45	π*	21.42	0.30	0.072
C43-C45	π	C38-C40	π*	22.68	0.30	0.073
C43-C45	π	C39-C41	π*	22.86	0.30	0.074
C81-C83	π	C25-C51	π*	22.94	0.30	0.077
C81-C83	π	C65-C66	π*	19.09	0.30	0.068
C85-C87	π	C21-C22	π*	15.92	0.29	0.067
S7	LP(2)	C3-C4	π*	27.51	0.25	0.078
S7	LP(2)	C5-C6	π*	21.53	0.27	0.069
S8	LP(2)	C1-C2	π*	26.50	0.28	0.077
S8	LP(2)	C3-C4	π*	23.66	0.26	0.072
S13	LP(2)	C9-C10	π*	25.06	0.28	0.076
S13	LP(2)	C12-C17	π*	21.67	0.28	0.071
S18	LP(2)	C15-C16	π*	20.37	0.27	0.070
S18	LP(2)	C75-C78	π*	22.86	0.28	0.072
O53	LP(2)	C20-C52	σ*	21.82	0.75	0.116
O53	LP(2)	C23-C52	σ*	22.38	0.71	0.115
N57	LP(1)	C55-C56	σ*	12.48	1.04	0.102
N59	LP(1)	C55-C58	σ*	12.65	1.04	0.103
N67	LP(1)	S18-C78	σ*	10.64	0.46	0.068
N67	LP(1)	C24-C50	π*	33.55	0.31	0.095
N67	LP(1)	C25-C51	π*	33.19	0.32	0.094
N67	LP(1)	C75-C78	π*	10.88	0.30	0.052
S68	LP(2)	C19-C20	π*	26.98	0.27	0.077
S68	LP(2)	C21-C22	π*	25.69	0.26	0.074
S89	LP(2)	C21-C22	π*	27.29	0.25	0.076
S89	LP(2)	C85-C87	π*	24.96	0.27	0.076

Table S29: Dipole moments, Linear polarizability and major contributing tensor (*a.u.*) of **CC10R** and **CC10D1-CC10D8**

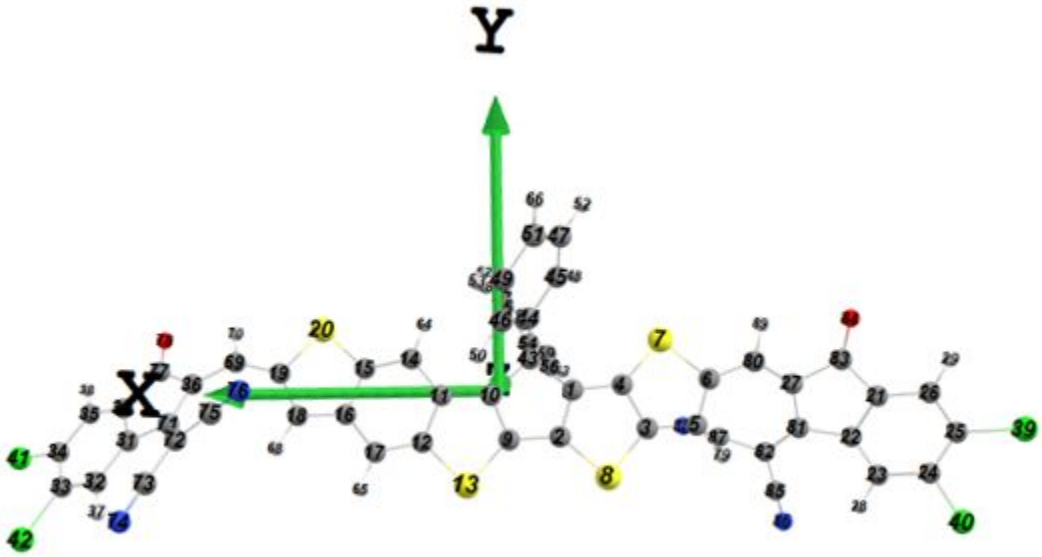
	Urea	**CC10R**	**CC10D1**	**CC10D2**	**CC10D3**	**CC10D4**	**CC10D5**	**CC10D6**	**CC10D7**	**CC10D8**
Dipole moments (in D)										
μ_x	0.000	0.266	1.334	4.422	2.625	3.955	1.186	4.700	-0.299	-0.513
μ_y	0.000	-0.650	0.447	1.395	0.815	1.177	0.476	1.440	0.188	-0.287
μ_z	0.000	-0.021	1.409	0.758	1.124	0.943	1.381	0.657	1.647	1.846
μ_{total}	**1.77**	**0.703**	**1.992**	**4.699**	**2.970**	**4.233**	**1.881**	**4.960**	**1.685**	**1.937**
Linear polarizability (in *a.u*)										
α_{xx}	38.232	2929.390	2117.600	2209.120	2090.560	2239.300	2142.840	2233.070	1741.980	1969.780
α_{yy}	39.274	1047.720	1115.160	1136.330	1103.580	1153.290	1162.160	1128.870	985.571	1078.170
α_{zz}	19.384	728.252	809.197	808.505	804.461	836.921	841.372	811.940	779.045	789.769
$\langle\alpha\rangle$	**32.296**	**2065.256**	**1199.509**	**1384.651**	**1332.867**	**1276.589**	**1181.677**	**1306.633**	**896.757**	**1090.098**

Table S30: The computed first-order hyperpolarizabilities (β_{tot}) and major contributing tensors (*a.u.*) of the studied compounds **CC10R** and **CC10D1-CC10D8**

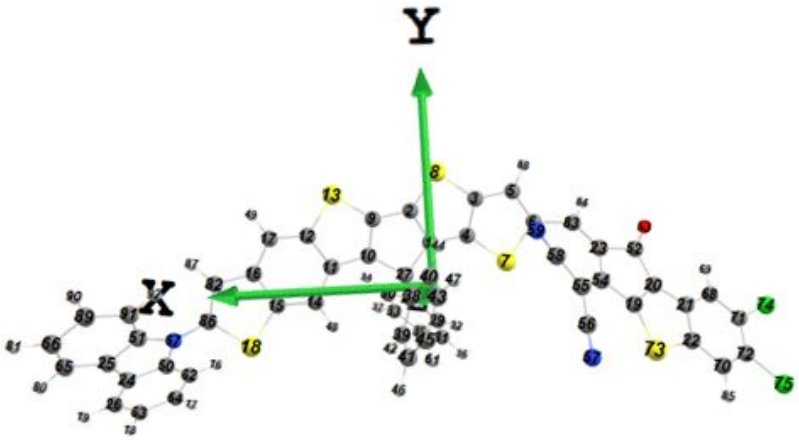
Tensors	Urea	CC10R	CC10D1	CC10D2	CC10D3	CC10D4	CC10D5	CC10D6	CC10D7	CC10D8
β_{xxx}	-0.05	-31820.60	120136.00	198324	147318.00	185596.00	131940.00	180448.00	92402.50	98284.10
β_{xxy}	-71.03	-9501.45	-3418.68	7245.43	-3342.87	-2326.52	-2434.92	6589.20	12007.50	2113.27
β_{xyy}	0.09	2748.37	-403.08	6533.57	2863.42	4897.83	2245.26	4127.74	4457.18	13.04
β_{yyy}	129.70	85.62	-1230.19	1491.06	-290.76	392.05	-527.89	940.58	1811.04	-855.33
β_{xxz}	-0.03	6538.55	17226.10	18835.00	17113.10	20072.30	16693.60	18671.30	5027.22	11661.40
β_{yyz}	-0.02	159.66	1477.40	1547.38	1144.16	1302.34	1326.24	1564.18	1935.20	1827.99
β_{xzz}	0.01	670.00	1613.43	2523.21	2052.07	2519.07	1870.62	2466.81	-485.44	204.77
β_{yzz}	17.88	-173.84	1169.09	1523.11	1345.94	1437.31	1262.54	1458.68	554.88	690.50
β_{zzz}	-0.01	121.95	380.69	273.52	315.32	320.81	94.42	369.43	-389.52	-11.34
β_{total}	**76.55**	**30743.49**	**122887.14**	**208659.3**	**153379.30**	**194229.03**	**137266.96**	**188388.61**	**97661.61**	**99438.83**

Table S31: The computed 2nd-order hyperpolarizabilities γ_{total} and major contributing tensors (*a.u.*) of the studied compounds **CC10R** and **CC10D1-CC10D8**

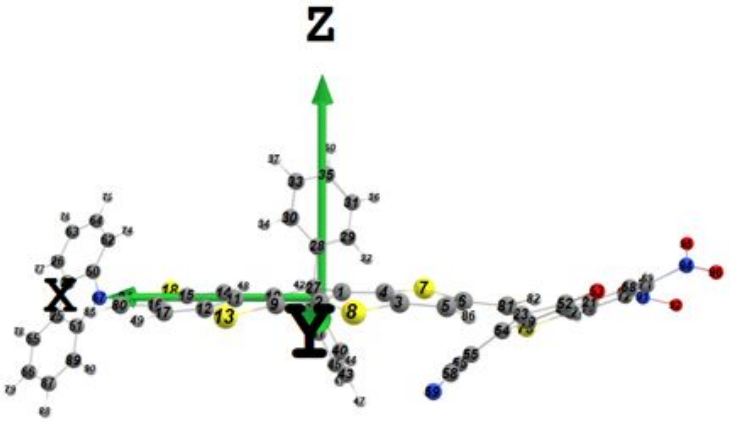
Tensors	Urea	CC10R	CC10D1	CC10D2	CC10D3	CC10D4	CC10D5	CC10D6	CC10D7	CC10D8
γ_X	1.97×10^{3}	5.78×10^{7}	2.10×10^{7}	3.37×10^{7}	2.33×10^{7}	3.00×10^{7}	2.19×10^{7}	2.96×10^{7}	1.34×10^{7}	1.67×10^{7}
γ_Y	9.80×10^{2}	3.64×10^{5}	7.95×10^{5}	1.40×10^{6}	8.43×10^{5}	1.09×10^{6}	9.15×10^{5}	1.06×10^{6}	5.71×10^{5}	6.50×10^{5}
γ_Z	1.89×10^{2}	3.37×10^{5}	3.72×10^{5}	4.15×10^{5}	3.67×10^{5}	4.14×10^{5}	3.68×10^{5}	4.12×10^{5}	1.65×10^{5}	2.54×10^{5}
$\langle\gamma\rangle$	**3.14×10^{3}**	**5.85×10^{7}**	**2.22×10^{7}**	**3.55×10^{7}**	**2.45×10^{7}**	**3.15×10^{7}**	**2.33×10^{7}**	**3.12×10^{7}**	**1.41×10^{7}**	**1.76×10^{7}**
Magnitude of γ	**2.22×10^{3}**	**5.78×10^{7}**	**2.10×10^{7}**	**3.37×10^{7}**	**2.33×10^{7}**	**3.00×10^{7}**	**2.20×10^{7}**	**2.97×10^{7}**	**1.34×10^{7}**	**1.67×10^{7}**



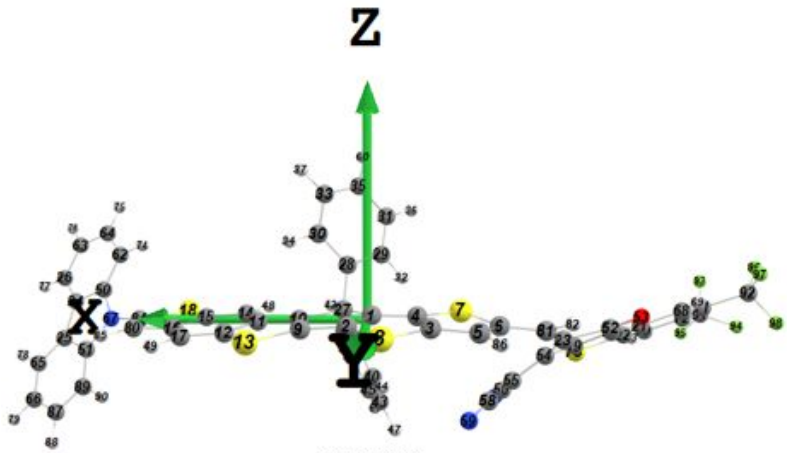
CC10R



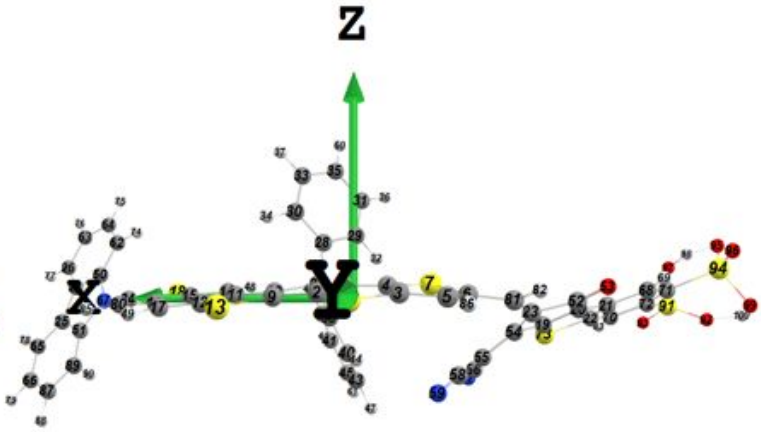
CC10D1



CC10D2



CC10D3



CC10D4

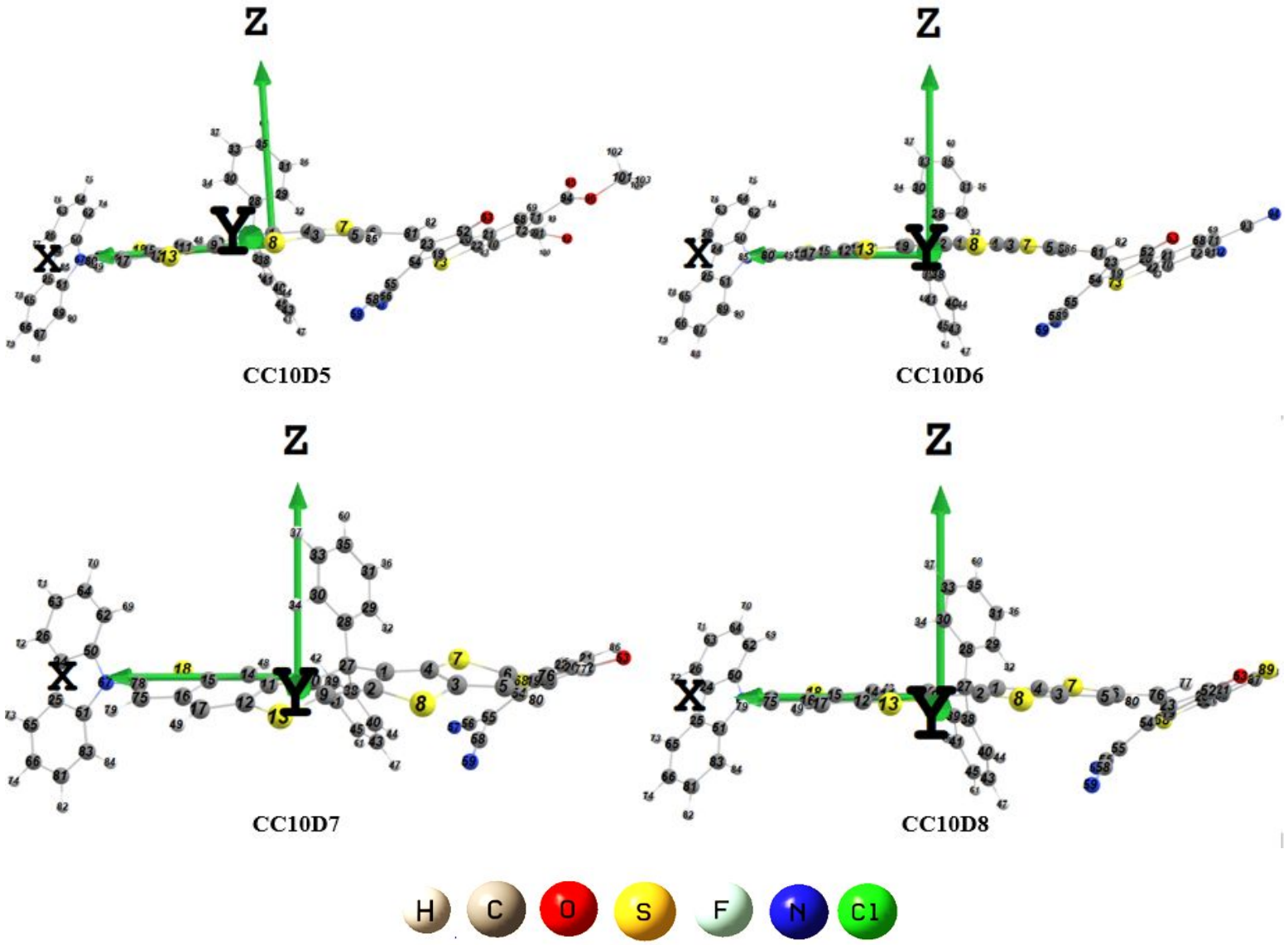


Figure S1: The optimized structures of studied compounds (**CC10R** and **CC10D1-CC10D8**)

IUPAC names

The acceptor (2-(5,6-dichloro-2-methylene-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile) from **CC10R** is replaced with donor moiety (9H-Carbazole) and we structurally modified (2-(2-methylene-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile) acceptor moiety of **CC10R** by introducing different electron withdrawing groups. Therefore, IUPAC names and abbreviations of acceptors in newly designed compounds are discussed as: 2-(2-methylene-6,7-dinitro-1-oxo-1,2-dihydro-3H-benzo[b]cyclopenta[d]thiophen-3-ylidene)malononitrile (**MDC**), 2-(2-methylene-1-oxo-6,7-bis(trifluoromethyl)-1,2-dihydro-3H-benzo[b]cyclopenta [d]thiophen-3-ylidene) malononitrile (**MCT**), 3-(dicyanomethylene)-2-

methylene-1-oxo-2,3-dihydro-1H-benzo[b]cyclopenta[d]thiophene-6,7-disulfonic acid (**DOD**), 2-(6,7-dimethyl-2-methylene-1-oxo-1,2-dihydro-3H-benzo[b]cyclopenta[d]thiophen-3-ylidene)malononitrile--carbon(IV) oxide (1/2) (**DMO**), 3-(dicyanomethylene)-2-methylene-1-oxo-2,3-dihydro-1H-benzo[b]cyclopenta[d]thiophene-6,7-dicarbonitrile (**MOD**), 2-(5-methylene-4-oxo-4,5-dihydro-6H-cyclopenta[b]thiophen-6-ylidene)malononitrile (**MCM**), 2-(6-methylene-7-oxo-6,7-dihydro-5H-cyclopenta[b]thieno[2,3-d]thiophen-5-ylidene)malononitrile (**MOC**).