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Linear and nonlinear optical properties of bis-TTF-Ge: Theoretical investigation

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Dalila Kamli[1,2], Douniazed Hannachi[1,3], Djamila Samsar[4], Henry Chermette[5]

[1]Laboratoire d'Electrochimie, d'Ingénierie Moléculaire et de Catalyse Redox (LEIMCR), Département d'Enseignement de Base en Technologie, Faculté de Technologie, Université Ferhat Abbas, Sétif-1, Algérie.

[2]Département des sciences de la matière, Faculté des Sciences, Université de khenchela, Algérie.

[3]Département de Chimie, Faculté des Sciences, Université Ferhat Abbas, Setif-1, Algérie.

[4]Institut D'Hygiène et Sécurité Industrielle, Département de Socle commun Hygiène et Sécurité Industrielle, Université de Batna-2, Algérie.

[5]Université de Lyon, Université Claude Bernard Lyon 1, Institut des Sciences Analytiques, UMR CNRS 5280, 69622 Villeurbanne Cedex, France.

E-mail: douniazed_hannachi@univ-setif.dz *(D.H.)*; *henry.chermette@univ-lyon1.fr (H.C.)*

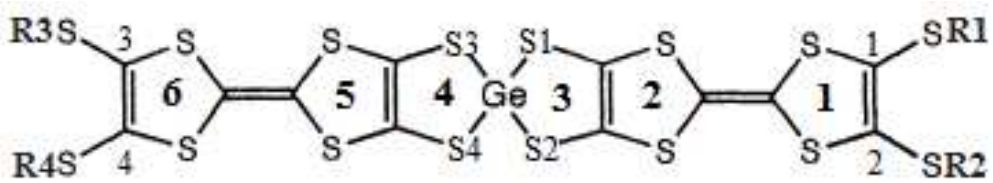

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Table S1. Vertical transition energy ($\Delta E_{0\to n}$, eV) and wavelength ($\Delta\lambda_{0\to n}$, nm), oscillator strengths ($f_{0\to n}$, dimensionless), charge transfer (q^{CT}), charge transfer distance (d^{CT}, Å) dipole moment variation ($\Delta\mu_{0\to n}$, D) and Sr index associated to the S0 → Sn transition, as calculated at the CAM-B3LYP/6-311g(d,p) of the studied **bis-TTF-Ge** compounds T0 to T36

Ti	Sn	E(eV)	λ(nm)	f	q^{ct}	d^{ct}	Sr	μ^{ct}	Transition	character
T0	S1	3.096	400	0.003	0.821	0.035	0.725	0.136	182→183 (65%)	CT from rings 1,2,5 and 6 to 4S+Ge
	S7	4.030	308	0.210	0.524	0.052	0.973	0.131	181 → 191(15%); 180 → 185(15%)	ICT in rings 1,2,5,and 6
	S11	4.249	291	0.209	0.651	0.045	0.827	0.145	180 → 183 (27%)	CT from rings 1,2,5 and 6 to 4S+Ge
	S17	4.649	267	1.030	0.493	0.037	0.979	0.089	182 → 193 (24%)	IC in rings 1,2,5,and 6
T1	S1	1.706	727	0.001	0.891	8.636	0.141	36.946	187→190(32%);185→190 (30%)	CT: from rings 1-3 to NO
	S7	3.218	385	0.079	0.707	9.586	0.571	32.559	189→190 (H→L) : (29%)	CT: from rings 1, 2, 5 and 6 to NO
	S10	4.034	307	0.207	0.534	1.278	0.966	3.255	186→193 (12%);188→193 (12%)	ICT: in rings 4-6
	S24	4.647	26	1.137	0.497	0.172	0.979	0.409	189→201(22%),188→199(18%)	ICT: in rings 1,2,5 and 6
	S2	3.043	407						189 -> 190 (33%) 188→190(20%)	
T2	S1	1.824	680	<0.001	0.829	8.451	0.231	33.661	195→197 (23%) 193→197(23%)	CT:1,2 to NO (at R1 and R2)
	S2	1.947	637	<0.001	0.804	8.564	0.234	33.090	193→198(22%),190→197(22%)	CT:rings1-3 to NO (R1,R2), ICT in 1-3
	S3	2.719	456	0.046	0.803	5.853	0.308	22.567	195→199 (74%)	CT: from rings 1-2 to NO (R1,R2)
	S16	4.036	307	0.126	0.618	6.649	0.674	19.741	194→203 (15%), 196→208(15%)	ICT: in rings1,2; CT: rings 6-5 to 1,2
	S18	4.088	303	0.114	0.559	0.710	0.965	1.905	195→ 202(10%), 196→204 (10%)	CT: from ring to NO and ICT in TTF rings
	S13	3.892	318	<0.001	0.999	16.977	0.000	81.427	196→197 H→L (98%)	CT: from rings 6-5 to NO (at R1, R2)
	S32	4.654	266	1.050	0.540	5.852	0.780	15.183	196→210(20%), 196→208(19%)	ICT: in rings 6,5
T3	S1	1.896	654	0.001	0.888	11.586	0.142	49.439	196→198 (18%)	CT: rings 6-5 to NO (at R3)
	S4	2.968	418	0.001	0.841	9.184	0.393	37.014	195→197(50%),196→197(H→L) (10%)	CT: rings 1-2 to NO (at R1) & 6-5 to NO (R1)
	S13	3.999	310	0.162	0.508	2.906	0.934	7.095	196→209(13%),194→203(13%)	ICT in TTF rings (1-6)
	S23	4.239	292	0.131	0.505	0.511	0.990	2.588	194 -> 199(15%)	CT from TTF to NO and 4S-Ge
	S29	4.620	268	0.804	0.486	1.481	0.961	3.454	195→207(20%),196→209(21%)	ICT and CT 1,2 to 6,5 and 6,5 to 1,2
	S46	5.098	243	0.126	0.518	0.383	0.996	0.951	194→203 (10%), 195→211(10%)	IC in TTF rings
T4	S1	1.833	676	<0.001	0.820	8.208	0.263	32.284	202→204 (25%)	CT:rings1,2 to 2NO
	S4	2.724	455	0.046	0.803	5.830	0.319	22.477	202→207 (72%)	CT:ring1,2 to 2 S-NO(R1+2)
	S17	3.921	316	<0.001	0.997	17.038	0.000	81.612	203→204(H→L) (98%)	CT: from rings 6,5 to NO (at R1+R2)
	S20	4.010	309	0.125	0.576	6.199	0.715	17.151	201→211(13%), 203→216 (13%)	CT:from rings1,2, R1+R2to ring5,6, 4S-Ge;R3

	S22 S33 S38	4.088 4.283 4.626	303 290 268	0.130 0.132 0.677	0.578 0.608 0.524	5.054 1.056 2.759	0.897 0.983 0.872	14.022 3.085 6.941	203 -> 213 (12%) 201→208(18%);201→206 (7%) 203→216 (22%),201→209 (12%)	CT from TTF to NO(R1,R2) and 4S-Ge CT: from ring 4-6 to NO(at R3) and 4S-Ge IC in rings 6-5 and 1-2
T5	S1 S3 S5 S11 S41 S47	1.831 1.945 2.725 3.096 4.297 4.677	677 637 455 400 289 265	<0.001 <0.001 0.046 0.003 0.202 1.521	0.805 0.775 0.794 0.809 0.567 0.462	6.489 2.195 1.452 0.207 0.132 0.106	0.900 0.925 0.935 0.720 0.943 0.988	25.050 8.166 5.526 0.803 0.359 0.236	208→2115(12.5%),210→211(H-L)(12.5%) 207→214(11%), 205→214(11%) 209→216(23%);210→215(22%) 210→217 (67%) 208→217(24%);209→225(12%) 209→226(23%);210→227(25%)	CT: from rings 1, 2,5,6 to NO groups CT: from rings 1, 2,5,6 to NO groups CT: from rings 1-2, 5-6 to NO (at R1-R4) CT: from rings 1-2,5-6 to 4S-Ge CT from ring1,2,,5 and 6 to 4S-Ge ICT in TTF rings

Ti	Sn	E(eV)	λ(nm)	F	q^{ct}	d^{ct}	Sr	μ^{ct}	Transition	character
T6	S1 S7 S10 S18 S29	3.070 4.003 4.141 4.658 5.122	404 307 292 266 240	0.003 0.167 0.141 0.628 0.145	0.872 0.631 0.705 0.582 0.573	6.729 7.18 6.049 6.743 5.910	0.375 0.628 0.636 0.637 0.766	28.067 21.766 20.478 18.866 16.212	188→189 (H→L) 68% 186→192 (20%) 186→189(15%),188→197(14%) 188→200(42%),186→192(10%) 187 → 197 (13%)	CT: rings 6, 5 to 4S-Ge CT:ring65 to 1,2 CT: ring 6,5,4 to 4S-Ge ICT in rings 6,5 ICT in rings
T7	S1 S7 S12 S16 S19 S22	3.051 4.028 4.260 4.489 4.662 4.815	406 308 291 276 266 258	0.002 0.163 0.174 0.234 0.488 0.360	0.871 0.623 0.618 0.639	6.634 5.961 1.550 2.380	0.351 0.663 0.847 0.904	27.747 17.829 4.597 7.298	194→195(H→L)(68%) 194→ 207(22%), 194→198(22%) 193→201(25%),193→206(24%) 193→199 (32%) 194→207 (33%) 193→203(26%),193→209(14%)	CT rings 6,5 to 4S-Ge ICT (in rings 6,5)+TC ring6-5 to 4S-Ge ICT in ring 1,2 3 and S-CN (at R1, R2) CT ring 1, 2 to S-CN (at R1, R2) ICT (in rings 6,5) ICT in TTF rings
T8	S1 S7 S11 S17 S19 S26	3.132 4.074 4.279 4.530 4.701 5.098	396 304 290 274 263 243	0.004 0.429 0.192 0.168 0.518 0.186	0.792 0.513 0.618 0.567 0.512	1.963 0.320 0.890 0.675 1.067	0.752 0.969 0.959 0.955 0.942	7.467 0.784 2.630 1.834 2.606	194→195 (H→L) (50%) 193→204(10%) 194→201(35%) 193→203 (35%) 194→205(25%) 193→201 (15%)	CT rings 6,5 to 4S-Ge CT ring 1,2 to Ge and CN (at R4) ICT in rings 6 and 5+ CT 6,5 to CN (at R4) IC in rings 1 and 2 + CT 1,2 to CN (at R1) IC in rings 6 and 5+ CT 6,5 to CN (at R4) CT from rings 1,2 to Ge+4,5, CN (at R4)
T9	S1 S5 S8 S12 S16	3.107 3.421 4.078 4.304 4.478	398 362 304 288 277	0.003 0.042 0.151 0.178 0.191	0.680 0.781 0.570 0.593 0.658	1.086 4.721 4.392 3.380 2.517	0.862 0.505 0.744 0.900 0.878	3.546 17.702 11.908 9.545 7.910	200→201(H→L) 84% 199 → 202 87% 200 → 212 (10%) 200→209 (20%) 197→201(28%),199→207 (17%)	CT from rings 5 and 6 to 4S-Ge CT+ICT: rings 1-2 to ring1&SCN(R1,R2) ICT in 6,5 and CT 6,5 to 1,2 CT from rings 6, 5 to 4S-Ge CT from 1-3 to CN (at R1, R2) and 4S-Ge

	S22	4.813	258	0.360	0.617	3.296	0.692	9.754	199→203 (20%)	ICT in rings 1-3
T10	S1 S3 S6 S13 S15 S22 S32	3.086 3.141 3.414 4.305 4.451 4.794 5.135	402 395 363 288 279 259 241	0.005 0.005 0.043 0.204 0.198 0.797 0.129	0.747 0.796 0.803 0.594 0.617 0.540 0.563	6.418 4.524 2.122 4.507 0.416 1.437 3.650	0.627 0.700 0.718 0845 0.952 0.926 0.891	23.035 17.24 8.182 12.859 1.234 3.725 9.870	206 → 210 (42%) 206→207 (H→L) 65% 205 → 208 (70%) 206→215 (20%) 204→207 (39%) 206→219 (13%) 206 → 208 (17%)	ICT in TTF rings CT from rings 5, 6 to 4S-G CT from ring 1-3 to C-S-COCN (R1,R2) CT from rings R6-R5 to 4S- Ge CT from TTF rings and to 4S- Ge IC in rings 6 and 5 CT rings 6,5 to C-S-COCN (at R1,R2) and C3-C4
T11	S1 S8 S13 S19 S20 S33	3.076 4.032 4.238 4.537 4.653 5.136	403 308 293 273 266 241	0.003 0.188 0.141 <0.001 0.919 0.186	0.861 0.530 0.601 0.993 0.505 0.588	6.645 3.260 4.082 17.300 1.946 2.846	0.388 0.922 0.917 0.000 0.950 0.802	27.478 8.295 11.783 82.506 4.718 8.024	195→197 (H→L) 65% 195→207(20%),193→200(18%) 193 -> 197 (23%) 195 → 196 (98%) 195-207(26%),194→205(9%) 194 → 208 (16%)	CT from 6 and 5 to 4S and Ge IC in rings 6 and 5 TC from ring 6,5 to 4S-Ge CT from 6 and 5 to COCN IC in rings 6 and 5 CT from rings 1 and 2 to COCN
T12	S1 S9 S14 S20 S31 s45	2.231 3.287 4.008 4.200 4.579 5.059	556 377 309 295 271 245	0.001 <0.001 0.182 0.205 0.394 0.190	0.675 0.998 0.660 0.708 0.622 0.560	1.966 17.102 7.786 7.483 0.991 5.439	0.662 0.000 0.719 0.590 0.856 0.791	6.372 81.95 24.679 25.392 2.958 14.630	206→215 (72%) 214 → 215 (H→L) 98% 118 ->216 (25%) 212→217 (32%) 211→217 (20%) 209 → 218 (25%)	IC in COCN group (at R1) CT from 6 and 5 rings to one COCN CT from ring 6,5 to ring 1, 2 and 4s-Ge CT from rings 6, 5,4 too 4S and Ge CT from rings 1,2,3 too 4S and Ge IC in COCN groups
T13	S1 S3 S6 S9 S17 S21	3.087 3.117 3.457 4.043 4.309 4.670	402 398 359 307 288 266	0.003 0.005 0.194 0.142 0.764 0.140	0.661 0.803 0.900 0.508 0.575 0.517	4.701 3.582 1.938 1.880 1.699 3.009	0.844 0.863 0.843 0.936 0.968 0.909	14.923 13.774 8.374 4.585 4.684 7.466	208→215(27%) 207→210 (63%) 207→220(35%),208→209(22%) 207→219 (24%) 208→221(22%);208→219(21%) 207→ 225(22%),206 → 215(13%)	CT in rings TTF CT from rings 5-6 to 4S-Ge CT from rings to COCN groups IC in rings CT from rings to 4S-Ge group IC in rings
T14	S1 S6 S9 S10 S19 S25	3.097 3.314 3.790 4.093 4.334 4.668	400 374 327 303 286 266	0.014 0.060 0.100 0.205 0.092 0.650	0.713 0.900 0.752 0.656 0.771 0.558	4.044 6.832 4.598 6.139 14.080 5.550	0.791 0.268 0.697 0.632 0.285 0.853	13.843 29.524 16.609 19.899 52.145 14.876	220→226(32%), 220→228(30%) 221→223 (79%) 220 -> 225 (42%) 221→230 (17%) 221 → 222 (H→L) 52% 221→236 (11%)	CT from ring1-3 to S-COCN (at R1,R2) CT from rings 4-6 to S-COCN (at R3) CT from ring1-3 to S-COCN (at R1,R2) IC in rings 6 and 5 CT from ring 6, 5 to S-COCN (at R1) IC in rings
T15	S1 S8 S11	3.098 3.528 4.133	400 351 300	0.015 0.041 0.197	0.722 0.912 0.567	2.246 6.937 1.482	0.739 0.248 0.901	7.784 30.399 4.037	234→235(H→L)32% 233 →237 (76%) 231→242 (16%)	CT from rings 1-3 to S-COCN (at R1,R2) CT from rings 4-6 to COCN (at R3) IC in rings 1, 2

	S28 S45	4.649 5.134	267 241	0.506 0183	0.602	2.818	0.758	8.147	233→246(30%),233→247(10%) 234 → 250 (10%)	IC IC
T16	S1 S7 S11 S18	3.082 4.020 4.246 4.644	402 308 292 267	0.003 0.221 0.179 1.066	0.858 0.610 0.665 0.519	6.540 3.628 5.202 1.651	0.400 0.823 0.800 0.963	26.862 10.635 16.581 4.120	189→190 (H→L) 65% 186→191 22% 187→190 (H-2→L) 28% 189→201(17%), 186→191(16%)	CT from ring 6, 5 to 4S-Ge IC in rings 1 and 2 CT from rings 1, 2 to 4S-Ge IC in rings
T17	S1 S7 S11 S19 S33	3.065 4.032 4.230 4.652 5.169	404 307 293 267 240	0.003 0.173 0.114 0.942 0.135	0.869 0.650 0.657 0.533 0.622	6.778 8.709 5.953 5.845 2.281	0.389 0.551 0.813 0.826 0.751	28.212 27.195 18.754 14.951 6.812	196→197 (H→L) 67% 196→209(20%), 194→201(12%) 194→197 (H-2→L) 34% 193→199 (20%)	CT from rings 6, 5 to 4s Ge IC in rings 6, 5 CT from rings 6,5 to 4s Ge IC in rings 6, 5
T18	S1 S7 S11 S19 S32	3.119 4.018 4.275 4.641 5.167	398 309 290 267 240	0.003 0.295 0.218 1.040 0.113	0.8004 0.558 0.639 0.536 0.549	1.281 0.723 0.862 0.250 0.656	0.739 0.963 0.946 0.968 0.941	4.946 1.945 2.647 0.643 1.729	196→197 (H→L)52% 194→199(14%),193→198(12%) 194→197(22%), 195→205(21%) 196→209 (17%) 196→214 (12%)	CT from rings 1,2,5,6 to 4s-Ge IC in rings 1,2,3,4,5,6 CT from rings 1,2,5,6 to 4s-Ge IC in rings 1,2,5,6 IC in rings 1,2,5,6
T19	S1 S8 S12 S20	3.117 4.091 4.285 4.651	398 303 289 267	0.004 0.172 0.194 0.779	0.831 0.669 0.596 0.572	5.726 5.704 2.085 3.518	0.537 0.670 0.965 0.871	22.867 18.314 5.959 9.611	203→204 (H→L) 65% 202→208 (23%) 203→212 (23%) 203→216 (24%)	CT from rings 6,5 to 4S-Ge CT from rings 1-3 to 4-6 Mixing IC in ring1+CT ring6,5 to 4S-Ge IC in rings 6 and 5
T20	S1 S7 S13 S21	3.125 4.074 4.316 4.666	397 304 278 266	0.004 0.386 0.247 0.928	0.786 0.581 0.593 0.527	3.243 0.315 0.270 0.041	0.805 0.942 0.973 0.972	4.816 0.879 0.769 0.104	210→211 (H→L) 56% 210→216 22% 210→220(14%), 208→211(14%) 210→225, 207→214 (22%)	CT from ring 6 and 5 to 4S-Ge CT from ring 6 and 5 to CHO groups CT from rings to 4S-Ge IC in rings

Ti	**Sn**	**E(eV)**	**λ(nm)**	**f**	**q^{ct}**	**d^{ct}**	**Sr**	**μ^{ct}**	**Transition**	**character**
T21	S1 S9 S12 S14 S21	2.854 4.035 4.092 4.207 4.653	434 307 303 295 266	0.083 0.145 0.125 <0.001 1.028	0.831 0.617 0.559 0.999 0.525	5.372 0.729 4.421 15.939 4.526	0.369 0.614 0.831 0.000 0.876	21.438 21.516 11.856 76.256 11.361	192→194 (87%) 193→205 (21%) 190→197 (22%) 193→194 (H→L) 98% 193→205(23%), 192→203 (8%)	CT from rings 1,2 to SNO_2 IC in rings 6 and 5 CT from rings 1,2 to SNO_2+CT Ring1,2 to ring6,5 CT from rings 6, 5 to SNO_2 group ICT in rings

T22	S1 S2 S6 S11 S12 S18 S23 S25	2.239 3.059 3.421 3.971 4.031 4.234 4.505 4.658	554 405 362 312 308 293 275 266	0.034 0.003 <0.001 0.113 0.127 0.171 0.116 0.907	0.830 0.869 0.969 0.883 0.610 0.666 0.613 0.532	5.647 6.583 15.746 6.229 5.523 6.057 3.561 5.594	0.251 0.349 0.000 0.283 0.699 0.803 0.872 0.738	22.492 27.489 73.084 26.408 16.182 19.384 10.485 5.620	203→205 (92%) 204→206(67%), 202→206(22%) 204 →205 (H→L) 95% 203→207 (54%) 204→218(23%),202→211(17%) 202→206(28%); 204→206(20%) 201→206 (39%) 204→218(35%), 202→211(11%)	CT from rings 1,2 to two NO_2 groups CT from 5-6 to 4S-Ge CT from rings 4-6 to two NO_2 groups CT from rings 1,2 to two NO_2 groups ICT in rings 5-6 CT from 5-6 to 4S-Ge CT from 1-2 to 4S-Ge ICT in rings 5-6 ICT in rings 1 and 2
T23	S1 S13 S19 S25 S34	2.867 4.084 4.316 4.666 4.990	432 304 287 266 248	0.123 0.312 0.261 1.139 0.211	0.829 0.522 0.604 0.920 0.570	3.650 0.578 0.426 0.332 0.611	0.885 0.969 0.856 0.970 0.959	14.512 1.446 1.228 0.782 1.671	204→205 (H→L) 34% 204→212(10%), 203→215(10%) 202→207 (20%) 204→217(20%),203→216(11%) 199→205 (16%)	CT from rings 1,2,5,6 to NO_2(at R1 and R4) ICT in rings 1,2,5,6 CT from rings 1,2,3,4,5,6, to 4S-Ge ICT in rings 1,2,5,6 CT from rings 6, 5 to NO_2 (at R1 and R4)
T24	S1 S2 S8 S13 S15 S28 S49	2.262 2.869 3.603 3.993 4.085 4.669 5.163	548 432 344 310 304 266 240	0.034 0.086 <0.001 0.121 0.171 1.171 0.117	0.832 0.828 0.999 0.875 0.627 0.535 0.607	5.627 5.318 15.685 6.053 6.106 5.627 4086	0.257 0.356 0.000 0.383 0.664 0.797 0.763	22.476 21.022 75.300 25.439 18.376 14.462 11.923	214→216 (92%) 215→217 (89 %) 215→216 (H→L) 98% 214→219 (54%) 215→225 (17%) 215→229 (17%) 212→ 223 (32%)	CT from rings 2-3 to NO_2 (at R1, R2) CT from rings 4-6 to NO_2 (at R3) CT from rings 4-6 to NO_2 (at R1, R2) CT from rings 2-3 to NO_2 (at R1, R2) ICT in rings 4, 5 and 6 ICT in rings 1,2 and 3 ICT in rings 1, 2 and 3
T25	S1 S2 S3 S9 S19 S29 S31	2.366 2.366 3.150 3.811 4.148 4.488 4.662	524 524 394 325 299 276 266	0.036 0.036 0.005 <0.001 0.337 0.124 0.790	0.838 0.838 0.787 0.916 0.582 0.603 0.555	7.662 7.626 0.129 13.204 0.718 0.321 2.508	0.529 0.550 0.757 0.143 0.931 0.836 0.954	30.850 30.538 0.487 58.126 2.004 0.928 6.658	225→227 (79%) 226 -> 222 (79%) 225→229 (37%), 226→229 (37%) 226→227 (H→L) 84% 225→238 (15%) 224 → 229 (40%) 215→228(12%); 216→227(12%)	CT from rings 2-3 to C-S-NO_2(R1, R2) CT from rings 5-6 to C-S-NO_2(R3, R4) CT from rings 1-2 and 5-6 to 4S-Ge CT from rings 5, 6 to C-S-NO_2(R1, R2) CT from rings 1-3 to 4-6 +ICT in rings 1-3 CT from rings to 4S-Ge CT from rings 2-3 and 5-6 to C-S-NO_2 (at R3 and R4) and ICT in rings1 and 6
T26	S1 S7 S12 S17 S52	3.083 4.030 4.239 4.623 5.795	402 308 293 268 214	0.003 0.332 0.169 0.870 0.028	0.857 0.536 0.659 0.544	6.448 4.420 4.690 6.905	0.454 0.907 0.811 0.754	26.428 11.286 14.780 17.888	186→187 (H→L) 63% 186→195 (16%) 184→187 (27%) 186→195 (16%) 183→192 (28%)	CT from rings 1, 2 to 4s-Ge Mixing IC in ring1,2, CT 1-3 To 4-6 CT from rings 1,2 to 4S-Ge Mixing: IC in rings 1,2; CT from 1, 2 to 6,5 IC in rings 6,5
T27	S1 S7 S11 S17	3.020 3.993 4.173 4.612	411 311 297 269	0.002 0.135 0.123 0.503	0.877 0.744 0.675 0.629	6.741 8.137 7.065 7.423	0.349 0.466 0.608 0.602	28.401 29.066 22.913 22.439	190→191 (H→L) 67% 190→193 (16%) 188→191 (25%)	CT from rings 1,2 to 4S-Ge CT from rings 1-3 to 4-6 CT from rings 1,2 to 4S-Ge Mixing:CT from rings 1,2 to 6,5+IC in 1,2

	S54	5.794	214	0.047					190→201 (26%) 180 →196 (10%)	IC in rings 6,5
T28	S1 S7 S17 S54	3.050 4.031 4.605 5.821	406 308 269 213	0.002 0.246 0.652 0.038	0.852 0.609 0.515	6.211 5.032 3.235	0.468 0.848 0.881	25.416 14.727 8.004	190→191 (H→L) 65% 190→192 (19%) 190→202 (20%) 180→193 (6%)	CT from rings 1-2, to 4S-Ge CT from rings 1-2 to 4S-Ge IC in rings 1,2 IC
T29	S1 S7 S8 S17 S51	3.026 4.002 4.045 4.611 5.687	410 309 307 269 218	0.002 0.151 0.165 0.723 0.029	0.874 0.738 0.573 0.509	6.746 8.838 6.394 3.931	0.373 0.461 0.699 0.891	28.277 31.299 17.853 9.598	194→195 (H→L) 67% 194→196 (19%) 193→204 (18%) 194→206 (20%) 188→195 (19%)	CT from rings 1,2 to 4S-Ge CT from rings 1,2 to 4S-Ge + 6, 5 rings IC in rings 6, 5 IC in rings 1; 2 IC
T30	S1 S7 S8 S19 S51	3.039 4.016 4.068 4.681 5.687	408 309 308 264 218	0.002 0.146 0.163 0.555 0.022	0.873 0.734 0.671 0.573	6.537 6.854 6.826 6.783	0.356 0.530 0.640 0.644	27.177 24.012 21.888 18.660	198→199 (H→L) 65% 198 -> 201 (27%) 197→201 (30%) 197→208 (30%) 188→ 204 (39%)	CT from rings 1-2 to 4S-Ge CT from rings 1-2 to 4S-Ge CT from rings 1,2 to 4S-Ge IC in rings 1, 2 IC

Ti	**Sn**	**E(eV)**	**λ(nm)**	**f**	**q^{ct}**	**d^{ct}**	**Sr**	**μ^{ct}**	**Transition**	**Character**
T31	S1	3.081	402	0.003	0.870	6.972	0.367	29.120	194→ 195 (H→L) 62%	CT from rings 1, 2 to 4S-Ge IC in rings 1 and 2 CT from rings 1-3 to 4-6 IC in rings 1,2 + CT: from rings 1,2 to 5, 6 IC
	S5 S7 S18 S53	3.855 4.023 4.616 5.788	321 308 268 214	0.068 0.319 0.720 0.038	0.599 0.593 0.551	1.022 7.924 8.192	0.788 0.639 0.654	2.942 22.565 21.668	194 → 199 (40%) 194 →203 (20%) 194→205 (15%) 184→200 (19%)	
T32	S1 S7 S19 S57	3.027 3.998 4.663 5.794	410 310 266 214	0.002 0.201 0.755 0.064	0.893 0.749 0.543	7.276 9.054 4.419	0.308 0.405 0.873	31.218 32.562 11.515	206→207 (H→L) 65% 206→209(16%), 206→208(16% 205→216(19%), 205→215(19% 195→211 (20%)	CT from rings 1,2 to 4S-Ge CT from rings 1-3 to 4-6 IC in rings 6, 5 IC in rings 6, 5
T33	S1 S7 S19 S51	3.089 4.021 4.614 5.711	401 308 269 217	0.003 0.420 0.777 0.227	0.843 0.522 0.492	4.628 3.447 1.358	0.657 0.943 0.969	18.658 8.593 3.195	206→207 (H→L) 65% 205→215 (20%) 206→217 (14%) 196→ 210 (13%)	CT from rings 1,2 to 4S-Ge CT from rings 1-3 to 4-6 IC in rings 1,2 + CT from rings 1,2 to 5.6 IC

T34	S1 S7 S19 S55	3.026 3.981 4.618 5.706	410 311 268 217	0.003 0.219 0.839 0.143	0.896 0.689 0.524	7.178 8.247 6.620	0.309 0.542 0.830	30.898 27.285 16.657	218→219 (H→L) 65% 218→227(16%),218→220(16% 217→227(16%), 215→220(16% 206 → 221 (13%)	CT from rings 1, 2 to 4S-Ge CT from rings 1-3 to 4-6 IC in rings 1, 2 IC in rings 1, 2
T35	S1 S7 S19 S20 S49	3.055 3.989 4.619 4.662 5.572	406 311 268 266 223	0.003 0.315 0.521 0.326 0.121	0.869 0.568 0.5523	5.083 2.059 7.036	0.645 0.951 0.831	21.208 5.619 17.671	230→231 (H→L) 65% 229→239(16%), 228→233(16% 230→240(10%), 226→236(10% 229→239(12%), 229→243(12% 228→237 (8%)	CT from rings 1, 2 to 4S-Ge IC in rings IC in rings IC in rings
T36	S1 S7 S17	3.083 4.062 4.672	401 305 265	0.003 0.400 0.966	0.843 0.618 0.513	4.578 0.034 0.070	0.669 0.908 0.975	18.492 0.102 0.173	198 → 199 (H→L) 65% 198 → 200 (16%) 197 → 207 (20%)	CT from one TTF to 4S-Ge group IC in rings IC n rings

Table S2. Static ($\lambda = \infty$) and dynamic ($\lambda = 1064$ nm) first hyperpolarizability (au) and depolarization ratio (DR), Electronic absorption energies (E, eV) , dipole moment variation ($\Delta\mu_{0\to n}$, D) associated to the S0 → Sn transition and dominant transition of the desired excited states for Ti calculated by the sum-over-states method

	Ti	$DR_{SOS}^{\lambda=\infty}$	$\beta_{HRS,SOS}^{\lambda=\infty}$	$DR_{SOS}^{\lambda=1064}$	$\beta_{SOS}^{\lambda=1064}$	S0 → Sn	Sn	$\Delta E_{0\to n}$	$\Delta\mu_{0\to n}$
a	T1	4.19	795	5.03	1930	S0 → S1	S1	1.706	0.124
						S0 → S7	S7	3.217	1.00
						S0 → S10	S10	4.033	1.446
						S0 → S17	*S17*	*4.245*	*1.117*
b	T2	5.51	1239	5.02	2801	S0 → S1	S1	1.824	0.078
						S0 → S16	S16	4.035	1.127
						S0 → S32	*S32*	*4.654*	*3.035*
c	T3	1.60	427	1.61	966	S0 → S1	S1	1.895	0.105
						S0 → S13	S13	3.998	1.284
						S0 → S23	S23	4.239	1.122
						S0 → S29	*S29*	*4.619*	*2.665*
d	T4	4.15	1046	2.98	2550	S0 → S1	S1	1.833	0.088
						S0 → S20	S20	4.009	1.128
						S0 → S22	S22	4.087	1.138
						S0 → S33	S33	4.282	1.119
						S0 → S38	*S38*	*4.626*	*2.444*
e	T5	1.81	776	1.15	2956	S0 → S1	S1	1.831	0.084
						S0 → S5	S5	2.724	0.828
						S0 → S27	S27	4.087	1.282
						S0 → S41	S41	4.297	1.387
						S0 → S47	*S47*	*4.676*	*3.642*
A	T6	4.28	555	4.39	889	S0 → S1	S1	3.069	0.190
						S0 → S7	S7	4.033	1.300
						S0 → S11	S11	4.240	1.163
						S0 → S18	*S18*	*4.658*	*2.345*
B	T7	4.95	690	5.60	1138	S0 → S1	S1	3.050	0.179
						S0→ S7	S7	4.028	1.285
						S0 → S12	S12	4.260	1.292
						S0 → S16	S16	4.488	1.459
						S0 → S19	*S19*	*4.662*	*2.066*

C	T8	2.07	297	1.88	460	S0 → S1 S0 → S7 S0 → S17	S1 S7 S17	3.132 4.073 4.530	0.219 2.073 1.229
						S0 → S19	*S19*	*4.700*	*2.121*
d	T9	3.08	480	2.83	751	S0 → S1 S0 → S8 S0 → S12 S0 → S16	S1 S8 S12 S16	3.107 4.077 4.304 4.477	0.217 1.229 1.297 1.318
						S0 → S22	*S22*	*4.812*	*1.748*
e	T10	2.83	751	1.45	836	S0 → S1 S0 → S6 S0 → S13	S1 S6 S13	3.086 3.414 4.305	0.261 0.716 1. 389
						S0 → S22	*S22*	*4.793*	*2.605*
a	T11	6.01	740	6.01	1304	S0 → S1 S0 → S8 S0 → S13	S1 S8 S13	3.075 4.031 4.237	0.187 1.378 1.165
						S0 → S20	*S20*	*4.652*	*2.839*
b	T12	5.55	2286	5.61	12563	S0 → S1 S0 → S14 S0 → S20	S1 S14 S20	2.230 4.000 4.200	0.142 1.365 1.410
						S0 → S31	*S31*	*4.578*	*1.874*
c	T13	**2.58**	**449**	**2.27**	**746**	S0 → S1 S0 → S9 S0 → S17	S1 S9 S17	3.087 4.043 4.309	0.180 1.200 1.354
						S0 → S21	*S21*	*4.669*	*2.583*
d	T14	2.30	515	2.04	1113	S0 → S1 S0 → S6 S0 → S9 S0 → S10	S1 S6 S9 S10	3.096 3.313 3.789 4.092	0.429 0.859 1.013 1.429
						S0 → S25	*S25*	*4.668*	*2.384*
e	T15	2.05	653	2.12	1461	S0 → S1 S0 → S8 S0 → S11 S0 → S28	S1 S8 S11 S28	3.098 3.527 4.132 4.649	0.438 0.685 1.395 2.107
						S0 → S45	*S45*	*5.134*	*1.205*
a	T16	4.30	695	4.25	1008	S0 → S1	S1	3.081	0.190

						S0 → S7 S0 → S11	S7 S11	4.019 4.246	1.496 1.311
						S0 → S18	*S18*	*4.644*	*3.060*
b	T17	3.74	566	4.40	996	S0 → S1 S0 → S7 S0 → S11 S0 → S19	S1 S7 S11 S19	3.065 4.032 4.230 4.651	0.183 1.324 1.049 2.876
						S0 → S33	*S33*	*5.168*	*1.031*
c	T18	3.34	352	2.83	507	S0 → S1 S0 → S7 S0 → S11	S1 S7 S11	3.119 4.017 4.274	0.203 1.731 1.441
						S0 → S19	*S19*	*4.641*	*3.024*
d	T19	2.44	225	1.97	403	S0 → S1 S0 → S8 S0 → S12	S1 S8 S12	3.115 4.090 4.285	0.196 1.311 1.358
						S0 → S20	*S20*	*4.651*	*2.610*
e	T20	**1.62**	**357**	**1.51**	**650**	S0 → S1 S0 → S7 S0 → S13	S1 S7 S13	3.125 4.073 4.316	0.226 1.967 1.527
						S0 → S21	*S21*	*4.666*	*2.849*
a	T21	3.58	1224	4.25	4107	S0 → S1 S0 → S9 S0 → S12	S1 S9 S12	2.854 4.034 4.091	1.089 1.211 1.115
						S0 → S21	*S21*	*4.652*	*3.003*
b	T22	5.02	1532	1.03	13348	S0→S1 S0→S11 S0→S18 S0→s23	S1 S11 S18 S23	2.238 3.971 4.233 4.504	0.783 1.079 1.283 1.026
						S0→25	*S25*	*4.657*	*2.819*
c	T23	2.84	1181	2.16	4049	S0 → S1 S0 → S13 S0 → S19	S1 S13 S19	2.866 4.083 4.315	1.325 1.765 1.569
						S0 → 25	*S25*	*4.666*	*3.156*
d	T24	1.89	1119	1.72	18404	S0 → S1 S0 → S2 S0 → S13	S1 S2 S13	2.261 2.869 3.992	0.787 1.104 1.110

						S0 → S15	S15	4.084	1.306
						S0 → S28	*S28*	*4.668*	*3.199*
e	T25	1.88	999	9.03	39343	S0→S1 S0→S2 S0→S19 S0→S29	S1 S2 S19 S29	2.365 2.366 4.148 4.487	0.783 0.782 1.821 1.061
						S0→S31	*S31*	*4.662*	*2.629*
a	T26	2.43	263	2.14	407	S0 → S1 S0 → S7 S0 → s12	S1 S7 S12	3.083 4.029 4.238	0.184 1.835 1.275
						S0 → S17	*S17*	*4.623*	*2.770*
b	T27	3.65	644	3.49	1048	S0 → S1 S0 → S7 S0 → S11	S1 S7 S11	3.019 3.992 4.173	0.167 1.172 1.095
						S0 → S17	*S17*	*4.611*	*2.109*
c	T28	3.79	493	3.98	791	S0 → S1 S0 → S7	S1 S7	3.050 4.030	0.176 1.578
						S0 → S17	*S17*	*4.605*	*2.404*
d	T29	3.44	452	3.41	806	S0 → S1 S0 → S7 S0 → S8	S1 S7 S8	3.026 4.001 4.044	0.169 1.242 1.291
						S0 → S17	*S17*	*4.611*	*2.529*
e	T30	2.83	462	2.82	803	S0 → S1 S0 → S7 S0 → S8	S1 S7 S8	3.039 4.016 4.067	0.169 1.217 1.278
						S0 → S19	*S19*	*4.680*	*2.199*
a	T31	3.75	304	303	432	S0 → S1 S0 → S7	S1 S7	3.081 4.023	0.186 1.799
						S0 → S18	*S18*	*4.615*	*2.523*
b	T32	6.63	494	6.11	726	S0 → S1 S0 → S7	S1 S7	3.027 3.997	0.168 1.433
						S0 → S19	*S19*	*4.662*	*2.570*
c	T33	3.11	230	3.03	319	S0 → S1 S0 → S7	S1 S7	3.088 4.021	0.197 2.064
						S0 → S19	*S19*	*4.613*	2.622

d	T34	4.49	305	5.98	425	S0 → S1 S0 → S7	S1 S7	3.026 3.981	0.196 1.498
						S0 → S19	*S19*	*4.618*	*2.723*
e	T35	1.66	256	1.66	259	S0 → S1 S0 → S7	S1 S7	3.054 3.988	0.183 1.795
						S0 → S19	*S19*	*4.619*	*2.166*

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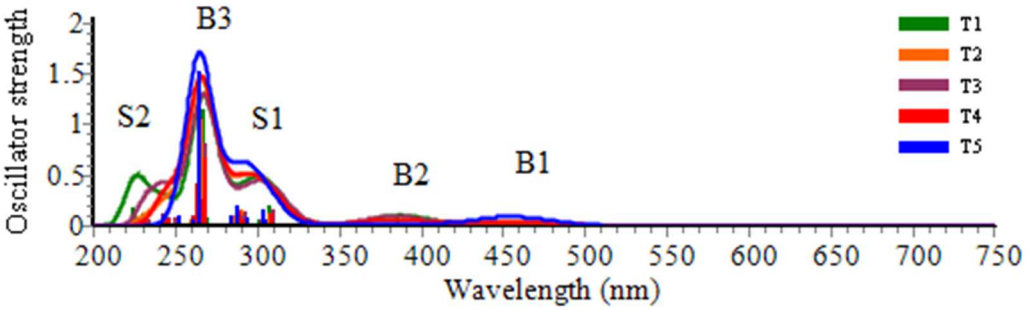

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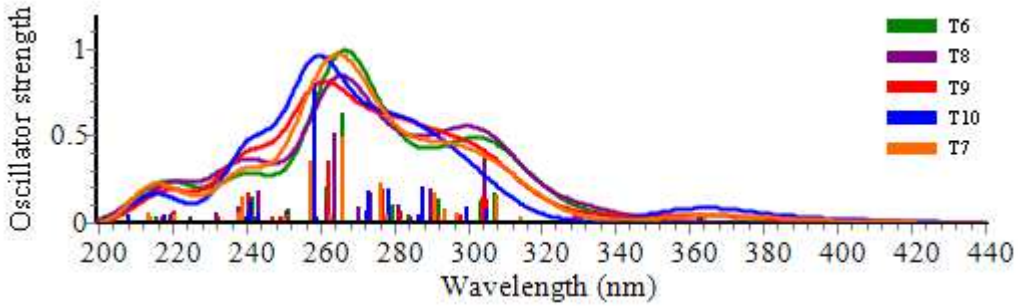

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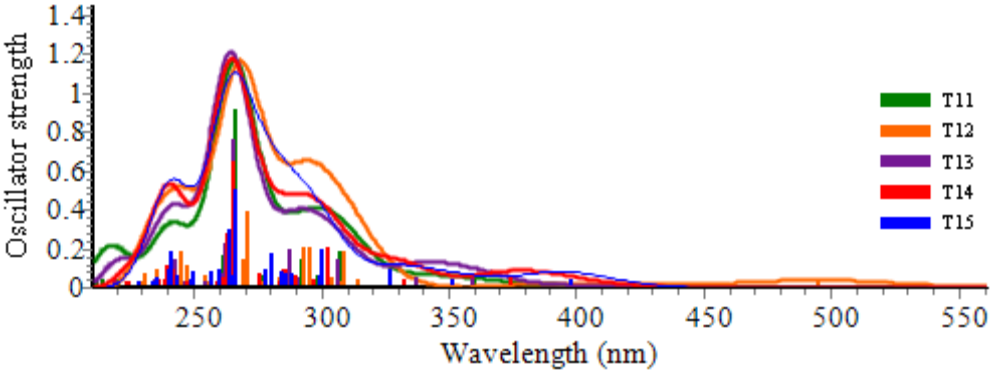

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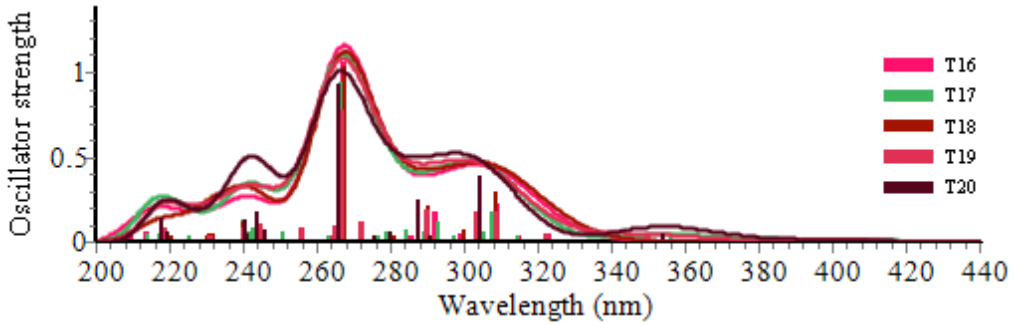

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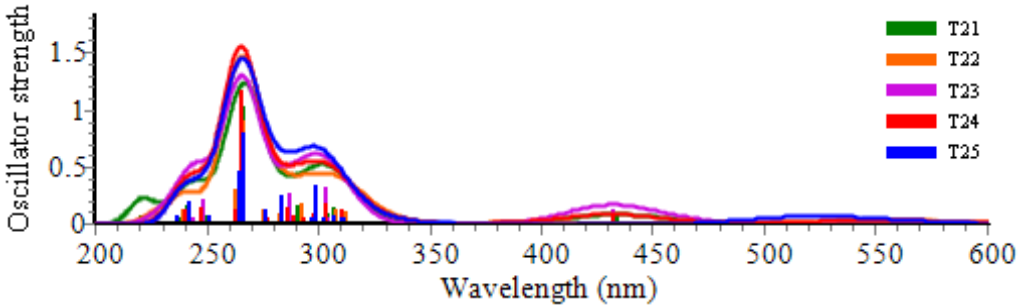

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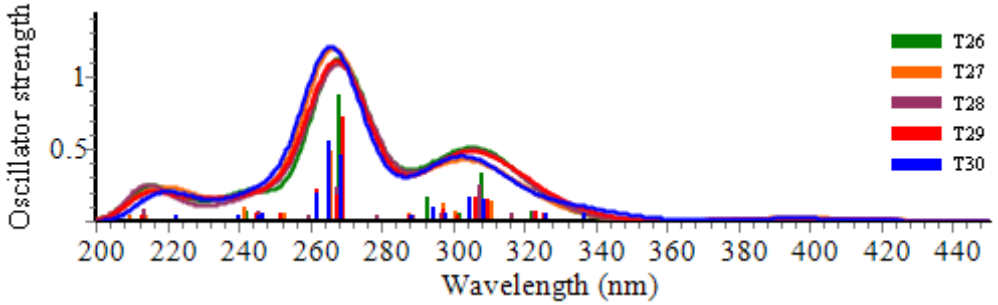

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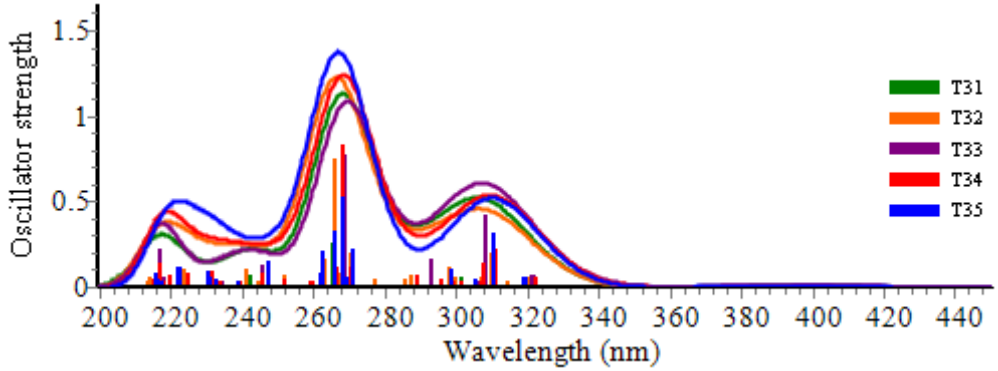

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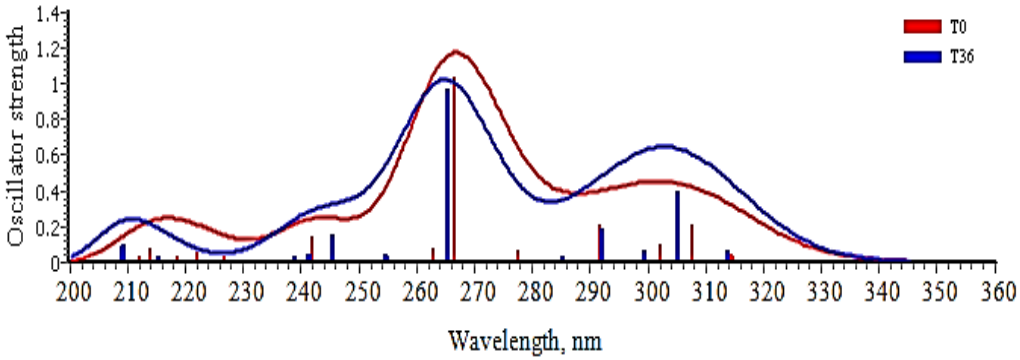
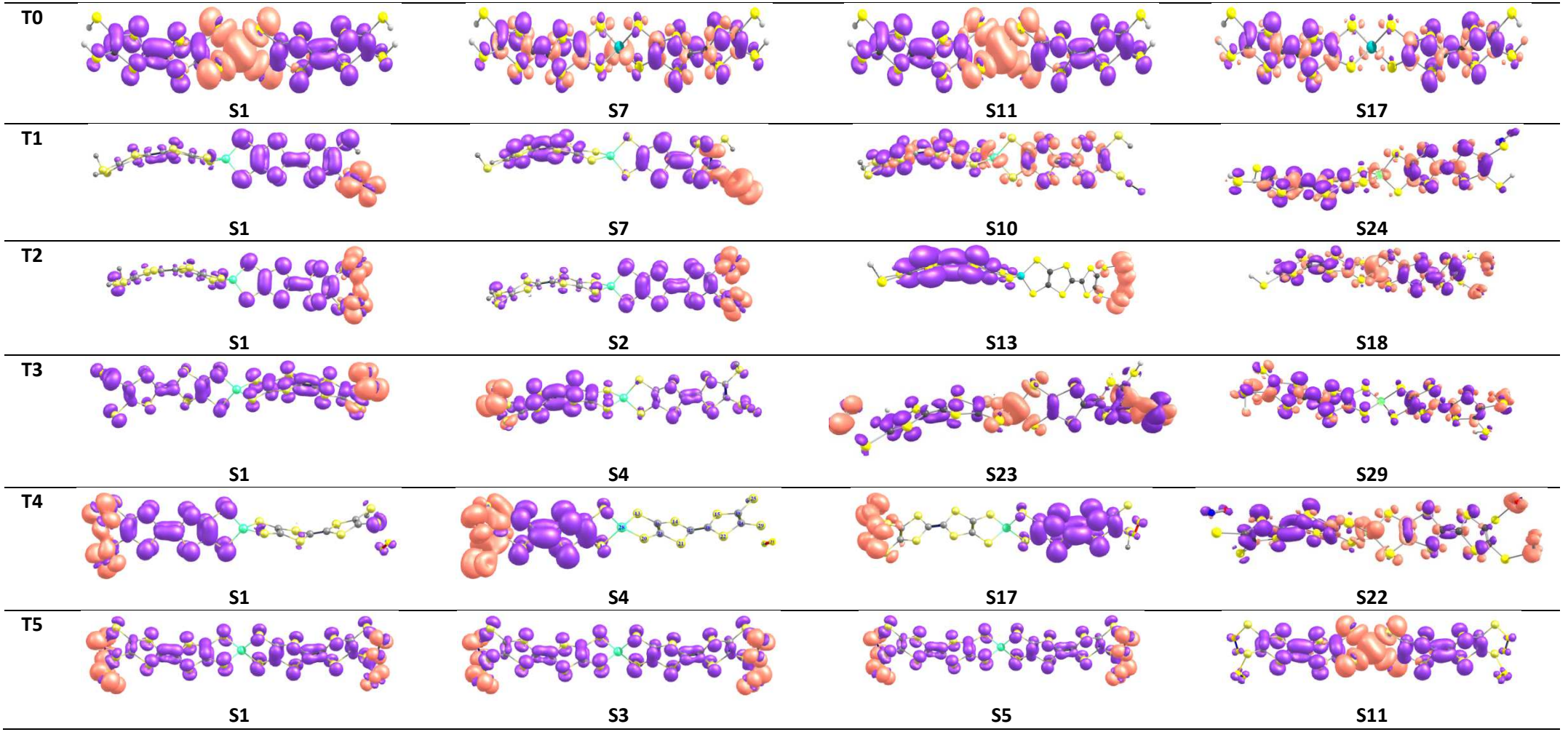
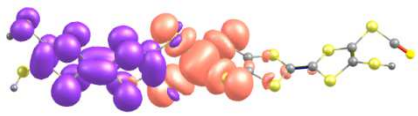
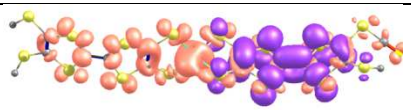
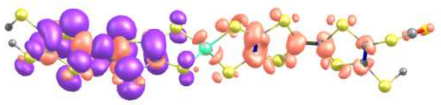
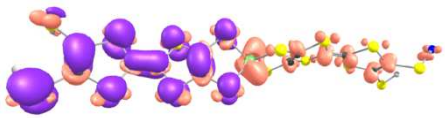


Figure S1. Calculated UV − vis absorption spectra of 36 bis-TTF-Ge compounds



T6				
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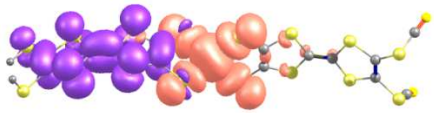
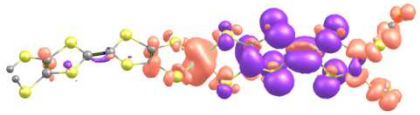
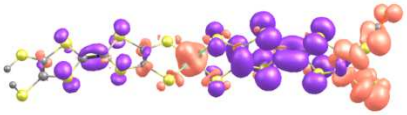
T7				
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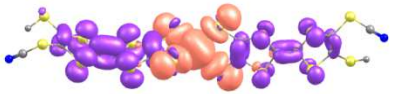
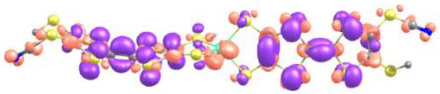
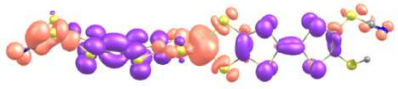
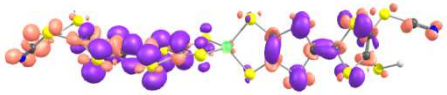
T8				
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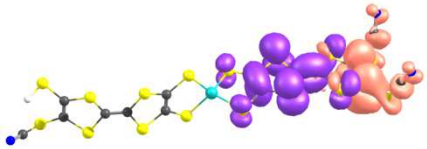
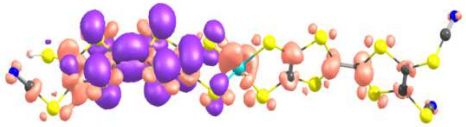
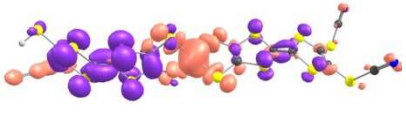
T9				
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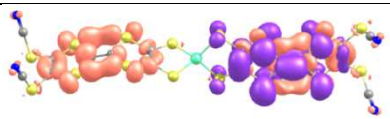
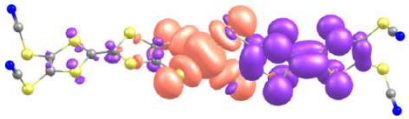
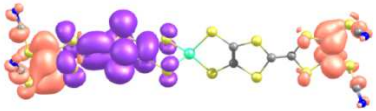
T10				
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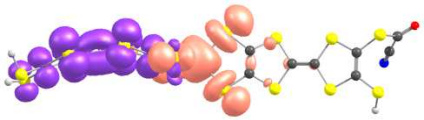
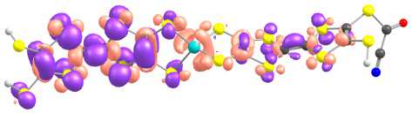
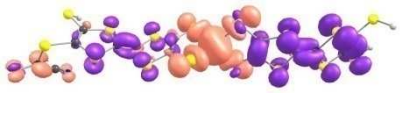
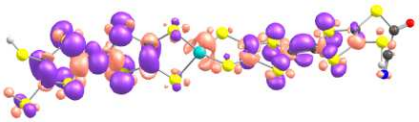
T11				

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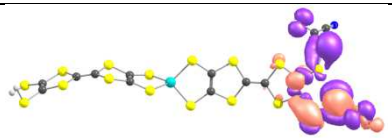
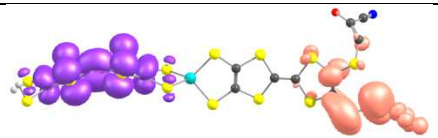
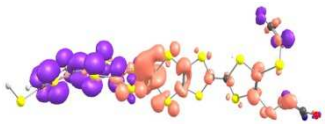
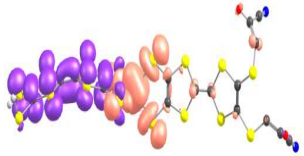
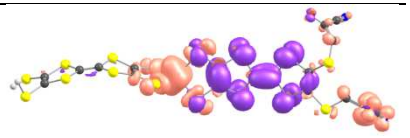
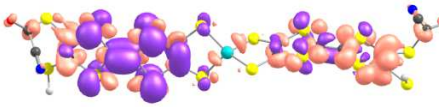
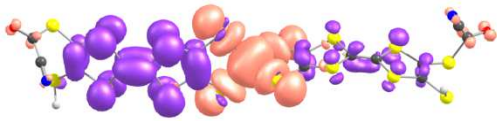
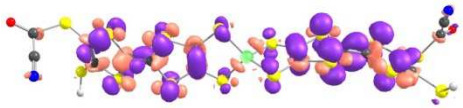
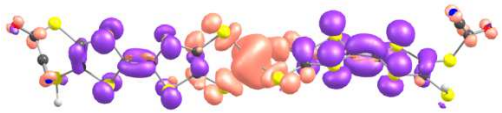
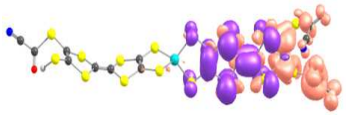
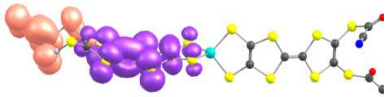
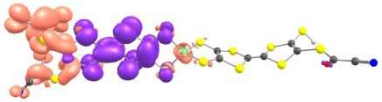
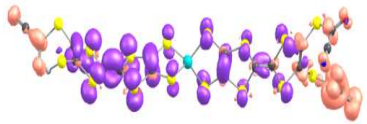
T12					
			S14	S20	
	S1	S9			S31
T13					
	S1	S3	S9		S17
T14					
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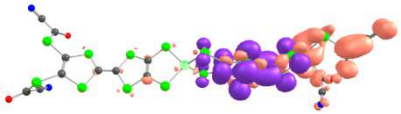
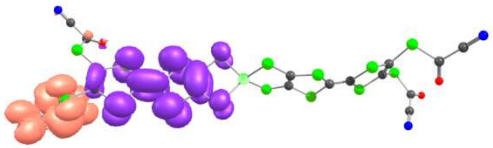
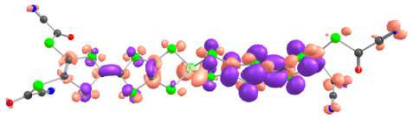
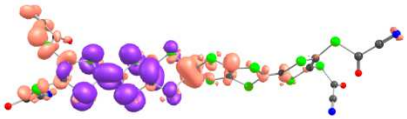
T15					
	S1	S8	S11		S28

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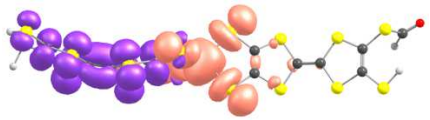
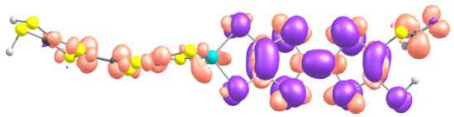
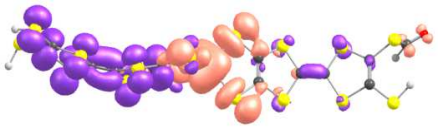
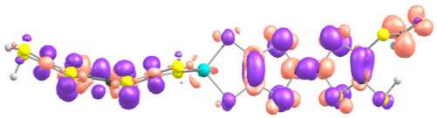
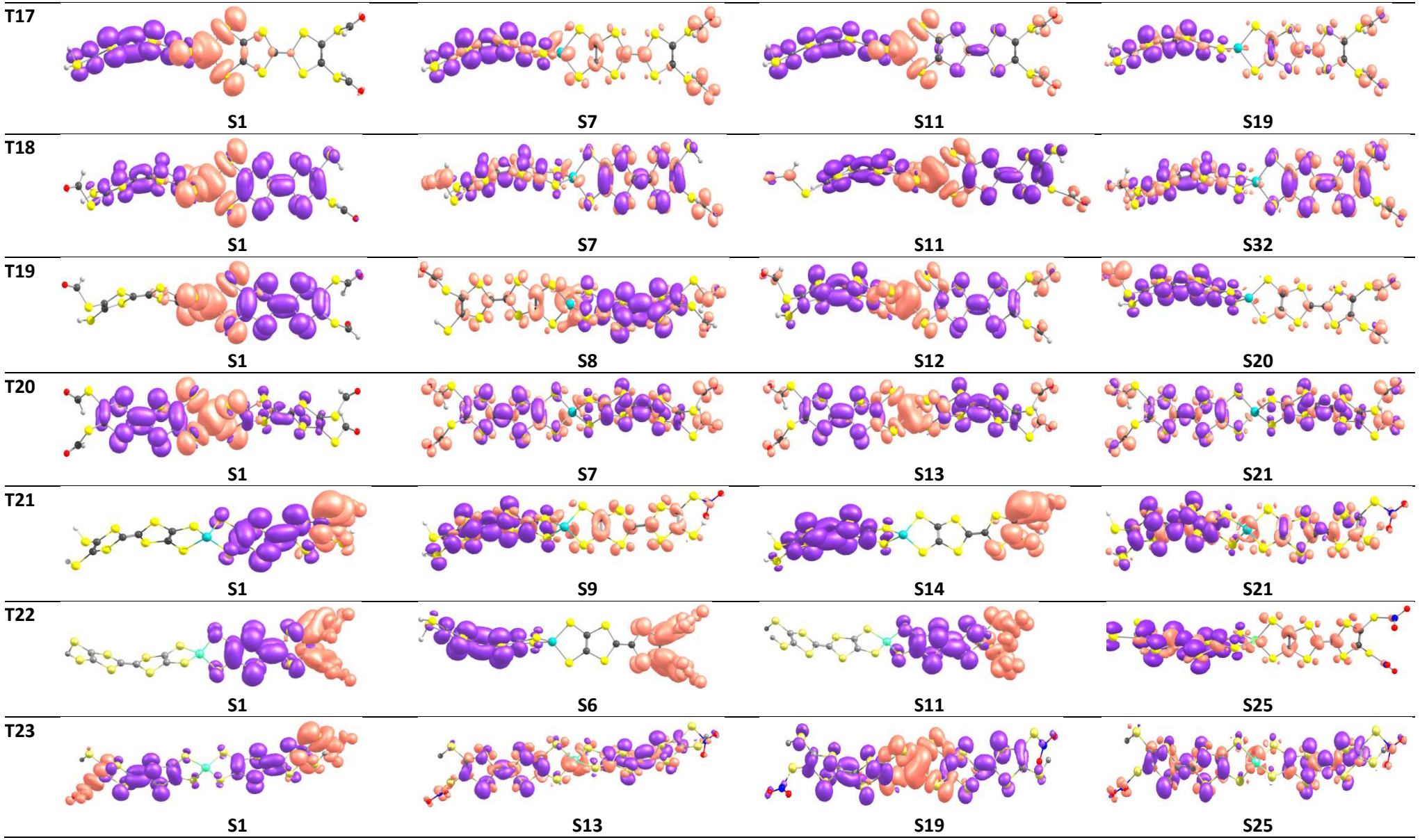
T16				
	S1	S7	S11	S18


T17
S1
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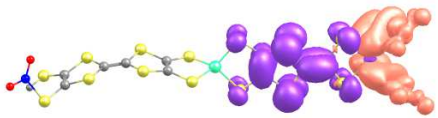
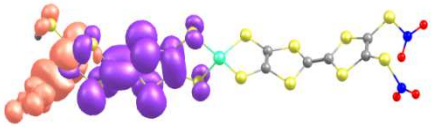
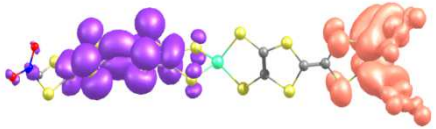
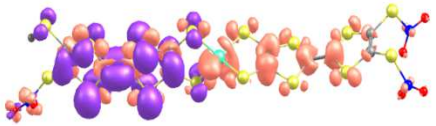
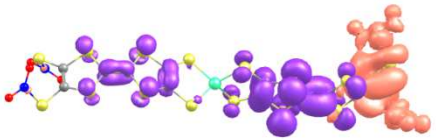
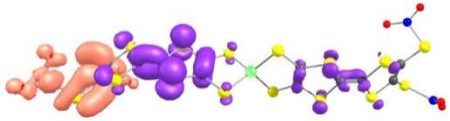
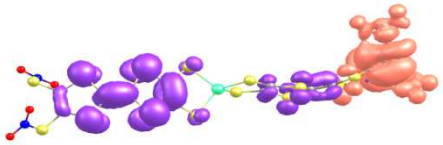
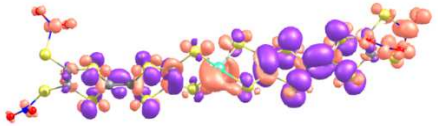
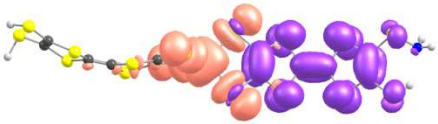
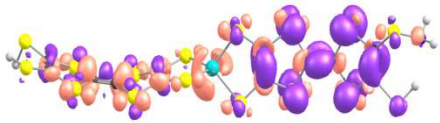
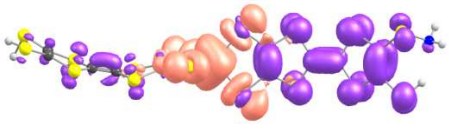
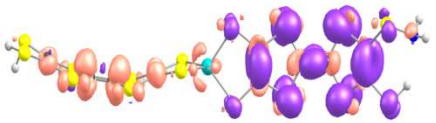
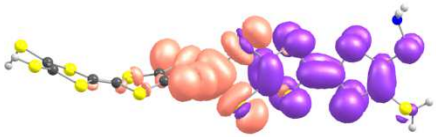
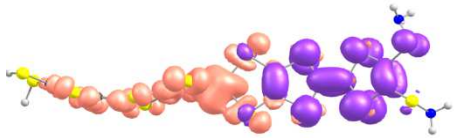
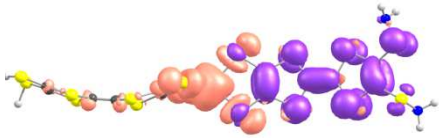
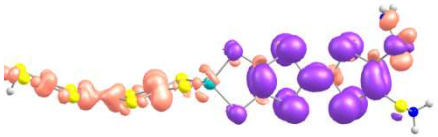
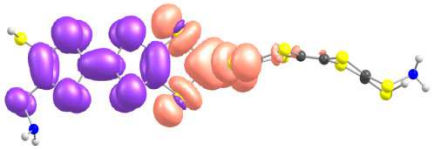
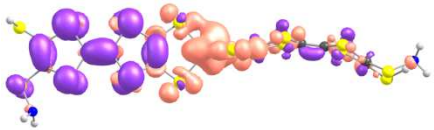
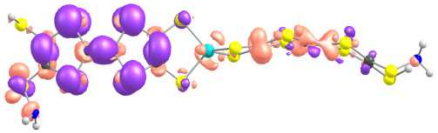
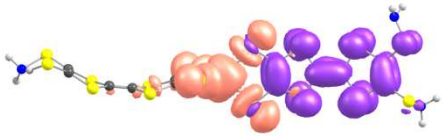
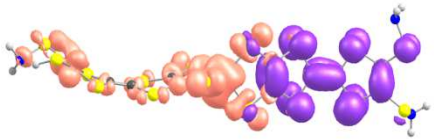
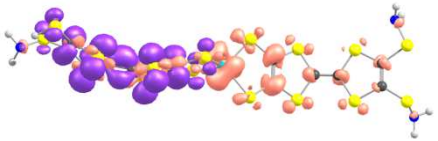
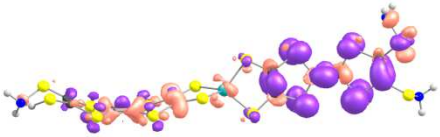
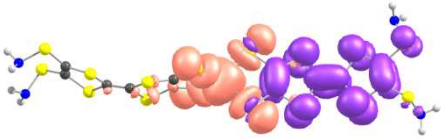
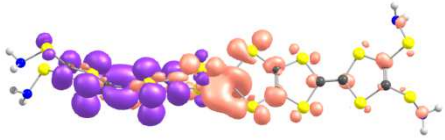
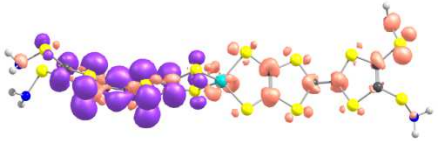
S19
S25

T24				
	S1	**S2**	**S8**	**S15**
T25				
	S1	**S2**	**S9**	**19**
T26				
	S1	**S7**	**S12**	**S17**
T27				
	S1	**S7**	**S11**	**S17**
T28				
	S1	**S7**	**S17**	
T29				
	S1	**S7**	**S8**	**S17**

T30				
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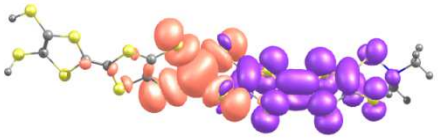
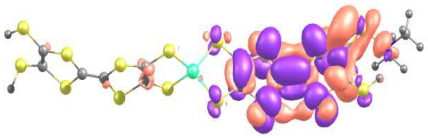
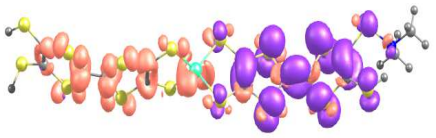
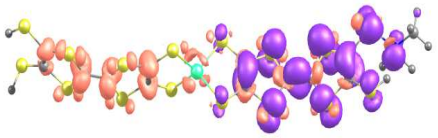
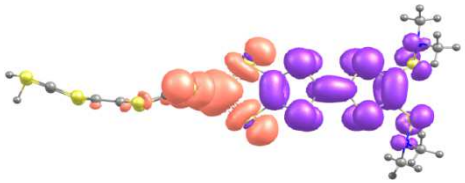
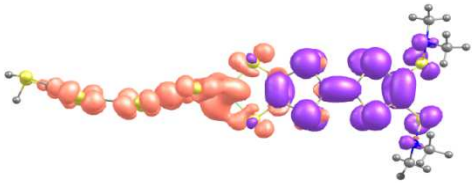
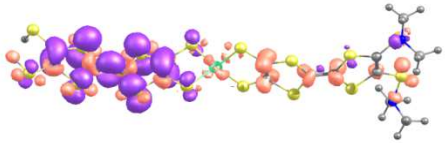
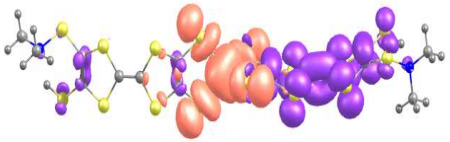
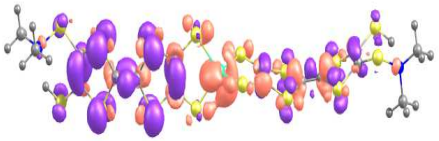
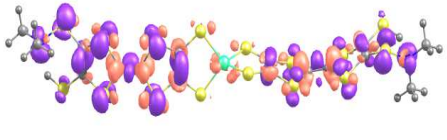
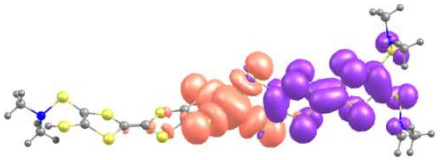
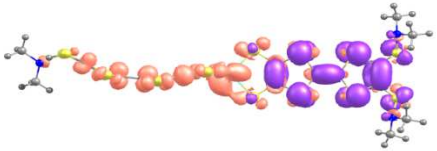
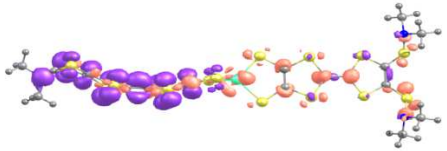
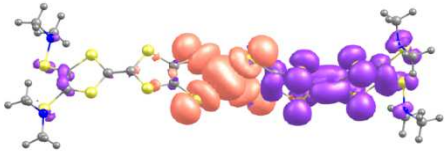
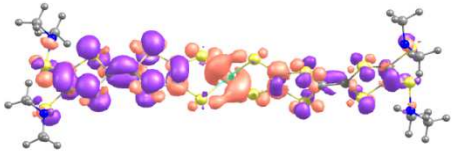
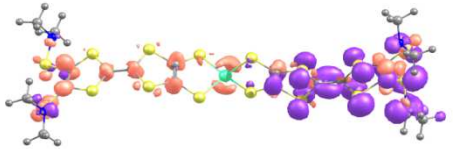
T31				
	S1	**S5**	**S7**	**S18**
T32				
	S1	**S7**	**S19**	
T33				
	S1	**S7**	**S19**	
T34				
	S1	**S7**	**S19**	
T35				
	S1	**S7**	**S19**	

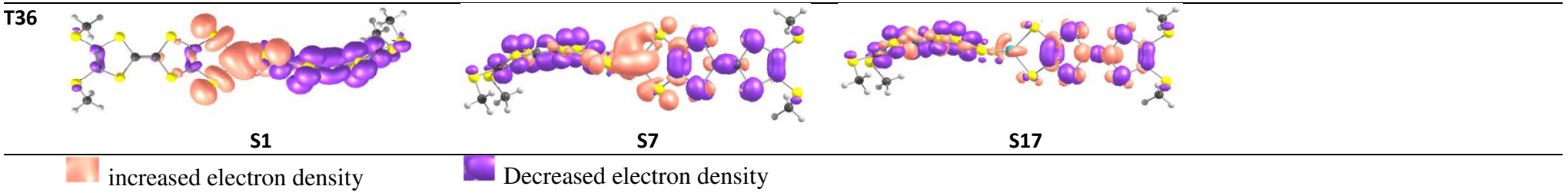


Figure S2. Electron density difference of bis-TTF-Ge derivatives from the ground state to the crucial excited state (Sn: S0 → Sn) plotted using 0.008 au isovalues

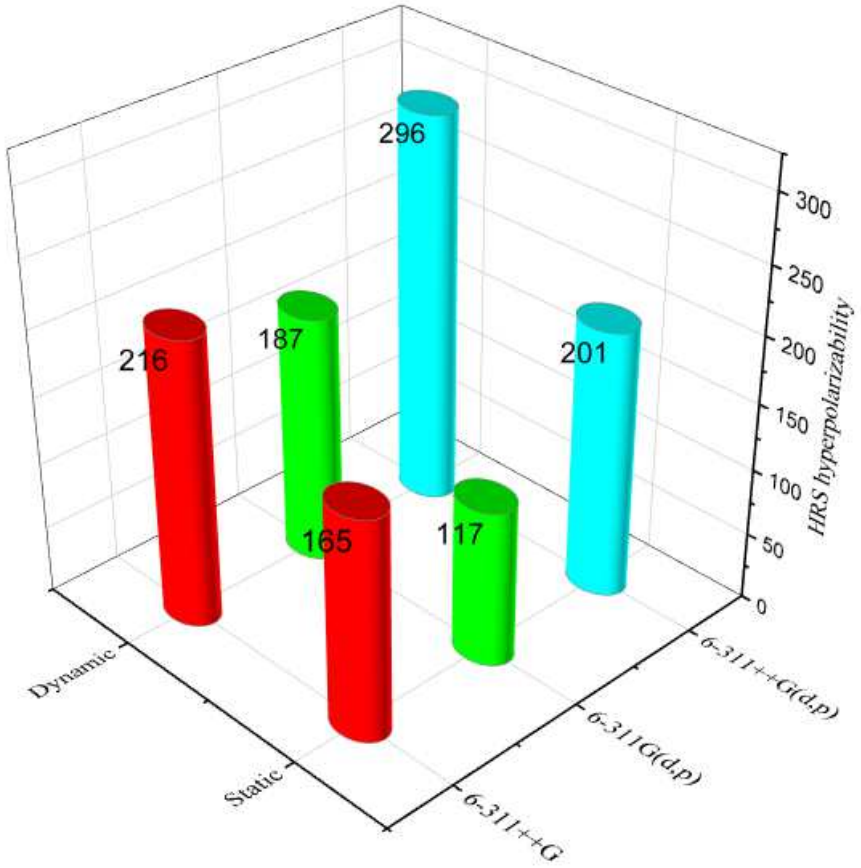


Figure S3. The calculated β_{HRS} values (a.u) using the CAM-B3LYP functional at the different basis sets level for T36

Influence of the basis set on the NLO of T36

Figure S3 reports the calculated β_{HRS} values in the static and dynamic regime using the CAM-B3LYP functional with different basis sets namely, 6-311++G, 6-311G(d,p) and 6-311++G(d,p) for the compounds T36. We can be seen that the 6-311++G(d,p) presented a larger value of hyperpolarizabilities than the 6-311++G and 6-311G(d,p), respectively. On the other hand, the difference between diffuse functional and 6-311G(d,p) is small. This is not to surprise because of the quasi linear shape of the molecule. The dynamic/static ratio of β_{HRS} is similar for all basis sets. Then, for the NLO calculation, the 6-311G(d,p) is a good choice for the title compounds.

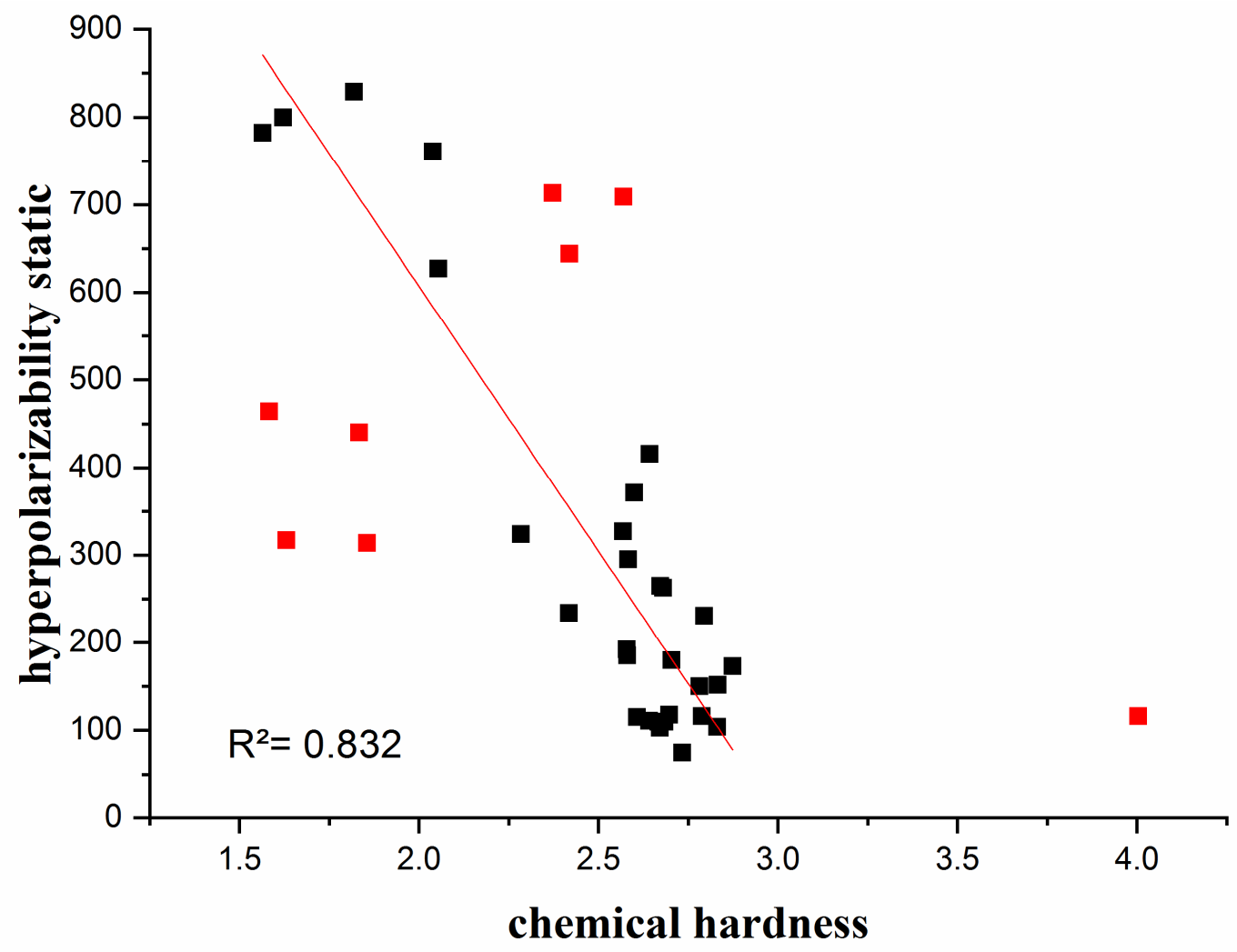
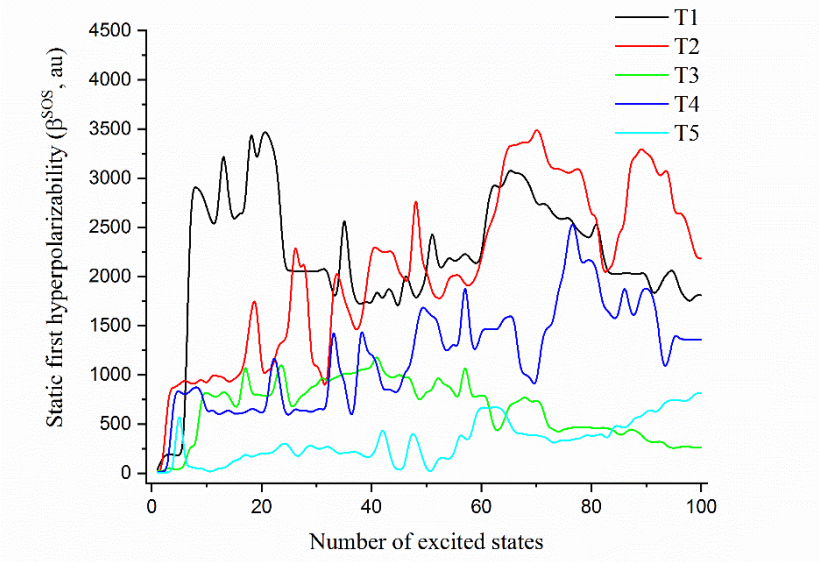
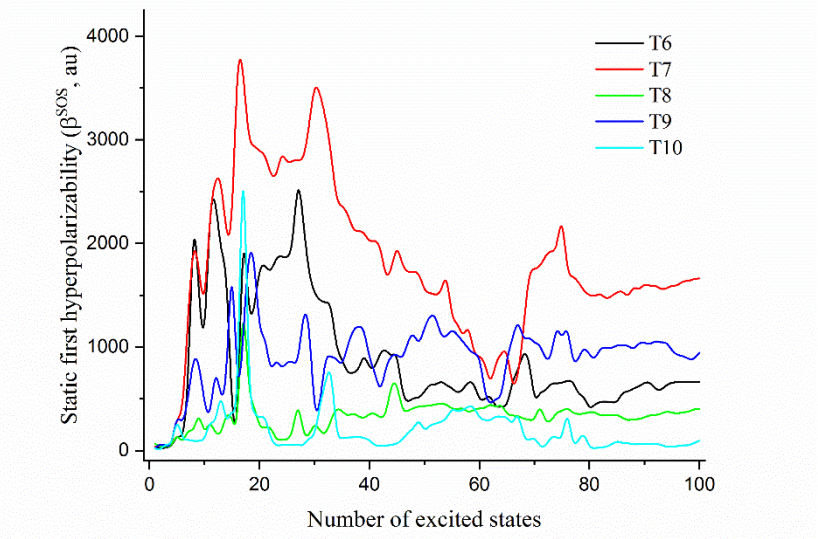
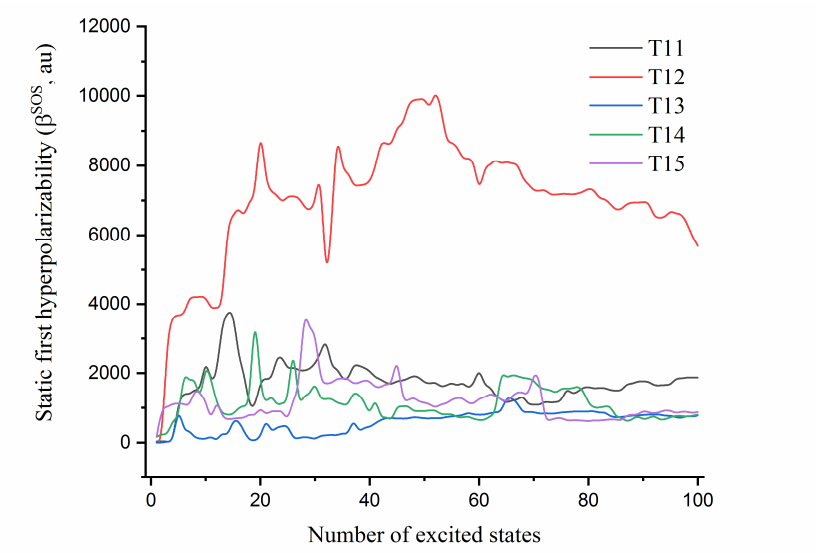
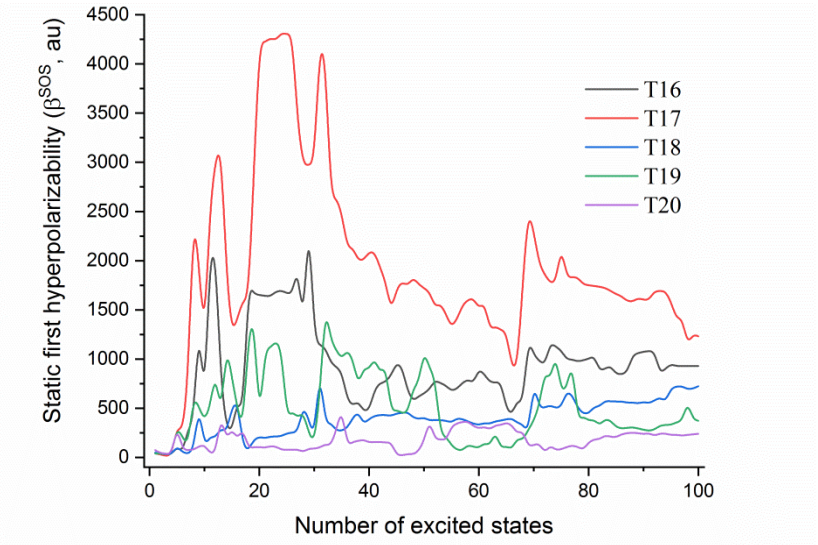


Figure S4. Correlation between static hyperpolarizability and hardness, T2,T4, T6, T7, T11, T13, T15 and T36 excepted


Static first hyperpolarizability (β^{SOS}, au)
Number of excited states
T1
T2
T3
T4
T5


Static first hyperpolarizability (β^{SOS}, au)
Number of excited states
T6
T7
T8
T9
T10


Static first hyperpolarizability (β^{SOS}, au)
Number of excited states
T11
T12
T13
T14
T15


Static first hyperpolarizability (β^{SOS}, au)
Number of excited states
T16
T17
T18
T19
T20

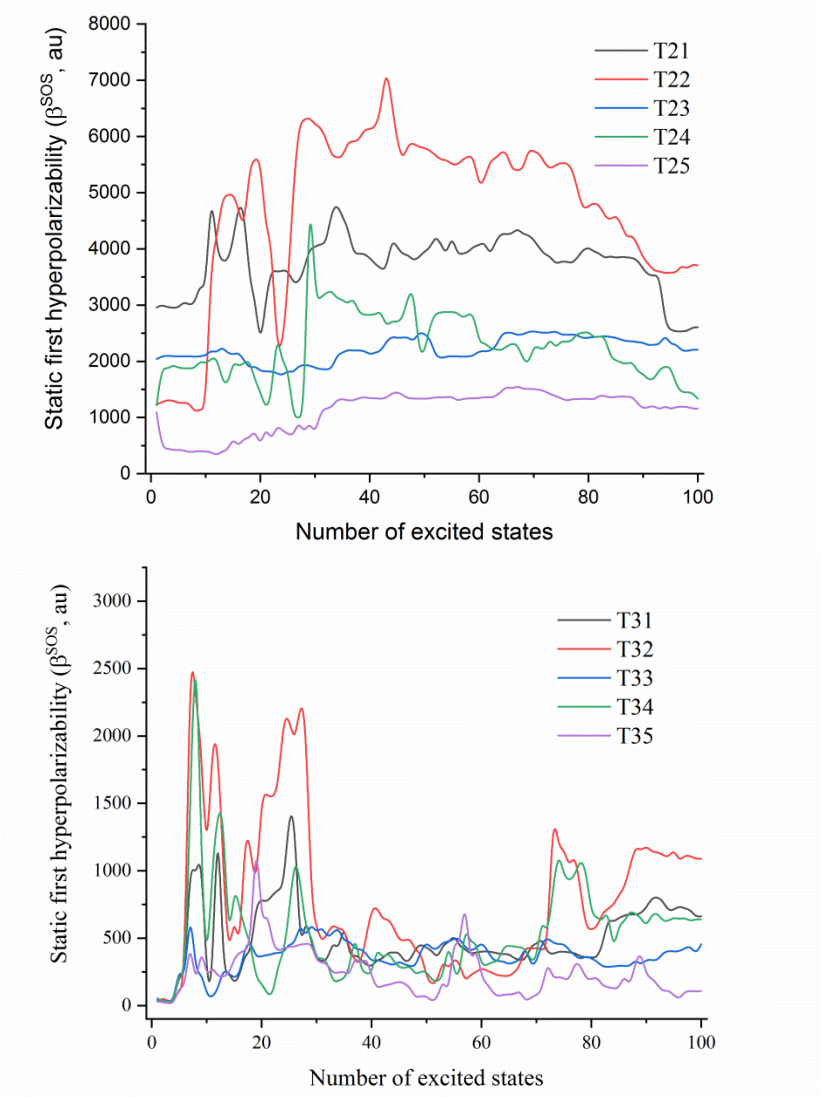


Figure S5. Relationship between the static first hyperpolarizability (β^{SOS}, a.u.) and the number of excited states

Reference

Full citation for Gaussian 09 program

Ref 40. Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

The optimized cartesian coordinates and energy of all structures

T0 : symmetry c1 -8907.9121123

0 1

S	-1.4518	1.19734	-1.19014
S	-4.37734	0.53762	-1.6365
S	-7.65602	0.90356	-1.36179
C	-2.88267	0.27134	-0.7048
C	-5.37739	-0.39156	-0.49355
C	-6.70988	-0.23574	-0.38519
C	-9.12089	0.7962	-0.3452
S	-1.52406	-1.20053	1.21629
S	-4.44077	-1.56469	0.46459
S	-7.70369	-1.19748	0.73702
C	-2.91033	-0.67884	0.24624
C	-9.13157	-0.15094	0.613
S	1.52406	-1.19644	-1.2203
S	4.44079	-1.5631	-0.4699
S	7.70365	-1.19492	-0.74119
C	2.91032	-0.67805	-0.24847
C	5.3774	-0.39324	0.49222
C	6.7099	-0.23706	0.38437
C	9.13154	-0.14882	-0.61361
S	1.45179	1.19319	1.19436
S	4.37736	0.53202	1.63836
S	7.65607	0.89885	1.36487

C	2.88266	0.26887	0.7058
C	9.1209	0.79501	0.34786
S	10.4107	-0.54282	-1.76878
H	11.31184	0.29363	-1.20731
S	-10.41826	1.96498	-0.65166
H	-10.9642	1.34381	-1.72486
Ge	0.00001	-0.04592	-0.00007
S	10.41828	1.96271	0.65831
H	10.96414	1.33791	1.72945
S	-10.41076	-0.54893	1.76677
H	-11.31185	0.28948	1.20818

T1 : symmetry c1 -9037.1901523

0 1

S	-2.14648300	0.96762400	-1.41737700
S	-5.05356500	0.16122900	-1.72586300
S	-8.33983100	0.51628100	-1.51737900
C	-3.55835700	0.12296500	-0.75827500
C	-6.03752500	-0.53973500	-0.41799500
C	-7.37265800	-0.38900600	-0.33802200
C	-9.80057500	0.59092000	-0.49154500
S	-2.17644100	-0.90185400	1.41986200
S	-5.07950800	-1.48033100	0.75220800
S	-8.34821600	-1.12581500	0.95676700
C	-3.56921600	-0.61848000	0.36346500
C	-9.79328800	-0.14669600	0.63591400

S	0.88507100	-1.31329000	-0.96079900
S	3.81019500	-1.43288200	-0.17603900
S	7.09731600	-1.08886600	-0.41366600
C	2.25355600	-0.56983200	-0.11944800
C	4.71115700	-0.08425900	0.55504000
C	6.04597700	0.04752200	0.44371000
C	8.45964900	0.07078300	-0.56990600
S	0.73984400	1.51180100	0.92464500
S	3.68163400	1.03848500	1.47540200
S	6.94262600	1.39303300	1.19587000
C	2.19647900	0.54890000	0.62398500
C	8.37227700	1.20447500	0.18986000
S	9.78797700	-0.35112900	-1.57578500
S	-11.11683200	1.65605200	-1.01662000
Ge	-0.67554700	0.02269800	-0.00058900
S	9.52941500	2.51551700	0.33302900
S	-11.06183500	-0.32613300	1.85408000
H	-11.97686100	0.37447600	1.14787300
H	-11.66148500	0.82261500	-1.93565800
H	10.47472300	1.89818200	-0.41074200
N	10.94969700	-1.27351700	-0.27777000
O	10.59445800	-1.27911300	0.86980700
O	11.93885600	-1.74187500	-0.77884400

T2 : symmetry c1 -9166.4711763

0 1

S	0.70527900	1.60810200	-0.52898200
S	3.64682700	1.50918500	0.19924000
S	6.90523000	1.33648800	-0.30730900
C	2.10603400	0.64621200	-0.03230800
C	4.58652000	0.00639100	0.37224500
C	5.91476500	-0.06178300	0.17130500
C	8.35173300	0.39572900	-0.72842900
S	0.64927500	-1.70278400	0.23534300
S	3.59754000	-1.39037500	0.86515500
S	6.86212500	-1.55463700	0.36297800
C	2.08478800	-0.66415100	0.26850900
C	8.32872400	-0.93729800	-0.42832700
S	-2.31274900	-0.42310300	-1.69162700
S	-5.22467500	0.42069400	-1.63361300
S	-8.48994400	0.00870400	-1.51748800
C	-3.71026100	0.11822700	-0.74590200
C	-6.18149000	0.60439500	-0.14274000
C	-7.51564400	0.43483400	-0.08891600
C	-9.93568000	-0.43764800	-0.59016600
S	-2.28127300	0.31050500	1.62476700
S	-5.19852900	1.06552700	1.26822300
S	-8.48296900	0.65301400	1.38190000
C	-3.69730900	0.41100200	0.56654900
C	-9.94346900	-0.13679100	0.72312300
S	-11.20484500	-1.18946100	-1.56476300
H	-12.12035000	-1.16441800	-0.57080900

S	9.66365800	1.26726800	-1.46823100
Ge	-0.80920300	-0.01401700	-0.06657400
S	-11.26080500	-0.49635000	1.85382600
H	-11.80169500	0.74521700	1.89379900
S	9.60288300	-2.08681000	-0.70096100
O	10.07552000	1.87386600	1.17687800
O	10.40087400	-0.98153500	1.67229300
N	10.53708900	2.13069600	0.15604000
N	10.72586500	-1.83370500	0.97096200

T3: symmetry c1 -9316.8630288

0 1

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S	7.66092	-1.45015	-0.89036
C	2.88827	-0.67421	-0.48815
C	5.37853	0.04936	-0.55774
C	6.71615	-0.0124	-0.42176
C	9.08054	-1.01395	0.05094
S	1.50858	1.42458	0.69547
S	4.42844	1.48551	-0.10976
S	7.72313	1.30709	0.19152
C	2.90573	0.57176	0.01678
C	9.12602	0.2513	0.56768
S	-1.43546	-0.69322	1.67474
S	-4.39076	-1.24971	1.30321

S	-7.6385	-0.80479	1.58792
C	-2.88402	-0.54827	0.66457
C	-5.39514	-0.53677	0.0183
C	-6.72535	-0.35997	0.12242
C	-9.04143	0.18137	1.19942
S	-1.53047	0.60441	-1.46606
S	-4.47569	-0.1124	-1.44465
S	-7.75387	0.28907	-1.16286
C	-2.92145	-0.03766	-0.57863
C	-9.11065	0.70415	-0.06224
S	-10.19987	0.32946	2.50866
H	-11.12417	0.96561	1.75437
S	10.28386	-2.28534	0.16716
H	11.20233	-1.50001	0.77354
Ge	0.00131	-0.11436	0.04042
S	-10.41509	1.63629	-0.6818
S	10.43841	0.91532	1.45698
N	-11.60975	0.20509	-1.32363
O	-11.28057	-0.92738	-1.09514
O	-12.58873	0.62334	-1.88503
N	11.56752	1.58826	-0.01286
O	11.21081	1.34449	-1.13373
O	12.54064	2.18227	0.37279

T4: symmetry c1 -9295.7520543

0 1

S	-1.11015500	-1.37855300	-0.91203100
S	-4.04951800	-1.51429000	-0.17869200
S	-7.31339400	-1.26202800	-0.61912900
C	-2.52173000	-0.59844700	-0.18153500
C	-5.00850600	-0.12047400	0.37709400
C	-6.33832700	-0.02057900	0.20106500
C	-8.76668900	-0.25646400	-0.79976200
S	-1.09619300	1.62297300	0.68198400
S	-4.03640400	1.11551500	1.21320500
S	-7.30336500	1.36124600	0.76763900
C	-2.51693300	0.58998400	0.44737800
C	-8.75793200	0.95658300	-0.17062600
S	1.86885500	0.93366400	-1.52054000
S	4.80061300	0.17527400	-1.67922700
S	8.05376400	0.63520800	-1.45005700
C	3.28358600	0.19985600	-0.74574900
C	5.76935200	-0.36882400	-0.28775400
C	7.09933500	-0.18828900	-0.19065200
C	9.52970200	0.76946500	-0.48399400
S	1.87242100	-0.63735500	1.49203200
S	4.80448600	-1.19937600	0.95738800
S	8.07573200	-0.74754100	1.18149900
C	3.28460700	-0.42395800	0.44555500
C	9.54671000	0.16185200	0.72725100
S	10.84654900	1.77634200	-1.10923400
H	10.64257100	1.47056900	-2.40927500

S	-10.06575500	-0.92105900	-1.74808800
Ge	0.38358700	0.09277400	-0.05171500
S	10.91457500	0.03815000	1.78794400
S	-10.03839500	2.13093700	-0.15660700
N	11.95930600	-1.37573500	0.73010600
N	-10.91985300	-2.20400500	-0.41479000
N	-11.21091300	1.42622500	1.34005200
O	11.49635800	-1.64328800	-0.28657900
O	-10.45870400	-2.22351000	0.63763100
O	-10.90230900	0.41246200	1.78864400

T5 : symmetry c1 -9425.0302378

0 1

S	-1.49438100	1.38398900	-1.13842300
S	-4.43296900	0.72395000	-1.47676200
S	-7.70122200	1.06696600	-1.10387100
C	-2.90628100	0.45869300	-0.59909800
C	-5.39161000	-0.21576500	-0.30632500
C	-6.72154000	-0.07779300	-0.15943400
C	-9.15257100	0.93969200	-0.08583900
S	-1.47795700	-1.01053900	1.27257500
S	-4.41890400	-1.37641700	0.63090700
S	-7.68170200	-1.02782400	0.99834400
C	-2.89892700	-0.49030000	0.35347400
C	-9.14748200	-0.03229600	0.87463400
S	1.47784300	-1.01055300	-1.27228300

S	4.41882900	-1.37650400	-0.63091700
S	7.68160100	-1.02779700	-0.99872100
C	2.89889700	-0.49043000	-0.35322600
C	5.39164200	-0.21595500	0.30633200
C	6.72155300	-0.07796700	0.15931700
C	9.14742600	-0.03227700	-0.87499800
S	1.49449800	1.38362000	1.13913400
S	4.43311800	0.72362400	1.47699400
S	7.70131900	1.06668200	1.10381100
C	2.90633400	0.45839900	0.59951500
C	9.15250500	0.93962200	0.08556300
S	10.44084000	-0.40393300	-1.97832200
S	-10.44880300	2.03959500	-0.44563300
Ge	0.00001100	0.14323300	0.00022700
S	10.44873600	2.03954300	0.44539400
S	-10.44100800	-0.40408200	1.97783300
N	11.59655100	0.91225400	1.67909800
N	-11.59650200	0.91175800	-1.67959700
N	-11.27547400	-2.03132800	1.07875700
O	11.26821100	-0.18231800	1.81440800
O	-11.26766000	-0.18262200	-1.81485600
O	-10.81100900	-2.35124400	0.07742900
N	11.27534100	-2.03155200	-1.07881800
O	10.81085100	-2.35109200	-0.07745900

T6 : symmetry c1 -9000.1158294

0 1

S	-1.8995	-0.55957	-1.6205
S	-4.82269	-1.20154	-1.12082
S	-8.09618	-0.71338	-1.22183
C	-3.29295	-0.50571	-0.5291
C	-5.76351	-0.55558	0.24587
C	-7.09364	-0.35535	0.19684
C	-9.52506	0.18017	-0.63021
S	-1.84069	0.5485	1.59047
S	-4.77024	-0.22989	1.68787
S	-8.02599	0.26037	1.58358
C	-3.2703	-0.065	0.74122
C	-9.48221	0.6299	0.6391
S	1.09188	1.54741	-0.53471
S	4.01955	1.11727	-1.18212
S	7.31585	1.23415	-0.89093
C	2.51003	0.48653	-0.48032
C	4.99882	-0.24087	-0.58007
C	6.3383	-0.18809	-0.46106
C	8.68279	0.74173	0.1377
S	1.11678	-1.65815	0.59732
S	4.04118	-1.69108	-0.19826
S	7.33686	-1.55194	0.1019
C	2.51908	-0.78193	-0.03487
C	8.70534	-0.53109	0.58255
S	9.90131	1.99318	0.47533

S	-10.85881	0.43833	-1.76924
Ge	-0.38534	-0.07072	-0.01006
S	9.93703	-1.33288	1.56912
S	-10.71388	1.51803	1.5446
H	-11.65073	1.40065	0.57732
H	-11.42329	-0.78857	-1.65976
H	10.99888	-1.0029	0.79914
C	11.24278	1.33939	-0.35277
N	12.18141	0.88975	-0.86182

T7: symmetry c1 -9092.3130741

0 1

S	0.75626	1.63294	-0.14531
S	3.69929	1.47745	0.55636
S	6.95775	1.51309	0.07351
C	2.18512	0.63012	0.15411
C	4.68239	-0.00088	0.446
C	6.01287	0.00988	0.24835
C	8.41914	0.70123	-0.50475
S	0.79975	-1.76568	-0.05125
S	3.73766	-1.49509	0.64462
S	6.999	-1.4714	0.14198
C	2.20145	-0.71386	0.19356
C	8.44044	-0.64554	-0.46477
S	-2.20073	0.04084	1.67063
S	-5.1265	-0.74083	1.47532

S	-8.38355	-0.24023	1.45118
C	-3.60883	-0.30036	0.65208
C	-6.08902	-0.6242	-0.0187
C	-7.41889	-0.41701	-0.03506
C	-9.82328	0.3909	0.62767
S	-2.19089	-0.07653	-1.72504
S	-5.11738	-0.83765	-1.49551
S	-8.38913	-0.33706	-1.51752
C	-3.60578	-0.34518	-0.69196
C	-9.83688	0.33815	-0.71855
S	-11.07958	0.96874	1.72913
H	-11.99467	1.1456	0.75015
S	9.73319	1.70023	-1.18178
Ge	-0.71262	-0.07319	-0.02976
S	-11.14822	0.92195	-1.75885
H	-11.70943	-0.2818	-2.0267
S	9.79356	-1.67894	-1.00986
C	10.10951	2.6724	0.17016
C	10.61165	-1.90695	0.4725
N	10.41064	3.38119	1.03416
N	11.21513	-2.10171	1.44058

T8 : symmetry c1 -9092.3194008

0 1

S	-1.43998	0.49446	-1.65653
S	-4.37559	-0.24992	-1.74231

S	-7.66603	0.1315	-1.70917
C	-2.8799	-0.07319	-0.79339
C	-5.38211	-0.54957	-0.30556
C	-6.71922	-0.39756	-0.29601
C	-9.05471	0.67607	-0.74953
S	-1.52988	-0.49213	1.59517
S	-4.45473	-1.11705	1.10307
S	-7.74472	-0.74831	1.11404
C	-2.91449	-0.46547	0.49216
C	-9.0776	0.28223	0.53991
S	1.50174	-1.67601	-0.5528
S	4.4171	-1.68725	0.27695
S	7.71348	-1.56237	-0.01625
C	2.90027	-0.7803	0.06093
C	5.37499	-0.22427	0.60701
C	6.71487	-0.177	0.49049
C	9.08744	-0.5632	-0.52594
S	1.47486	1.57029	0.45505
S	4.39399	1.15642	1.15283
S	7.69199	1.25974	0.86963
C	2.89046	0.50431	0.45761
C	9.06491	0.72548	-0.12955
S	10.32324	-1.40432	-1.47372
H	11.38097	-1.04733	-0.71013
S	-10.24408	1.6509	-1.62607
H	-11.32851	0.91106	-1.30046

Ge	0.00112	-0.0644	-0.01945
S	10.28919	1.9606	-0.50471
S	-10.32684	0.68911	1.7396
C	11.62288	1.33316	0.35574
C	-11.66156	-0.14351	1.07781
N	12.55632	0.89898	0.88723
N	-12.59425	-0.6556	0.61939

T9: symmetry c1 -9184.51656

0 1

S	-1.13805	-1.64103	-0.1414
S	-4.08675	-1.48684	0.53802
S	-7.33753	-1.51637	0.00606
C	-2.56909	-0.6388	0.15099
C	-5.0673	-0.0068	0.42254
C	-6.39469	-0.01497	0.20533
C	-8.80244	-0.69965	-0.5547
S	-1.17936	1.75666	-0.02937
S	-4.12315	1.4852	0.64214
S	-7.3768	1.46868	0.09422
C	-2.58459	0.70503	0.19765
C	-8.82254	0.64688	-0.50721
S	1.79771	-0.05867	1.72003
S	4.729	0.69698	1.56364
S	8.02055	0.33062	1.57059

C	3.21873	0.27841	0.71874
C	5.7096	0.62346	0.08035
C	7.04748	0.47812	0.08592
C	9.39958	-0.43302	0.75768
S	1.82776	0.07706	-1.67659
S	4.7551	0.81045	-1.40994
S	8.04748	0.46169	-1.38446
C	3.23137	0.3303	-0.62471
C	9.39898	-0.38118	-0.58977
S	10.61048	-1.14639	1.83359
H	11.68333	-0.51051	1.31048
S	-10.12145	-1.69657	-1.22558
Ge	0.3281	0.06328	0.00164
S	10.63289	-1.07447	-1.66779
S	-10.17813	1.68126	-1.0432
C	11.97199	-0.09822	-1.25953
C	-10.50534	-2.65453	0.13456
C	-10.94817	1.96428	0.45542
N	12.90797	0.51554	-0.96036
N	-11.51874	2.19697	1.435
N	-10.81206	-3.35284	1.00506

T10 : symmetry c1 -9276.7136587

0 1

S	1.4778	1.47503	0.82444
S	4.41396	0.8793	1.28959

S	7.67901	1.17562	0.92135
C	2.89697	0.48898	0.44181
C	5.38578	-0.22075	0.28328
C	6.71739	-0.10424	0.13464
C	9.16759	0.81512	0.0395
S	1.49205	-1.24954	-1.20563
S	4.42543	-1.50299	-0.49171
S	7.68609	-1.21734	-0.86824
C	2.90335	-0.58817	-0.36351
C	9.17017	-0.26274	-0.76946
S	-1.51501	0.97996	-1.49559
S	-4.45499	1.36793	-0.87213
S	-7.70797	0.90774	-1.15521
C	-2.91477	0.55684	-0.49528
C	-5.39206	0.33069	0.22925
C	-6.71918	0.14309	0.11762
C	-9.16471	-0.02911	-0.8025
S	-1.45639	-1.06998	1.21657
S	-4.40325	-0.42032	1.50394
S	-7.65402	-0.89385	1.22766
C	-2.89051	-0.25199	0.57875
C	-9.14072	-0.84022	0.27347
S	-10.5365	0.11316	-1.93668
S	10.53626	1.9446	0.24633
Ge	-0.00105	0.04033	-0.11961
S	-10.4769	-1.91349	0.7782

S	10.54041	-0.75199	-1.80448
C	-11.07101	-1.04171	2.12177
C	11.09345	1.46098	1.78711
C	11.00123	-2.20394	-1.03191
N	-11.52169	-0.50863	3.04481
N	11.36342	-3.20091	-0.56908
N	11.52076	1.19035	2.828
C	-11.05381	1.70319	-1.58789
N	-11.45353	2.77514	-1.4133

T11: symmetry c1 -9113.4275079

0 1

S	-2.29456	1.35599	-1.1576
S	-5.20061	0.62	-1.61545
S	-8.48403	0.85522	-1.2572
C	-3.68322	0.34352	-0.72395
C	-6.14815	-0.42276	-0.52686
C	-7.48251	-0.31947	-0.38361
C	-9.92463	0.6246	-0.22643
S	-2.24354	-1.21106	1.06926
S	-5.15531	-1.6299	0.32685
S	-8.42173	-1.39252	0.68294
C	-3.66188	-0.67338	0.15556
C	-9.88536	-0.38906	0.66025
S	0.77689	-0.90332	-1.38349

S	3.7041	-1.22912	-0.66093
S	6.96735	-0.74074	-0.8873
C	2.14737	-0.4106	-0.37768
C	4.60417	-0.11371	0.3944
C	5.93228	0.08043	0.3019
C	8.40491	0.25166	-0.55576
S	0.63097	1.30102	1.19769
S	3.57548	0.70223	1.59599
S	6.82313	1.19353	1.37329
C	2.09015	0.46377	0.64253
C	8.3366	1.13596	0.46135
S	9.79866	0.00567	-1.61795
S	-11.2652	1.76764	-0.42503
H	-11.81363	1.20474	-1.52867
Ge	-0.78392	0.0907	-0.07191
S	9.62256	2.27045	0.90509
H	9.44327	2.15683	2.2396
S	-11.1274	-0.9127	1.80418
H	-12.0664	-0.06703	1.32449
C	10.82058	-1.16616	-0.69391
O	11.85436	-1.56346	-1.1497
C	10.33662	-1.57603	0.62735
N	10.00829	-1.92858	1.67531

T12 : symmetry c1 -9394.9283441

0 1

S	0.36387	-1.71034	0.54361
S	-2.57781	-1.36682	1.16892
S	-5.86485	-1.55907	0.96096
C	-1.08432	-0.69365	0.4735
C	-3.59431	-0.03238	0.58296
C	-4.93545	-0.11315	0.49545
C	-7.2936	-1.07705	0.02656
S	0.24528	1.48877	-0.60781
S	-2.68124	1.43315	0.16503
S	-5.96508	1.23044	-0.07275
C	-1.1307	0.5714	0.0205
C	-7.34453	0.18759	-0.43553
S	3.29815	0.4803	1.60568
S	6.20627	1.18467	1.09642
S	9.46906	0.72933	1.21578
C	4.69094	0.45181	0.51166
C	7.15766	0.54299	-0.26587
C	8.48937	0.35169	-0.22206
C	10.909	-0.14461	0.65709
S	3.25795	-0.64113	-1.60138
S	6.17016	0.19975	-1.70738
S	9.44584	-0.25412	-1.58691
C	4.6758	0.00655	-0.75725
C	10.90934	-0.58212	-0.61721
S	12.18247	-0.27457	1.87625
H	13.08826	-0.79244	1.01688

S	-8.51394	-2.37542	-0.20184
Ge	1.797	-0.05369	0.00247
S	12.21779	-1.49197	-1.39352
H	12.76211	-0.46162	-2.08472
S	-8.71505	0.84275	-1.48861
C	-9.94688	-1.61878	-0.14921
C	-8.97181	2.39178	-1.26335
C	-11.19232	-2.26755	-0.46262
O	-11.62114	-2.3832	-1.59551
C	-8.44663	3.46113	-0.47911
O	-7.47032	4.12658	-0.78001
C	-9.27051	3.77571	0.70372
N	-9.87989	4.00526	1.65627
C	-11.97461	-2.65451	0.72515
N	-12.56629	-3.0006	1.65335

T13: symmetry c1 -9318.9428393

0 1

S	1.46336	1.54757	-1.06026
S	4.41924	1.72167	-0.41031
S	7.65584	1.44876	-0.95883
C	2.89674	0.8002	-0.33488
C	5.39665	0.35546	0.17841
C	6.71917	0.2409	-0.04045
C	9.13291	0.48251	-1.06025
S	1.50092	-1.37987	0.66484

S	4.45255	-0.8376	1.10252
S	7.70053	-1.11713	0.5534
C	2.911	-0.35703	0.3501
C	9.15606	-0.67447	-0.36607
S	-1.43649	1.08943	1.38258
S	-4.36931	0.37051	1.66902
S	-7.62411	0.85032	1.50705
C	-2.87792	0.32547	0.69535
C	-5.38109	-0.24369	0.33969
C	-6.71109	-0.05305	0.27014
C	-9.13362	0.92288	0.58953
S	-1.54014	-0.65844	-1.53021
S	-4.4598	-1.1527	-0.88254
S	-7.72662	-0.67175	-1.05117
C	-2.92004	-0.36448	-0.45821
C	-9.18272	0.22407	-0.56386
S	-10.44035	1.94381	1.21257
H	-10.28762	1.57951	2.50493
S	10.4415	1.06655	-2.10166
H	10.33883	2.36138	-1.72856
Ge	-0.00195	0.1383	-0.09179
S	-10.56751	0.13641	-1.66239
S	10.5053	-1.81823	-0.3062
C	11.55203	-1.15318	1.01063
O	12.56095	-1.71483	1.32798
C	-11.56999	-1.19426	-0.95789

O	-12.59193	-1.52999	-1.48422
C	11.12029	0.09957	1.63679
N	10.83262	1.08708	2.15868
C	-11.08629	-1.80877	0.28156
N	-10.75716	-2.32277	1.26023

T14: symmetry c1 -9524.4583333

0 1

S	-0.7903	-1.4794	-0.77293
S	-3.75025	-1.62559	-0.14274
S	-7.01111	-1.4026	-0.64434
C	-2.2274	-0.7041	-0.08562
C	-4.73089	-0.24648	0.40501
C	-6.05811	-0.15928	0.20272
C	-8.42391	-0.36363	-0.89965
S	-0.83867	1.513	0.84139
S	-3.79222	0.98998	1.27386
S	-7.04779	1.20643	0.77569
C	-2.24542	0.47813	0.55466
C	-8.42471	0.83323	-0.27186
S	2.12449	-0.89897	1.62591
S	5.05077	-0.14154	1.861
S	8.34777	-0.47841	1.73235
C	3.55293	-0.14669	0.89827
C	6.04665	0.4539	0.51147
C	7.38514	0.32198	0.46603

C	9.75564	-0.75702	0.69438
S	2.18743	0.73502	-1.35355
S	5.10532	1.28294	-0.75123
S	8.3947	0.96765	-0.84712
C	3.57844	0.49785	-0.2815
C	9.76514	-0.11337	-0.49127
S	10.9872	-1.84946	1.35181
H	11.96454	-0.91754	1.41867
S	-9.66839	-0.9099	-2.03516
Ge	0.67093	-0.02096	0.12801
S	10.99099	-0.23175	-1.75475
S	-9.61178	2.13759	-0.44353
C	-11.054	1.46223	0.40586
O	-11.17093	0.35479	0.84571
C	-10.72276	-2.02641	-1.05974
O	-11.72997	-2.44918	-1.54717
C	12.39812	0.57612	-0.98113
O	12.46583	0.95663	0.15668
C	-12.11379	2.46773	0.47448
N	-12.94476	3.26588	0.52802
C	-10.25717	-2.42719	0.26488
N	-9.90544	-2.81751	1.29117
C	13.513	0.6903	-1.92226
N	14.38931	0.78401	-2.66657

T15: symmetry c1 -9729.9671302

0 1

S	1.60324	1.37553	0.7797
S	4.52958	0.75307	1.2466
S	7.81214	0.81517	0.95166
C	2.9865	0.30979	0.47815
C	5.45176	-0.48817	0.36633
C	6.78912	-0.45034	0.22393
C	9.16088	0.527	-0.17112
S	1.50316	-1.54692	-0.95634
S	4.44215	-1.80922	-0.26648
S	7.72953	-1.68708	-0.63985
C	2.94587	-0.84656	-0.20645
C	9.13881	-0.63477	-0.86614
S	-1.43559	-0.81761	1.50399
S	-4.38396	-1.26159	0.95835
S	-7.64698	-0.80628	1.18203
C	-2.84404	-0.50724	0.47786
C	-5.32814	-0.36105	-0.25069
C	-6.6581	-0.17952	-0.15997
C	-9.05948	0.19811	0.81477
S	-1.39513	0.89607	-1.43067
S	-4.3486	0.24516	-1.60677
S	-7.61488	0.69187	-1.38411
C	-2.8288	0.17301	-0.68207
C	-9.03002	0.89712	-0.34143
S	-10.34552	0.30491	2.02798

S	10.39592	1.75746	-0.49838
Ge	0.06857	-0.06673	-0.01532
S	-10.21775	2.08259	-0.91049
S	10.34462	-1.1722	-2.04887
C	11.6356	-1.92855	-1.02433
O	12.60512	-2.40627	-1.5375
C	10.57249	2.58632	1.08169
O	9.9607	2.35683	2.08748
C	-11.62227	1.0355	-1.34682
O	-11.72171	-0.14181	-1.15331
C	-11.36809	-1.17321	1.74743
O	-12.39315	-1.29426	2.35198
C	11.43402	-1.91205	0.42496
N	11.32293	-1.9219	1.57298
C	11.58129	3.64205	0.983
N	12.37893	4.47218	0.91227
C	-10.85864	-2.19994	0.84292
N	-10.47342	-3.06306	0.18264
C	-12.67463	1.83738	-1.96969
N	-13.49953	2.47493	-2.46312

T16 : symmetry c1 -9021.2197938

0 1

S	-1.94924	-0.39607	1.64893

S	-4.88357	0.37386	1.59987
S	-8.15023	-0.13441	1.42587
C	-3.35302	0.1471	0.71638
C	-5.83276	0.58182	0.108
C	-7.16031	0.36953	0.04303
C	-9.57326	-0.57847	0.44175
S	-1.91384	0.46696	-1.63718
S	-4.85226	1.12512	-1.27598
S	-8.10306	0.61404	-1.44794
C	-3.33969	0.48633	-0.58477
C	-9.54058	-0.24728	-0.86383
S	1.04383	-1.51676	-0.44059
S	3.97033	-1.49774	0.34566
S	7.25618	-1.38811	-0.04005
C	2.45435	-0.59465	0.10699
C	4.93717	-0.0226	0.58313
C	6.27291	0.01415	0.42246
C	8.67991	-0.41477	-0.5125
S	1.04161	1.77611	0.4
S	3.96851	1.38238	1.08881
S	7.23959	1.48436	0.70279
C	2.45244	0.70764	0.44159
C	8.65996	0.89511	-0.18322
S	9.98368	-1.2455	-1.36381
S	-10.88769	-1.45147	1.24992
Ge	-0.44641	0.10536	0.03046

S	9.871	2.14274	-0.49688
S	-10.77007	-0.50911	-2.10694
H	-11.69567	-0.96772	-1.23518
H	-11.47742	-0.38	1.83293
H	10.77394	1.29032	-1.0282
C	11.01483	-1.76564	0.05771
O	12.02964	-2.37038	-0.08328
H	10.57894	-1.44327	1.02185

T17: symmetry c1 -9134.5248035

0 1

S	0.65916	1.73731	-0.11457
S	3.59485	1.47801	0.59543
S	6.8666	1.40887	0.12818
C	2.05464	0.68797	0.17594
C	4.53219	-0.02919	0.46187
C	5.86407	-0.05692	0.27611
C	8.31194	0.56462	-0.45911
S	0.59521	-1.66137	-0.07352
S	3.53819	-1.49652	0.62681
S	6.80939	-1.56297	0.15882
C	2.03009	-0.65634	0.19022
C	8.28588	-0.7873	-0.44514
S	-2.34414	0.00215	-1.71753
S	-5.26846	0.77893	-1.513
S	-8.52632	0.29007	-1.51983

C	-3.75643	0.31469	-0.69332
C	-6.23871	0.62623	-0.02726
C	-7.56943	0.42418	-0.02398
C	-9.97137	-0.3609	-0.7214
S	-2.34915	0.01931	1.68044
S	-5.27386	0.79669	1.4594
S	-8.54876	0.30906	1.45027
C	-3.75789	0.32369	0.65138
C	-9.99254	-0.34357	0.62564
S	-11.22202	-0.90792	-1.8449
H	-12.14307	-1.10939	-0.87631
S	9.62884	1.58795	-1.05738
Ge	-0.86207	0.05688	-0.02566
S	-11.31057	-0.95297	1.6426
H	-11.87227	0.24391	1.93856
S	9.56252	-1.87302	-1.02029
C	10.48618	-2.14682	0.52983
O	11.43905	-2.85725	0.57626
H	10.06024	-1.5826	1.38059
C	10.55989	1.86542	0.48766
O	11.53763	2.54211	0.51896
H	10.11312	1.33741	1.35089

T18: symmetry c1 -9134.5274149

0 1

S	-1.48174	1.77815	-0.35525
S	-4.39549	1.38429	-1.09852
S	-7.6716	1.48577	-0.757
C	-2.89095	0.70877	-0.42573
C	-5.37163	-0.02236	-0.61189
C	-6.70946	0.0141	-0.46951
C	-9.10692	0.89135	0.10096
S	-1.49627	-1.51751	0.47397
S	-4.40806	-1.4984	-0.3659
S	-7.69887	-1.39011	-0.02701
C	-2.89768	-0.59472	-0.09577
C	-9.13161	-0.41999	0.42402
S	1.43432	0.46887	1.73306
S	4.38172	1.11091	1.43609
S	7.63991	0.66642	1.6514
C	2.88122	0.48399	0.71009
C	5.3894	0.58696	0.06539
C	6.71996	0.40232	0.14872
C	9.0657	-0.24156	1.1107
S	1.53451	-0.38628	-1.55501
S	4.46969	0.36524	-1.442
S	7.74231	-0.07881	-1.21876
C	2.92018	0.14787	-0.59121
C	9.12483	-0.57216	-0.19765
S	10.22885	-0.57256	2.39873
H	11.15184	-1.11831	1.5775

S	-10.32442	2.13658	0.39851
H	-11.23488	1.2812	0.91202
Ge	-0.001	0.10804	0.03629
S	10.44233	-1.44464	-0.98355
S	-10.44966	-1.25572	1.24798
C	11.51167	-0.03978	-1.47147
O	12.5432	-0.19749	-2.04272
H	11.08049	0.93146	-1.1645
C	-11.45473	-1.77015	-0.19451
O	-12.47115	-2.37653	-0.07447
H	-11.00197	-1.44271	-1.14909

T19: symmetry c1 -9247.837081

0 1

S	1.05919	1.50752	-0.87722
S	4.01202	1.68593	-0.21752
S	7.27502	1.45953	-0.704
C	2.49429	0.75582	-0.15894
C	4.99616	0.31792	0.35694
C	6.32354	0.22612	0.1578
C	8.69886	0.42571	-0.92552
S	1.109	-1.45299	0.79231
S	4.05549	-0.90231	1.24843
S	7.31455	-1.13232	0.74292
C	2.51313	-0.4142	0.50333

C	8.72495	-0.74977	-0.26325
S	-1.8679	0.96529	1.51212
S	-4.7917	0.19637	1.75025
S	-8.06671	0.53743	1.59791
C	-3.28885	0.19012	0.7945
C	-5.77803	-0.42487	0.40498
C	-7.11517	-0.28731	0.33758
C	-9.50393	0.7513	0.5788
S	-1.90872	-0.73113	-1.43202
S	-4.82673	-1.28387	-0.82989
S	-8.11445	-0.93964	-0.9749
C	-3.30585	-0.47972	-0.37128
C	-9.53804	0.07057	-0.58741
S	-10.71102	1.84078	1.2698
H	-11.62499	1.6225	0.29958
S	9.95453	1.05188	-2.00459
Ge	-0.40094	0.06049	0.04116
S	-10.86052	0.08914	-1.75601
S	10.02029	-1.95566	-0.29992
C	11.13618	1.75798	-0.82452
O	11.07102	1.69353	0.36585
H	11.94669	2.25952	-1.38234
C	11.04996	-1.38404	1.10994
O	12.02386	-1.98192	1.43937
H	10.66571	-0.45574	1.5621
C	-11.87256	-1.29799	-1.11796

O	-12.89271	-1.62715	-1.63388
H	-11.42013	-1.75875	-0.21998

T20: symmetry c1 -9361.1371729

0 1

S	1.49063	-1.46211	-0.84655
S	4.42705	-0.87561	-1.3207
S	7.69937	-1.12571	-0.93103
C	2.90202	-0.44923	-0.50581
C	5.38869	0.27518	-0.36142
C	6.72103	0.17512	-0.2061
C	9.16209	-0.78128	0.01129
S	1.48051	1.35501	1.0551
S	4.41768	1.58767	0.34832
S	7.69078	1.33346	0.73877
C	2.89876	0.66407	0.2483
C	9.15826	0.33741	0.77092
S	-1.48836	-0.90883	1.47754
S	-4.42712	-1.37003	0.90098
S	-7.69645	-0.96704	1.17141
C	-2.90292	-0.55644	0.47028
C	-5.39125	-0.40313	-0.24137
C	-6.72238	-0.24301	-0.13305
C	-9.15596	-0.01519	0.83944
S	-1.48474	1.0128	-1.32677

S	-4.42438	0.30776	-1.55616
S	-7.69459	0.70917	-1.28324
C	-2.90073	0.20195	-0.64007
C	-9.15516	0.74741	-0.27723
S	-10.45325	-0.12493	2.04107
S	10.46682	-1.97447	-0.10276
Ge	-0.00064	-0.00893	0.04721
S	-10.44963	1.83106	-0.81526
S	10.45568	0.88741	1.84497
C	-11.38653	-1.55205	1.38878
O	-12.35407	-1.97356	1.93705
H	-10.95069	-1.94919	0.45292
C	-11.37574	0.71553	-1.92455
O	-12.33801	1.08007	-2.52095
H	-10.94179	-0.30131	-1.9599
C	11.38405	-1.32294	-1.5406
O	12.35171	-1.86687	-1.96745
H	10.93882	-0.39188	-1.93861
C	11.36945	1.99653	0.71912
O	12.33069	2.59958	1.07531
H	10.92934	2.025	-0.29529

T21 : symmetry c1 -9112.3876197

0 1

S	-2.14648	0.96762	-1.41738
S	-5.05356	0.16123	-1.72586

S	-8.33983	0.51628	-1.51738
C	-3.55836	0.12297	-0.75828
C	-6.03752	-0.53974	-0.418
C	-7.37266	-0.38901	-0.33802
C	-9.80058	0.59092	-0.49155
S	-2.17644	-0.90185	1.41986
S	-5.07951	-1.48033	0.75221
S	-8.34822	-1.12582	0.95677
C	-3.56922	-0.61848	0.36347
C	-9.79329	-0.1467	0.63591
S	0.88507	-1.31329	-0.9608
S	3.8102	-1.43288	-0.17604
S	7.09732	-1.08887	-0.41367
C	2.25356	-0.56983	-0.11945
C	4.71116	-0.08426	0.55504
C	6.04598	0.04752	0.44371
C	8.45965	0.07078	-0.56991
S	0.73984	1.5118	0.92465
S	3.68163	1.03849	1.4754
S	6.94263	1.39303	1.19587
C	2.19648	0.5489	0.62399
C	8.37228	1.20448	0.18986
S	9.78798	-0.35113	-1.57579
S	-11.11683	1.65605	-1.01662
Ge	-0.67555	0.0227	-0.00059
S	9.52942	2.51552	0.33303

S	-11.06184	-0.32613	1.85408
H	-11.97686	0.37448	1.14787
H	-11.66149	0.82262	-1.93566
H	10.47472	1.89818	-0.41074
N	10.9497	-1.27352	-0.27777
O	10.59446	-1.27911	0.86981
O	11.93886	-1.74188	-0.77884

T22: symmetry c1 -9316.8550138

0 1

S	-0.20054	-1.65338	-0.24308
S	-3.15162	-1.5103	0.42541
S	-6.41501	-1.5504	-0.08803
C	-1.63708	-0.65646	0.04045
C	-4.14079	-0.03513	0.31039
C	-5.46988	-0.05216	0.10806
C	-7.89067	-0.75495	-0.63326
S	-0.25805	1.74427	-0.14881
S	-3.20245	1.46349	0.51395
S	-6.46637	1.42176	0.00373
C	-1.65903	0.6874	0.08014
C	-7.91438	0.61099	-0.59079
S	2.71887	-0.05106	1.62428
S	5.64565	0.73739	1.47972
S	8.90418	0.24906	1.5124
C	4.14337	0.29398	0.63027

C	6.63426	0.62432	0.00261
C	7.96496	0.42214	0.00943
C	10.35954	-0.37879	0.71435
S	2.76742	0.06695	-1.7712
S	5.68774	0.83464	-1.49086
S	8.96151	0.34568	-1.45573
C	4.16347	0.33904	-0.71359
C	10.39666	-0.32607	-0.63143
S	11.59769	-0.95355	1.83784
H	12.53082	-1.12709	0.87544
S	-9.18317	-1.77317	-1.21944
Ge	1.25952	0.05793	-0.10204
S	11.72763	-0.90661	-1.64839
H	12.29048	0.29854	-1.90636
S	-9.24267	1.61766	-1.11318
N	-10.14062	1.92505	0.57144
O	-9.68194	1.41464	1.55468
O	-11.10685	2.63031	0.44534
N	-10.07627	-2.20626	0.43932
O	-9.63948	-1.73675	1.4525
O	-11.01713	-2.93587	0.26789

T23: symmetry c1 -9316.8630288

0 1

S	1.46768	-1.72691	-0.57862
S	4.39213	-1.26854	-1.23445

S	7.66092	-1.45015	-0.89036
C	2.88827	-0.67421	-0.48815
C	5.37853	0.04936	-0.55774
C	6.71615	-0.0124	-0.42176
C	9.08054	-1.01395	0.05094
S	1.50858	1.42458	0.69547
S	4.42844	1.48551	-0.10976
S	7.72313	1.30709	0.19152
C	2.90573	0.57176	0.01678
C	9.12602	0.2513	0.56768
S	-1.43546	-0.69322	1.67474
S	-4.39076	-1.24971	1.30321
S	-7.6385	-0.80479	1.58792
C	-2.88402	-0.54827	0.66457
C	-5.39514	-0.53677	0.0183
C	-6.72535	-0.35997	0.12242
C	-9.04143	0.18137	1.19942
S	-1.53047	0.60441	-1.46606
S	-4.47569	-0.1124	-1.44465
S	-7.75387	0.28907	-1.16286
C	-2.92145	-0.03766	-0.57863
C	-9.11065	0.70415	-0.06224
S	-10.19987	0.32946	2.50866
H	-11.12417	0.96561	1.75437
S	10.28386	-2.28534	0.16716
H	11.20233	-1.50001	0.77354

Ge	0.00131	-0.11436	0.04042
S	-10.41509	1.63629	-0.6818
S	10.43841	0.91532	1.45698
N	-11.60975	0.20509	-1.32363
O	-11.28057	-0.92738	-1.09514
O	-12.58873	0.62334	-1.88503
N	11.56752	1.58826	-0.01286
O	11.21081	1.34449	-1.13373
O	12.54064	2.18227	0.37279

T24 : symmetry c1 -9521.3302842

0 1

S	-0.89472	-1.55163	-0.59677
S	-3.82904	-1.52069	0.16159
S	-7.09656	-1.42705	-0.30457
C	-2.31116	-0.62206	-0.085
C	-4.80077	-0.04166	0.35198
C	-6.13215	-0.00506	0.16779
C	-8.56638	-0.52551	-0.67204
S	-0.90703	1.76005	0.17199
S	-3.84006	1.3785	0.83014
S	-7.11219	1.46995	0.36521
C	-2.31705	0.68817	0.21725
C	-8.5737	0.80597	-0.36396
S	2.05614	0.5546	-1.79721
S	4.98561	-0.22051	-1.78136

S	8.25137	0.17704	-1.72611
C	3.47873	0.04515	-0.87145
C	5.96818	-0.41213	-0.30948
C	7.30516	-0.26012	-0.27935
C	9.67656	0.68606	-0.83148
S	2.08803	-0.18841	1.51824
S	5.01533	-0.86917	1.1222
S	8.30932	-0.50966	1.15605
C	3.49106	-0.25166	0.44002
C	9.72006	0.38774	0.50226
S	10.888	1.49448	-1.80986
H	11.8083	1.53124	-0.82004
S	-9.87313	-1.39471	-1.43854
Ge	0.58664	0.10595	-0.15171
S	11.03695	0.72592	1.55401
S	-9.89248	1.91012	-0.66776
N	12.14599	-0.88012	1.27213
O	11.77904	-1.65919	0.43469
O	13.11861	-0.91264	1.98013
N	-10.75002	-2.15819	0.10671
O	-10.29571	-1.91384	1.18906
O	-11.69963	-2.8296	-0.20004
N	-10.7879	1.87494	1.0454
O	-10.33754	1.16541	1.90067
O	-11.7444	2.60377	1.0692

T25: symmetry c1 -9725.8030333

0 1

S	-1.54262	-1.48431	-1.1543
S	-4.44757	-1.78054	-0.34489
S	-7.74246	-1.5111	-0.47905
C	-2.91315	-0.88853	-0.20531
C	-5.36789	-0.56601	0.57363
C	-6.70771	-0.46071	0.51978
C	-9.11783	-0.40025	-0.47686
S	-1.43196	1.08187	1.07365
S	-4.3501	0.46838	1.60229
S	-7.64784	0.7301	1.45192
C	-2.87017	0.12741	0.6742
C	-9.07143	0.63467	0.41243
S	1.42005	0.91452	-1.36603
S	4.34799	0.26664	-1.78973
S	7.6383	0.59108	-1.66486
C	2.86665	0.04418	-0.82819
C	5.3719	-0.59522	-0.61725
C	6.70983	-0.46492	-0.57187
C	9.06054	0.66567	-0.61749
S	1.54894	-1.30119	1.21068
S	4.46074	-1.67699	0.46142
S	7.75315	-1.34159	0.57426
C	2.91681	-0.83333	0.18911
C	9.11108	-0.22475	0.41621
S	10.29722	1.81659	-1.04022

S	-10.43546	-0.76734	-1.55453
Ge	-0.00097	-0.23975	-0.05553
S	10.48237	-0.45204	1.4671
S	-10.37897	1.7465	0.71344
N	-9.724	3.29572	-0.22754
O	-10.44241	4.2513	-0.09295
O	-8.70659	3.18218	-0.85492
N	-11.70339	-1.54303	-0.31999
O	-11.44851	-1.50012	0.85326
O	-12.66535	-1.99585	-0.88131
N	9.84873	0.45616	3.04462
O	10.61523	0.36142	3.96703
O	8.79568	1.02894	2.97683
N	11.59383	0.65704	-1.88117
O	11.40566	-0.5286	-1.83472
O	12.50183	1.27225	-2.37369

T26: symmetry c1 -8963.2455633

0 1

S	-1.78283	1.37248	1.07425
S	-4.70346	1.61538	0.28998
S	-7.9792	1.24418	0.59912
C	-3.16386	0.72616	0.1744
C	-5.62799	0.32905	-0.52231
C	-6.95927	0.18184	-0.38981
C	-9.39369	0.15311	0.5844

S	-1.68635	-1.29309	-1.03014
S	-4.61837	-0.71903	-1.5488
S	-7.87734	-1.08826	-1.23606
C	-3.12633	-0.33023	-0.65665
C	-9.3364	-0.91002	-0.24134
S	1.21981	-0.97088	1.33042
S	4.1445	-0.24963	1.6684
S	7.44107	-0.55872	1.46104
C	2.64125	-0.10123	0.7257
C	5.13187	0.55149	0.42166
C	6.46922	0.42121	0.3421
C	8.8083	-0.72619	0.32297
S	1.26068	1.11607	-1.35178
S	4.18059	1.58168	-0.67592
S	7.47346	1.26091	-0.86281
C	2.65655	0.72589	-0.33399
C	8.82012	0.10742	-0.73473
S	10.00188	-1.95202	0.76601
S	-10.73348	0.53352	1.68143
Ge	-0.24634	0.09936	-0.00041
S	10.06772	0.24441	-1.98069
S	-10.551	-2.16315	-0.5241
H	-11.49582	-1.55632	0.22814
H	-11.31738	1.49068	0.92077
H	11.09479	0.1358	-1.10314
N	11.48209	-1.03098	0.75284

H	11.78557	-0.81309	1.69623
H	12.19932	-1.57207	0.28137

T27: symmetry c1 -9018.5789986

0 1

S	1.05323	1.69016	-0.37845
S	3.97347	1.63948	0.45189
S	7.23028	1.49859	-0.10004
C	2.45562	0.75186	0.1597
C	4.93311	0.14526	0.59882
C	6.2584	0.09048	0.36645
C	8.69282	0.55132	-0.48222
S	1.03244	-1.62444	0.36202
S	3.95513	-1.25954	1.09721
S	7.18924	-1.4265	0.53833
C	2.44819	-0.56109	0.45052
C	8.66029	-0.76099	-0.18646
S	-1.90137	-0.38258	-1.62937
S	-4.82695	0.41357	-1.6433
S	-8.09295	-0.01692	-1.61859
C	-3.33106	0.13256	-0.71803
C	-5.82526	0.58473	-0.17858
C	-7.15949	0.40869	-0.16251
C	-9.5576	-0.48178	-0.73071
S	-1.96773	0.3351	1.69005
S	-4.88549	1.04643	1.26112

S	-8.16832	0.61724	1.28199
C	-3.35652	0.41938	0.59547
C	-9.60273	-0.18577	0.58294
S	-10.79345	-1.243	-1.74044
H	-11.7367	-1.22534	-0.77265
S	10.07076	1.34649	-1.24797
Ge	-0.44305	0.04234	0.03562
S	-10.94596	-0.56229	1.67719
H	-11.49808	0.67455	1.70981
S	10.01952	-1.87987	-0.45421
N	9.34984	-3.28998	0.26558
H	9.24539	-4.04638	-0.39814
H	9.85965	-3.58461	1.08843
N	10.79158	2.17815	0.08858
H	11.70265	1.79875	0.31448
H	10.85033	3.17233	-0.09192

T28: symmetry c1 -9018.5808153

0 1

S	1.41041	-0.11974	-1.71612
S	4.35149	0.6119	-1.67061
S	7.63925	0.19019	-1.69027
C	2.85104	0.28885	-0.76782
C	5.3562	0.64903	-0.20101
C	6.69108	0.47648	-0.2121
C	9.00503	-0.55019	-0.82611

S	1.49723	0.30311	1.65497
S	4.42734	0.98938	1.27956
S	7.71639	0.56912	1.23607
C	2.88445	0.45909	0.56528
C	9.04311	-0.38154	0.50954
S	-1.53795	1.82545	-0.26463
S	-4.44913	1.69499	0.58644
S	-7.71567	1.60304	0.09566
C	-2.93396	0.83992	0.19988
C	-5.40626	0.1929	0.62064
C	-6.73704	0.15719	0.41903
C	-9.18466	0.68905	-0.33431
S	-1.50636	-1.54179	0.17626
S	-4.42104	-1.25134	0.96788
S	-7.66839	-1.36739	0.48375
C	-2.92224	-0.49372	0.37221
C	-9.1498	-0.64248	-0.16321
S	-10.5684	1.5691	-1.00979
H	-11.10144	1.9883	0.16296
S	10.20495	-1.36166	-1.84096
H	11.26458	-0.82884	-1.18525
Ge	-0.03404	0.15118	-0.00977
S	-10.51906	-1.7287	-0.50024
S	10.27007	-0.94359	1.65067
N	11.73417	-0.3261	0.93332
H	12.0661	0.49511	1.4283

H	12.44352	-1.05092	0.96295
N	-9.82281	-3.20811	0.02873
H	-10.31231	-3.60242	0.82163
H	-9.73039	-3.87992	-0.72225

T29: symmetry c1 -9073.9124224

0 1

S	-1.31945	-1.73646	-0.36171
S	-4.22983	-1.62652	0.49711
S	-7.49331	-1.47404	-0.01226
C	-2.70698	-0.76527	0.15604
C	-5.17337	-0.11867	0.60308
C	-6.50132	-0.05942	0.3878
C	-8.95191	-0.52672	-0.40914
S	-1.25793	1.60146	0.25886
S	-4.17588	1.29378	1.03685
S	-7.41521	1.4722	0.51651
C	-2.6834	0.55714	0.39931
C	-8.90263	0.79521	-0.16262
S	1.64903	0.25671	-1.70365
S	4.57915	-0.51896	-1.69836
S	7.8732	-0.14994	-1.69688
C	3.08308	-0.22307	-0.77918
C	5.58247	-0.65152	-0.23336
C	6.91996	-0.50014	-0.23579
C	9.24829	0.5249	-0.79447

S	1.72771	-0.34828	1.63934
S	4.64773	-1.05591	1.22714
S	7.9434	-0.68601	1.20488
C	3.11319	-0.4653	0.54284
C	9.28333	0.28421	0.53016
S	10.45943	1.37353	-1.7646
H	11.51167	0.79387	-1.13715
S	-10.34841	-1.33583	-1.12505
Ge	0.19849	-0.09234	-0.01584
S	10.51639	0.76844	1.70006
S	-10.25512	1.91692	-0.45206
N	-9.56011	3.34693	0.20125
H	-9.45811	4.0755	-0.49326
H	-10.05392	3.67923	1.01948
N	-11.05948	-2.10761	0.25217
H	-11.96392	-1.71063	0.47451
H	-11.13027	-3.10737	0.11114
N	11.97355	0.17339	0.95033
H	12.6913	0.88718	1.01906
H	12.29551	-0.67724	1.40015

T30: symmetry c1 -9129.241849

0 1

S	1.55805	1.67146	-0.59532
S	4.47811	1.69307	0.23721
S	7.73556	1.44812	-0.28292

C	2.95016	0.79278	0.05767
C	5.42124	0.21969	0.57519
C	6.74656	0.12236	0.35773
C	9.18655	0.44189	-0.53793
S	1.5014	-1.52373	0.5547
S	4.42731	-1.10125	1.24267
S	7.6605	-1.36898	0.72912
C	2.9282	-0.47298	0.51116
C	9.13874	-0.82068	-0.07502
S	-1.41113	-0.50901	-1.59404
S	-4.34017	0.2693	-1.70734
S	-7.61206	-0.20721	-1.6163
C	-2.84357	0.11099	-0.75424
C	-5.34156	0.60238	-0.27181
C	-6.67343	0.41298	-0.23423
C	-9.03165	-0.64674	-0.64496
S	-1.48372	0.61139	1.61234
S	-4.40596	1.2484	1.09924
S	-7.69501	0.78934	1.16864
C	-2.87184	0.55601	0.51418
C	-9.06902	-0.20793	0.62919
S	-10.20719	-1.64118	-1.53174
S	10.57392	1.11423	-1.39863
Ge	0.04197	0.10302	0.01449
S	-10.39952	-0.49121	1.76067
S	10.48343	-1.98197	-0.19599

N	9.80635	-3.26967	0.71931
H	9.69109	-4.11147	0.17013
H	10.31772	-3.44925	1.57372
N	11.30132	2.10831	-0.18192
H	12.20676	1.75127	0.09682
H	11.37336	3.06852	-0.49375
N	-11.35744	0.91466	1.46964
H	-12.14752	0.70509	0.87171
H	-11.62777	1.36096	2.33607
N	-11.71511	-0.84465	-1.23478
H	-12.10021	-0.48504	-2.10097
H	-12.36082	-1.49427	-0.80144

T31: symmetry c1 -9041.8279617

0 1

S	-2.28646	0.98169	1.4245
S	-5.22377	1.4218	0.80583
S	-8.48716	0.91231	1.0244
C	-3.67641	0.64777	0.37991
C	-6.14912	0.45967	-0.37205
C	-7.47558	0.25314	-0.27522
C	-9.88887	-0.13813	0.67335
S	-2.20036	-0.83605	-1.44561
S	-5.148	-0.17248	-1.70231
S	-8.396	-0.68383	-1.4781
C	-3.64301	-0.0736	-0.75425

C	-9.83608	-0.86916	-0.45723
S	0.72986	-1.29259	0.85993
S	3.65029	-0.69327	1.40682
S	6.94653	-0.87553	1.10544
C	2.13899	-0.25607	0.57338
C	4.6212	0.4903	0.49708
C	5.95974	0.41063	0.37899
C	8.31208	-0.63249	-0.02372
S	0.73122	1.56868	-0.97326
S	3.65196	1.81523	-0.19305
S	6.94821	1.61963	-0.47444
C	2.13878	0.87704	-0.1501
C	8.30959	0.50924	-0.74195
S	9.53508	-1.901	-0.01811
S	-11.21024	-0.16379	1.85506
Ge	-0.75645	0.14803	-0.025
S	9.56196	1.06845	-1.85252
S	-11.0416	-1.98069	-1.11819
H	-11.98066	-1.66669	-0.19826
H	-11.81715	0.98314	1.46526
H	10.56058	0.50595	-1.10797
N	11.00422	-0.95418	0.26146
C	11.20585	-0.61195	1.67516
H	12.06845	0.05669	1.74667
H	10.33098	-0.08087	2.05001
H	11.38539	-1.49455	2.30469

C	12.15827	-1.65328	-0.319
H	13.03587	-1.01148	-0.20986
H	12.37378	-2.61387	0.17172
H	11.98263	-1.83161	-1.38063

T32: symmetry c1 -9175.7413647

0 1

S	-0.23704	-1.746	-0.0842
S	-3.16465	-1.62291	0.70538
S	-6.42994	-1.62842	0.19745
C	-1.66103	-0.75946	0.29275
C	-4.1518	-0.14142	0.62586
C	-5.47859	-0.14401	0.39742
C	-7.87048	-0.77483	-0.43257
S	-0.28161	1.6441	0.13384
S	-3.20247	1.34125	0.90585
S	-6.44359	1.35834	0.36418
C	-1.67746	0.5821	0.38142
C	-7.87403	0.56833	-0.33669
S	2.76168	-0.21525	1.72128
S	5.66955	0.61897	1.49264
S	8.94064	0.23918	1.38337
C	4.14092	0.18558	0.68645
C	6.60148	0.59142	-0.02446
C	7.93731	0.43515	-0.07526
C	10.37545	-0.3286	0.50662

S	2.67402	0.02777	-1.66538
S	5.59249	0.8257	-1.47233
S	8.87926	0.44696	-1.57872
C	4.10719	0.28004	-0.65452
C	10.35849	-0.22557	-0.83667
S	11.66854	-0.91793	1.55868
H	12.56973	-1.02537	0.55709
S	-9.13645	-1.69448	-1.23667
Ge	1.22574	-0.04353	0.06035
S	11.66127	-0.73782	-1.92463
H	12.18459	0.4892	-2.1622
S	-9.18397	1.62703	-0.89774
N	-8.69916	3.07835	-0.07976
N	-9.37718	-2.95745	-0.0554
C	-8.47633	4.21251	-0.98176
H	-8.01424	5.01976	-0.4072
H	-7.79203	3.91813	-1.77648
H	-9.40335	4.59703	-1.43237
C	-9.51621	3.41449	1.09053
H	-9.02754	4.23247	1.62712
H	-10.53634	3.73021	0.82795
H	-9.57328	2.55374	1.75613
C	-10.43967	-2.66905	0.91065
H	-11.44536	-2.67806	0.46373
H	-10.40232	-3.42371	1.70165
H	-10.26378	-1.69258	1.36193

C	-9.49546	-4.28186	-0.6681
H	-9.47496	-5.02968	0.12934
H	-10.42606	-4.41995	-1.24104
H	-8.64673	-4.45732	-1.32882

T33: symmetry c1 -9175.7437607

0 1

S	1.48387	1.71344	-0.57117
S	4.39384	1.78558	0.27897
S	7.68764	1.69566	-0.02129
C	2.89084	0.85278	0.07374
C	5.37181	0.33987	0.63138
C	6.71166	0.30426	0.50669
C	9.06349	0.6992	-0.54197
S	1.49731	-1.51058	0.50476
S	4.40668	-1.03813	1.21494
S	7.71188	-1.10876	0.90497
C	2.89729	-0.42307	0.4974
C	9.07889	-0.58233	-0.12145
S	-1.41049	-0.52705	-1.66332
S	-4.3451	0.21589	-1.81589
S	-7.63178	-0.17744	-1.82928
C	-2.86619	0.05702	-0.83767
C	-5.37742	0.53419	-0.40019
C	-6.71368	0.37184	-0.40698
C	-9.02518	-0.73445	-0.878

S	-1.55572	0.52398	1.56348
S	-4.47336	1.14071	1.00891
S	-7.7673	0.7392	0.97543
C	-2.92302	0.47525	0.4389
C	-9.0911	-0.31865	0.40348
S	-10.22346	-1.69658	-1.74582
H	-11.26325	-1.12962	-1.06314
S	10.31056	1.52605	-1.47774
H	11.31453	0.81102	-0.88639
Ge	0.00329	0.08845	-0.02239
S	-10.36369	-0.64427	1.57799
S	10.32046	-1.79837	-0.41295
N	11.7747	-0.92423	0.0916
N	-11.80026	-0.16523	0.66053
C	11.96795	-0.92417	1.54726
H	12.81824	-0.27691	1.78045
H	11.08279	-0.51247	2.03204
H	12.16251	-1.92784	1.95016
C	12.94026	-1.44887	-0.63195
H	13.80826	-0.84037	-0.36678
H	13.16792	-2.49615	-0.38417
H	12.77022	-1.37008	-1.70647
C	-12.96657	-0.91353	1.14732
H	-13.23101	-0.67364	2.18777
H	-13.82068	-0.66382	0.51318
H	-12.77268	-1.98419	1.07097

C	-12.02212	1.28632	0.66003
H	-12.8576	1.50557	-0.01095
H	-12.25362	1.68106	1.65908
H	-11.13505	1.79008	0.27614

T34: symmetry c1 -9309.6571512

0 1

S	0.96032	1.65649	-0.08725
S	3.89401	1.5171	0.6715
S	7.15743	1.59886	0.22246
C	2.39947	0.66499	0.20998
C	4.8981	0.05317	0.51235
C	6.22907	0.08488	0.31275
C	8.62643	0.80509	-0.41365
S	1.04028	-1.73664	-0.08174
S	3.96356	-1.45481	0.68718
S	7.22473	-1.39129	0.23982
C	2.43025	-0.67949	0.21535
C	8.65712	-0.54092	-0.39657
S	-1.94148	-0.02278	1.75727
S	-4.86852	-0.7994	1.60462
S	-8.16056	-0.46304	1.66122
C	-3.36954	-0.34013	0.75969
C	-5.86727	-0.67142	0.13607
C	-7.2057	-0.53011	0.16076
C	-9.53987	0.35927	0.90098

S	-2.00619	-0.03963	-1.64122
S	-4.92681	-0.80391	-1.37
S	-8.22605	-0.45076	-1.29156
C	-3.39651	-0.34375	-0.58435
C	-9.57334	0.36874	-0.44741
S	-10.76749	0.99412	1.9986
H	-11.78594	0.66716	1.14782
S	9.88737	1.8184	-1.11343
Ge	-0.48489	-0.06564	0.01904
S	-10.82103	1.04782	-1.48998
S	9.98083	-1.53029	-1.02645
N	9.69859	-2.95998	-0.07826
N	9.7725	3.17454	-0.02541
N	-12.27519	0.303	-0.8085
C	9.64935	-4.1839	-0.88205
H	9.29503	-4.99739	-0.2433
H	8.94378	-4.05493	-1.70205
H	10.62761	-4.47337	-1.29511
C	10.55461	-3.07473	1.10632
H	10.18645	-3.90281	1.71858
H	11.60963	-3.2635	0.85944
H	10.48812	-2.1594	1.69392
C	10.7223	3.12784	1.08942
H	11.76663	3.26823	0.77329
H	10.46221	3.91963	1.79772
H	10.63487	2.16969	1.60146

C	9.76036	4.4615	-0.72451
H	9.51533	5.2415	0.00137
H	10.72594	4.71694	-1.18791
H	8.99053	4.45188	-1.49557
C	-13.43393	1.17111	-1.05586
H	-13.67253	1.28019	-2.12413
H	-14.30138	0.73233	-0.55685
H	-13.24777	2.15962	-0.63399
C	-12.4899	-1.071	-1.28001
H	-13.34128	-1.49121	-0.73693
H	-12.69363	-1.12314	-2.35857
H	-11.61059	-1.67471	-1.05558

T35: symmetry c1 -9443.5705262

0 1

S	1.51277	1.01642	1.3598
S	4.43136	0.21768	1.60738
S	7.69034	0.57107	1.31224
C	2.90594	0.15344	0.68815
C	5.37773	-0.51345	0.28566
C	6.70926	-0.36562	0.15302
C	9.12388	0.60432	0.25606
S	1.45827	-0.94549	-1.41088
S	4.38379	-1.49241	-0.82332
S	7.6524	-1.16981	-1.11949
C	2.88535	-0.6215	-0.41051

C	9.10708	-0.16553	-0.84845
S	-1.48157	1.35621	-0.98862
S	-4.4057	1.64751	-0.23231
S	-7.66481	1.40168	-0.63878
C	-2.89809	0.70148	-0.14736
C	-5.38446	0.34001	0.48171
C	-6.71531	0.22862	0.31194
C	-9.10966	0.36067	-0.70295
S	-1.50286	-1.42883	0.95518
S	-4.42372	-0.78616	1.47385
S	-7.68982	-1.0299	1.10165
C	-2.90546	-0.39939	0.62456
C	-9.12057	-0.74276	0.06837
S	-10.3965	0.82455	-1.82792
S	10.4421	1.69733	0.71186
Ge	-0.00346	-0.00829	0.02263
S	-10.39575	-1.95667	0.03524
S	10.36977	-0.15095	-2.07468
N	10.41592	-1.85537	-2.44301
N	10.05416	1.86835	2.39613
N	-10.43765	-2.35254	1.73286
N	-10.01292	2.51339	-1.96476
C	10.47096	-2.1181	-3.88253
H	10.32688	-3.19055	-4.03903
H	9.66443	-1.58356	-4.38382
H	11.42869	-1.83154	-4.34475

C	11.41847	-2.60188	-1.67878
H	11.25942	-3.67022	-1.85139
H	12.45203	-2.35039	-1.9603
H	11.28518	-2.40459	-0.61513
C	10.88977	1.06378	3.29277
H	11.92872	1.42011	3.34902
H	10.45429	1.10177	4.29524
H	10.89021	0.02657	2.95897
C	9.92015	3.26433	2.82217
H	9.50675	3.27422	3.83426
H	10.87701	3.80759	2.83642
H	9.22846	3.78427	2.16047
C	-9.85628	2.96131	-3.35139
H	-9.44676	3.97497	-3.33851
H	-9.15308	2.31021	-3.8693
H	-10.80356	2.98063	-3.91114
C	-10.86784	3.39334	-1.16218
H	-10.43579	4.39796	-1.1747
H	-11.89982	3.45157	-1.53805
H	-10.88746	3.04212	-0.13092
C	-11.43882	-1.60188	2.49506
H	-12.47266	-1.88199	2.24337
H	-11.27511	-1.79074	3.55993
H	-11.30877	-0.53505	2.31368
C	-10.48829	-3.7961	1.97416
H	-10.34089	-3.96819	3.04375

H	-11.44569	-4.25611	1.68328
H	-9.68197	-4.28722	1.43003

T36: symmetry c1 -9065.1056921

0 1

S	1.39657	1.13777	-1.08354
S	4.30727	0.56387	-1.70924
S	7.60472	0.88442	-1.56018
C	2.85017	0.17584	-0.76183
C	5.35614	-0.48733	-0.72513
C	6.69373	-0.35149	-0.66658
C	9.04386	0.79621	-0.50396
S	1.57185	-1.51966	1.02545
S	4.46115	-1.76614	0.13334
S	7.75981	-1.42679	0.26237
C	2.91866	-0.87722	0.07124
C	9.1153	-0.26382	0.3312
S	-1.5623	-1.27138	-1.28057
S	-4.46186	-1.71129	-0.50405
S	-7.75575	-1.33013	-0.60805
C	-2.92025	-0.8651	-0.21862
C	-5.36875	-0.65832	0.61042
C	-6.70475	-0.50396	0.56196
C	-9.10454	-0.17023	-0.43545
S	-1.4164	0.83069	1.38632
S	-4.33435	0.13315	1.82577

S	-7.62926	0.5012	1.69793
C	-2.86358	-0.03186	0.83485
C	-9.04617	0.67007	0.62136
S	-10.46688	-0.342	-1.54431
S	10.31462	1.99212	-0.76887
Ge	-0.00306	-0.24948	0.00653
S	-10.317	1.78528	1.12792
S	10.49774	-0.69187	1.34139
C	-9.44786	3.40106	1.02974
H	-9.14275	3.60712	0.00489
H	-10.17937	4.14418	1.3491
H	-8.58872	3.4308	1.69766
C	-9.68019	0.04562	-3.15867
H	-10.47677	-0.04488	-3.89802
H	-9.29638	1.06469	-3.15988
H	-8.88734	-0.66186	-3.39512
C	9.4589	3.54782	-0.29638
H	9.16527	3.5169	0.75181
H	10.19324	4.34	-0.44648
H	8.59366	3.73365	-0.93036
C	9.75017	-0.66868	3.01948
H	10.55917	-0.93462	3.70077
H	9.385	0.32875	3.25962
H	8.9493	-1.4007	3.10816