FC geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.014650	-0.001209	0.031775
2	6	0	0.002027	0.000096	1.393331
3	6	0	1.247831	0.001284	2.161440
4	6	0	2.460343	0.000452	1.357559
5	6	0	2.411884	-0.000789	0.005814
6	6	0	1.198188	-0.001577	-0.744418
7	1	0	-0.952852	-0.001937	-0.490097
8	1	0	-0.914535	0.000468	1.959220
9	8	0	1.259043	0.003061	3.391930
10	1	0	3.400168	0.001045	1.883165
11	1	0	3.340721	-0.001314	-0.545168
12	6	0	1.263769	-0.001598	-2.147565
13	6	0	0.616299	0.000335	-4.558592
14	6	0	-1.597987	0.000018	-4.153399
15	1	0	-2.646082	0.000357	-4.381109
16	6	0	0.301798	-0.001571	-3.136268
17	1	0	2.262578	-0.001486	-2.556424
18	8	0	1.667072	0.001469	-5.168609
19	7	0	-1.099040	-0.001812	-2.973606
20	7	0	-0.640114	0.001593	-5.154465
21	1	0	-0.791424	0.003115	-6.134628

FS geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016202	0.001012	-0.030664
2	6	0	-0.012176	0.000312	1.364834
3	6	0	1.185652	-0.000779	2.156830
4	6	0	2.435202	-0.000496	1.388998
5	6	0	2.452274	0.000177	0.047206
6	6	0	1.243421	0.000742	-0.747896
7	1	0	-0.901497	0.001733	-0.581856
8	1	0	-0.952793	0.000491	1.887980
9	8	0	1.205335	-0.001776	3.400465
10	1	0	3.350735	-0.000872	1.956372
11	1	0	3.397273	0.000384	-0.473060
12	6	0	1.370099	0.000725	-2.192288
13	6	0	0.578610	-0.000128	-4.594635
14	6	0	-1.614139	-0.000425	-4.100343
15	1	0	-2.670435	-0.000654	-4.271965
16	6	0	0.326033	0.000490	-3.159707
17	1	0	2.363679	0.000689	-2.601278

18	8	0	1.622103	-0.000052	-5.234538
19	7	0	-1.039308	0.000240	-2.934968
20	7	0	-0.695920	-0.000673	-5.133008
21	1	0	-0.885313	-0.001140	-6.106592

TI1 geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.259174	-1.101849	0.185748
2	6	0	0.224074	-0.785727	1.498932
3	6	0	1.106258	0.230575	2.053449
4	6	0	2.010115	0.880375	1.115816
5	6	0	2.024018	0.539205	-0.218229
6	6	0	1.158142	-0.468827	-0.741702
7	1	0	-0.406542	-1.849112	-0.217110
8	1	0	-0.463947	-1.268896	2.177183
9	8	0	1.093097	0.534232	3.254224
10	1	0	2.660922	1.648808	1.507567
11	1	0	2.685288	1.036757	-0.909729
12	6	0	1.183606	-0.829406	-2.161088
13	6	0	0.459296	-0.426071	-4.542184
14	6	0	-1.061536	1.142182	-4.004243
15	1	0	-1.832061	1.865254	-4.147088
16	6	0	0.402056	-0.179693	-3.129567
17	1	0	1.878508	-1.561453	-2.503675
18	8	0	1.141172	-1.174457	-5.235144
19	7	0	-0.552254	0.791355	-2.866473
20	7	0	-0.504926	0.438336	-5.054947
21	1	0	-0.689415	0.538412	-6.021849

TI2 geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.028613	0.672052	-0.195499
2	6	0	-0.179613	0.790520	1.164603
3	6	0	0.926737	1.079943	2.045206
4	6	0	2.206340	1.219677	1.367173
5	6	0	2.328392	1.089265	0.027961
6	6	0	1.228051	0.813387	-0.846032
7	1	0	-0.901048	0.470884	-0.785352
8	1	0	-1.146252	0.679827	1.619302
9	8	0	0.809605	1.206497	3.272583
10	1	0	3.062487	1.433339	1.982408
11	1	0	3.302729	1.203413	-0.418036

12	6	0	1.439735	0.717226	-2.234879
13	6	0	-0.030557	-0.845857	-3.761532
14	6	0	-1.174478	0.866120	-4.648133
15	1	0	-1.903250	1.375907	-5.254404
16	6	0	0.402647	0.472930	-3.224778
17	1	0	2.434214	0.871932	-2.598127
18	8	0	0.355857	-1.976139	-3.546793
19	7	0	-0.335845	1.455611	-3.832874
20	7	0	-1.038592	-0.501591	-4.651369
21	1	0	-1.577424	-1.158839	-5.168278

CI geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.121456	-0.863535	0.042475
2	6	0	0.097213	-0.420959	1.324996
3	6	0	1.193633	0.331295	1.894216
4	6	0	2.307460	0.557679	0.992974
5	6	0	2.304260	0.085563	-0.293909
6	6	0	1.223845	-0.664381	-0.817528
7	1	0	-0.716302	-1.414282	-0.342346
8	1	0	-0.741198	-0.617656	1.965595
9	8	0	1.189783	0.746932	3.058681
10	1	0	3.134132	1.125400	1.375874
11	1	0	3.145965	0.283748	-0.931443
12	6	0	1.209042	-1.133756	-2.207866
13	6	0	0.671619	0.693869	-3.995048
14	6	0	-1.520352	0.170395	-4.089442
15	1	0	-2.548339	0.225992	-4.399586
16	6	0	0.319000	-0.412743	-3.119286
17	1	0	2.089436	-1.621260	-2.586488
18	8	0	1.733049	1.246554	-4.246688
19	7	0	-1.034841	-0.687343	-3.237834
20	7	0	-0.550510	1.020098	-4.586396
21	1	0	-0.673483	1.770064	-5.227373

$TS_{FS->TI2}$ geometry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.613813	-.125263	1.388140
2	6	0	-.642319	-.249526	2.765502
3	6	0	.536870	-.117767	3.579394
4	6	0	1.778480	.145670	2.834735
5	6	0	1.805301	.263586	1.502973
6	6	0	.610735	.143522	.678261

7	1	0	-1.522539	-.204809	.826218
8	1	0	-1.572024	-.438082	3.275523
9	8	0	.549657	-.203939	4.815987
10	1	0	2.677763	.244973	3.419432
11	1	0	2.739241	.461045	1.000266
12	6	0	.724713	.326406	-.710227
13	6	0	-.073779	-.189435	-3.096178
14	6	0	-2.250536	.171223	-2.692501
15	1	0	-3.301398	.236276	-2.879773
16	6	0	-.336612	.138929	-1.712627
17	1	0	1.701868	.510649	-1.119264
18	8	0	.972812	-.412496	-3.696980
19	7	0	-1.674264	.361574	-1.535306
20	7	0	-1.338207	-.155230	-3.669034
21	1	0	-1.522693	-.339093	-4.626613

Table 2. Two-root state-average excited state CASSCF/6-31+G* absolute energies and Dipole moments for the GFP fluorophore model **3**

	CASSCF (u.a)	Dipole (Debyes)
FC(S_0)	-641.551841	6.521
FC(S_1)	-641.419064	5.044
FS	-641.426342	5.168
TI1	-641.439484	10.794
TI2	-641.442345	9.538
CI	-641.424948	6.5517

Table 3. Two-root state-average excited state CASSCF/6-31G* absolute energies and Dipole moments

for the GFP fluorophore model **3**

	CASSCF (u.a)	Dipole (Debyes)
FC(S_0)	-641.52282	6.30
FC(S_1)	-641.38770	5.33
FS	-641.39495	5.38
TI1	-641.40868	11.06
TI2	-641.41289	9.26
CI	-641.39483	5.98

Table 4. Ground and excited state two-root state-average CASSCF/6-31G* absolute energies for the GFP fluorophore model **3**. Values in brackets correspond to three-root state average.

Structure	*State*	*CASSCF energy (au)*
FC	S_0	-641.52282
	S_1	-641.38770
FS	S_0	-641.50047
		(-641.50683)
	S_1	-641.39495
		(-641.39110)
	S_2	(-641.34282)
TI1	S_0	-641.46445
	S_1	-641.40868
$TS_{FS \rightarrow TI2}$	S_0	-641.49574
	S_1	-641.39463
TI2	S_0	-641.45181
	S_1	-641.41289
CI	S_0	-641.40186
	S_1	-641.39483