A stable triplet diradical emitter

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Content

General Procedures S2

Preparation of **3** S3

Preparation of **4** S3

Table S1. Crystal data and structure refinement for compounds **3** and **4** S4

Table S2. Selected bond lengths (Å) of **1**, **2**, **3** and **4** S5

Table S3. Selected bond angles (°) of **1**, **2**, **3** and **4** S6

EPR spectra S7

Figure S1. Powder EPR spectrum of **4** at 90K with the forbidden transition at the half magnetic field.. ..... S7

Figure S2. Absorption spectra of **3** in THF before and after irradiation at 365 nm for 0, 10, 20, 30, 40, 50, 60 min S8

Figure S3. Absorption spectra of **4** in THF before and after irradiation at 365 nm for 0, 10, 20, 30, 40, 50, 60 min S8

Computational Details. S9

Table S4. Energy correction of **3** S9

Table S5. Energy correction of **4** S9

Table S6. The UV-vis absorption information for diradical **3** according to experiment and TDDFT calculation. S10

Table S7. The UV-vis absorption information for diradical **4** according to experiment and TDDFT calculation. S11

Coordinates of the studied molecules S12

3-CS S12

3-OS S14

3-T S16

4-CS S19

4-OS S21

4-T S22

Reference S24

General Procedures

All experiments and manipulations were carried out under N_2 atmosphere using standard Schlenk techniques or in a N_2-filled glovebox. Solvents were dried by the proper drying agents; NaK/benzophenone (tetrahydrofuran, toluene, and n-hexane), and degassed before use. 2,7-di-tert-butylpyrene-4,5,9,10-tetraone,[1] 2,7-dibromopyrene-4,5,9,10-tetraone,[2] chlorobis(perfluorophenyl)borane[3] were synthesized according to published procedures. UV/Vis spectra were recorded on the Lambda 750 spectrometer at room temperature. Fluorescence data were measured at room temperature with a HORIBA Fluorolog-3 spectrofluorometer with a 1 cm quartz cuvette. Cyclic voltammetry was performed on a CHI660E electrochemical workstation with platinum as the working and counter electrode, and a $Ag/AgNO_3$ electrode as reference. Freshly distilled THF was used as the solvent and n-Bu_4NPF_6 (10^{-1} M) was used as electrolyte. EPR spectra were obtained using Bruker EMX-10/12 variable-temperature apparatus. Magnetic measurements were performed using a Quantum Design SQUID VSM magnetometer with a field of 0.1 T. Element analyses were performed on an Elementar Vario EL III instrument at Shanghai Institute of Organic Chemistry, the Chinese Academy of Science. For the single crystal X-ray structure analyses, the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data were collected on Bruker D8 CMOS detectors at 193 K. The structures were solved by direct methods and all refined on F^2 with the SHELX-2014/7 software package.

Preparation of 3

30 ml THF was added to a mixture of 2,7-di-tert-butylpyrene-4,5,9,10-tetraone (0.5 mmol, 187 mg), chlorobis(perfluorophenyl)borane (1 mmol, 380 mg) and potassium (1 mmol, 39 mg) at room temperature. After addition, the mixture was stirred for 48 h. All the volatiles were evaporated under vacuum, and the remaining solid was extracted with toluene and filtered through Celite. The filtrate was concentrated and kept at room temperature for 48 h to afford **3** as dark red crystalline solid. Yield: 128 mg, 0.12 mmol, 24%. Elemental analysis for $C_{48}H_{22}B_2F_{20}O_4 \cdot (C_7H_8)$: Cacld: C 57.12, H 2.61; Found: C 57.78, H 3.08.

Preparation of 4

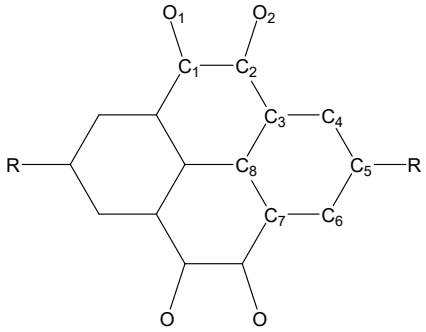
30 ml THF was added to a mixture of 2,7-dibromopyrene-4,5,9,10-tetraone (0.5 mmol, 210 mg), chlorobis(perfluorophenyl)borane (1 mmol, 380 mg) and potassium (1 mmol, 39 mg) at room temperature. After addition, the mixture was stirred for 48 h. All the volatiles were evaporated under vacuum, and the remaining solid was extracted with toluene and filtered through Celite. The filtrate was concentrated and kept at room temperature for 48 h to afford **4** as dark red crystalline solid. Yield: 140 mg, 0.13 mmol, 25%. Elemental analysis for $C_{40}H_4B_2Br_2F_{20}O_4 \cdot (2C_7H_8)$: Cacld: C 50.12, H 1.56; Found: C 50.14, H 1.50.

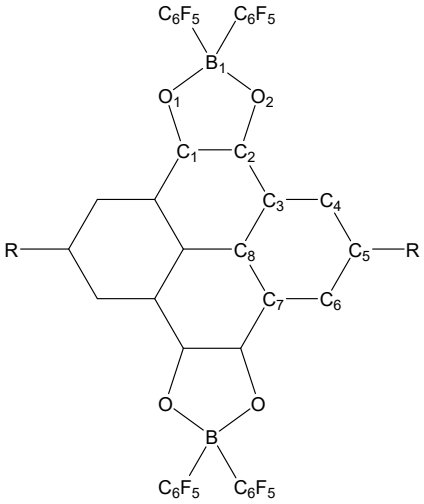
Table S1. Crystal data and structure refinement for compounds **3** and **4**

	3	**4**
Formula	$C_{62}H_{38}B_2F_{20}O_4$	$C_{40}H_4B_2Br_2F_{20}O_4$
Formula weight	1248.54	1109.87
Temp. (K)	193(2)	193(2)
Crystal system	triclinic	triclinic
Space group	*P* -1	*P* -1
a (Å)	9.6004(6)	9.4968(4)
b (Å)	12.4461(7)	12.6034(7)
c (Å)	12.6370(7)	12.6524(6)
α(°)	74.158(3)	65.579(2)
β(°)	81.407(4)	79.789(2)
γ(°)	71.642(3)	78.572(2)
V [Å^3]	1375.35(14)	1343.83(12)
Z	1	1
ρ_{calcd}(g·cm^{-3})	1.507	1.371
μ(mm-1)	0.784	1.610
F(000)	632.0	536.0
Collected data	5001	6119
Unique data	3398	4366
GOF on F^2	1.053	1.040
Final *R* indexes [I > 2σ(I)]	*R1* = 0.0474 *ωR2* = 0.1226	*R1* = 0.0395 *ωR2* = 0.0957
R indexes (all data)	*R1* = 0.0768 *ωR2* = 0.1391	*R1* = 0.0595 *ωR2* = 0.1035
Completeness	0.991	0.990

Table S2. Selected bond lengths (Å) of **1**, **2**, **3** and **4**

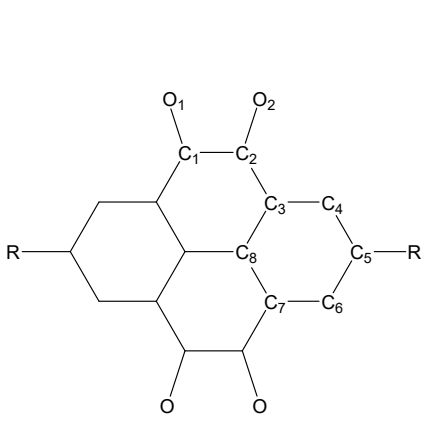
Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Center as supplementary publication CCDC- 2079823 for **3**, and CCDC- 2079824 for **4**.

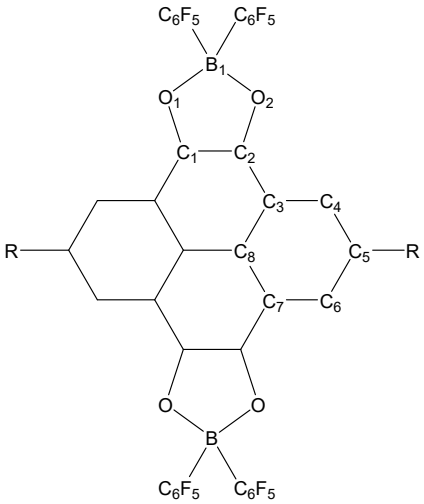




	1[1]	**2**[2]	**3**	**4**
B1-O1	-	-	1.542(3)	1.542(3)
B1-O2	-	-	1.540(3)	1.535(3)
C1-O1	1.207(8)	1.212(3)	1.304(2)	1.300(2)
C2-O2	1.221(7)	1.207(4)	1.305(3)	1.302(3)
C1-C2	1.546(1)	1.537(4)	1.411(3)	1.399(3)
C2-C3	1.473(9)	1.496(3)	1.431(3)	1.425(3)
C3-C4	1.384(1)	1.397(4)	1.392(3)	1.400(3)
C3-C8	1.401(8)	1.396(3)	1.418(3)	1.417(3)
C4-C5	1.396(9)	1.391(3)	1.400(3)	1.385(3)
C5-C6	1.384(7)	1.376(4)	1.392(3)	1.382(3)
C6-C7	1.390(1)	1.399(4)	1.396(3)	1.394(3)
C7-C8	1.416(9)	1.417(3)	1.418(3)	1.416(3)

Table S3. Selected bond angles (°) of **1**, **2**, **3** and **4**





	1[1]	**2**[2]	**3**	**4**
O1-B1-O2	-	-	100.81(16)	100.90(16)
B1-O1-C1	-	-	107.90(16)	107.43(17)
B1-O2-C2	-	-	107.91(17)	107.69(18)
O1-C1-C2	119.66(19)	119.88(15)	111.72(19)	112.08(19)
O2-C2-C1	118.26(17)	118.36(15)	111.65(17)	111.89(18)
O1-B1-C13	-	-	108.74(18)	109.5(2)
O2-B1-C19	-	-	110.64(18)	110.09(19)

EPR spectra

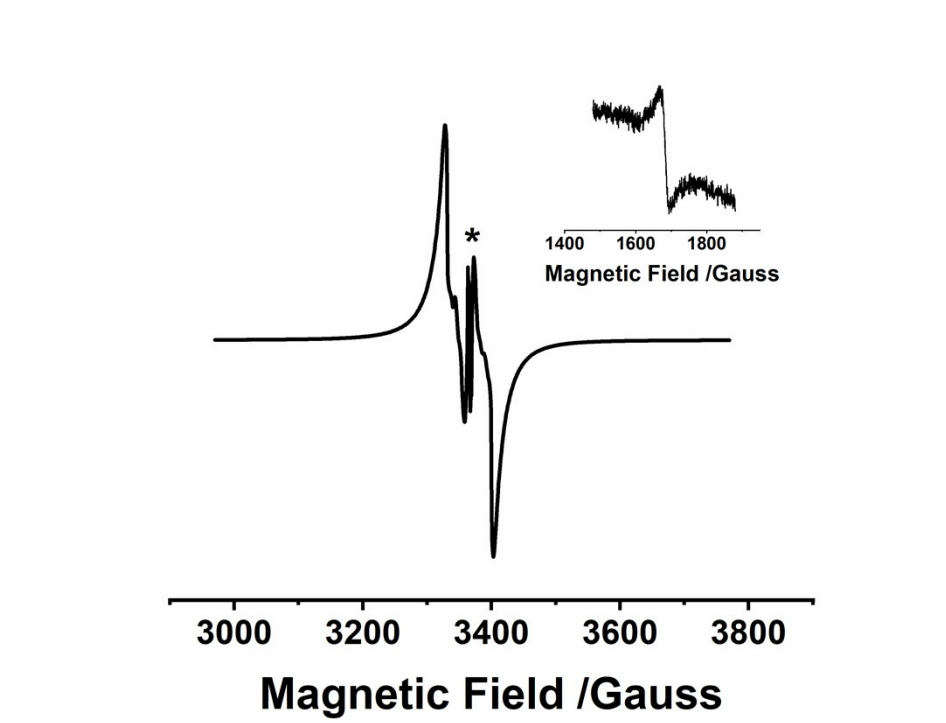


Figure S1. Powder EPR spectrum of **4** at 90K with the forbidden transition at the half magnetic field. The star (*) show the signal derived from monoradical impurities.

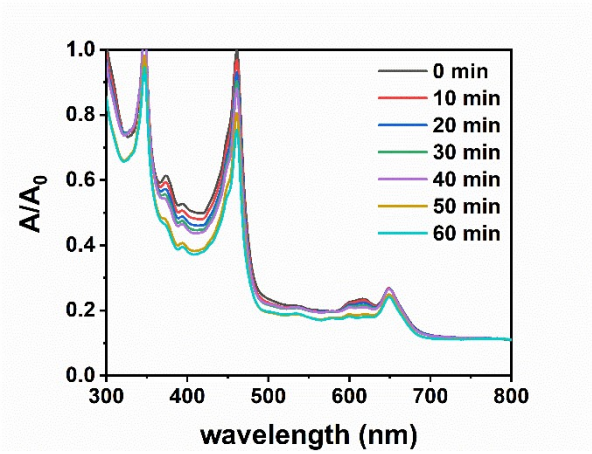


Figure S2. Absorption spectra of **3** in THF before and after irradiation at 365 nm for 0, 10, 20, 30, 40, 50, 60 min

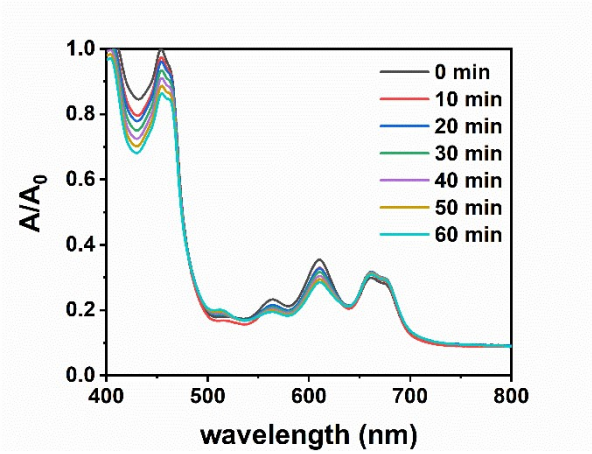


Figure S3. Absorption spectra of **4** in THF before and after irradiation at 365 nm for 0, 10, 20, 30, 40, 50, 60 min

Computational Details.

All the geometry optimizations were performed with the (U)B3LYP functional. Frequency calculations were carried out to confirm that all optimized geometries correspond to energy minima. All calculations were performed with the Gaussian 09 program suite.

Table S4. Energy correction of 3

3	Energy/a.u.	$<S^2>$	$\triangle E_{x\text{-}OS}$/ kcal•mol^{-1} (X = CS, OS, T)
CS	-4189.138122		5.800058166
OS	-4189.147349	0.8969	0
T	-4189.147329	2.0199	0.022573596

Table S5. Energy correction of 4

4	Energy/a.u.	$<S^2>$	$\triangle E_{x\text{-}OS}$/ kcal•mol^{-1} (X = CS, OS, T)
CS	-9017.067231		6.751622135
OS	-9017.078522	0.938	0
T	-9017.079135	2.0196	-0.718256904

Table S6. The UV-vis absorption information for diradical **3** according to experiment and TDDFT calculation. The orbital contributions are shown with transition percent. The corresponding orbitals ("a" means spin up, "b" means spin down) are displayed in Figure 8A

Experimental Absorption (nm)	Calculated Absorption (nm)	Oscillator strength (*f*)	Transition Configuration
347	376	0.11	255a -> 267a 46% 255b -> 267b 46%
461	427	0.14	256a -> 267a 25% 256b -> 267b 25% 266a -> 268a 19% 266b -> 268b 19%
618	-	-	-
649	684	0.01	261a -> 267a 49% 261b -> 267b 49%

Table S7. The UV-vis absorption information for diradical **4** according to experiment and TDDFT calculation. The orbital contributions are shown with transition percent. The corresponding orbitals ("a" means spin up, "b" means spin down) are displayed in Figure 8B

Experimental Absorption (nm)	Calculated Absorption (nm)	Oscillator strength (*f*)	Transition Configuration
359	378	0.003	265a -> 270a 49% 265b -> 270b 49%
454	474	0.031	258a -> 269a 49% 258b -> 269b 49%
612	-	-	-
663	-	-	-

Coordinates of the studied molecules

3-CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	4.641390	-0.085293	0.026085
2	6	0	2.436162	-0.061085	-0.696677
3	6	0	2.432191	-0.074716	0.732532
4	6	0	1.219078	-0.050293	1.464299
5	6	0	1.190086	-0.065191	2.876108
6	1	0	2.145294	-0.093700	3.388038
7	6	0	-0.004551	-0.043656	3.603486
8	6	0	-1.199704	-0.002476	2.865255
9	1	0	-2.156920	0.013827	3.377775
10	6	0	-1.224294	0.016876	1.459438
11	6	0	-0.000133	-0.008457	0.717253
12	6	0	-0.052081	-0.062255	5.141533
13	6	0	1.356027	-0.119295	5.762922
14	1	0	1.900524	-1.022803	5.465251
15	1	0	1.271065	-0.133096	6.854373
16	1	0	1.961669	0.753442	5.493045
17	6	0	-0.845200	-1.305543	5.611057
18	1	0	-1.874179	-1.305367	5.235531
19	1	0	-0.894561	-1.326659	6.705528
20	1	0	-0.364309	-2.231298	5.275779
21	6	0	-0.756902	1.220850	5.643508
22	1	0	-0.211565	2.118913	5.332443
23	1	0	-0.806859	1.217012	6.738203
24	1	0	-1.782363	1.301971	5.267275
25	6	0	5.447651	1.318531	0.023498
26	6	0	5.771953	2.009432	1.191677
27	6	0	6.458974	3.221791	1.191402
28	6	0	6.859158	3.780294	-0.018471
29	6	0	6.575027	3.115152	-1.207769
30	6	0	5.886351	1.906046	-1.164350
31	6	0	5.510728	-1.454134	0.016686
32	6	0	6.906217	-1.519872	0.036802
33	6	0	7.611096	-2.724060	0.028919
34	6	0	6.915224	-3.927510	-0.000003

35	6	0	5.522837	-3.913713	-0.019939
36	6	0	4.860603	-2.691492	-0.010983
37	9	0	5.436709	1.508315	2.397138
38	9	0	6.738119	3.850174	2.342106
39	9	0	7.517056	4.944263	-0.038663
40	9	0	6.966241	3.640197	-2.377276
41	9	0	5.664128	1.292458	-2.344102
42	9	0	7.654550	-0.402158	0.067451
43	9	0	8.949953	-2.729329	0.049320
44	9	0	7.575132	-5.089193	-0.007825
45	9	0	4.841739	-5.067441	-0.046979
46	9	0	3.507932	-2.738779	-0.029525
47	8	0	3.652065	-0.089738	-1.166150
48	8	0	3.648741	-0.111442	1.206105
49	5	0	-4.641108	0.084710	0.002083
50	6	0	-2.435703	0.058296	0.720238
51	6	0	-2.432174	0.075448	-0.708922
52	6	0	-1.218828	0.050815	-1.440609
53	6	0	-1.189771	0.066939	-2.852360
54	1	0	-2.144872	0.098808	-3.364316
55	6	0	0.004779	0.042675	-3.579793
56	6	0	1.199837	-0.001365	-2.841573
57	1	0	2.156929	-0.020895	-3.354243
58	6	0	1.224501	-0.019627	-1.435789
59	6	0	0.000359	0.007299	-0.693599
60	6	0	0.052332	0.061321	-5.117850
61	6	0	-1.355580	0.122768	-5.739237
62	1	0	-1.897453	1.027721	-5.441195
63	1	0	-1.270621	0.136693	-6.830685
64	1	0	-1.963772	-0.748302	-5.469706
65	6	0	0.849211	1.302224	-5.587337
66	1	0	1.878322	1.298596	-5.212158
67	1	0	0.898360	1.323433	-6.681811
68	1	0	0.371331	2.229420	-5.251721
69	6	0	0.753306	-1.223835	-5.619981
70	1	0	0.205270	-2.120295	-5.309022
71	1	0	0.803264	-1.220025	-6.714679
72	1	0	1.778502	-1.308133	-5.243742
73	6	0	-5.447967	-1.318483	-0.027644
74	6	0	-5.881353	-1.885508	-1.227365
75	6	0	-6.571071	-3.093016	-1.294156
76	6	0	-6.861514	-3.777827	-0.117627
77	6	0	-6.466495	-3.240246	1.103367
78	6	0	-5.778519	-2.028726	1.127081

79	6	0	-5.510019	1.453728	0.022916
80	6	0	-6.905556	1.519537	0.039207
81	6	0	-7.610049	2.723865	0.055561
82	6	0	-6.913716	3.927394	0.056516
83	6	0	-5.521264	3.913514	0.041860
84	6	0	-4.859426	2.691151	0.025836
85	9	0	-5.653066	-1.252560	-2.395426
86	9	0	-6.957466	-3.597878	-2.474085
87	9	0	-7.520488	-4.940570	-0.160564
88	9	0	-6.751404	-3.887640	2.242076
89	9	0	-5.448276	-1.548299	2.342569
90	9	0	-7.654345	0.401710	0.041347
91	9	0	-8.948976	2.729179	0.070621
92	9	0	-7.573246	5.089211	0.072258
93	9	0	-4.839735	5.067303	0.043852
94	9	0	-3.506678	2.738338	0.014135
95	8	0	-3.651871	0.084972	1.189950
96	8	0	-3.648471	0.114527	-1.182177

3-OS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-4.633949	0.086752	0.021995
2	6	0	-2.429146	0.060215	-0.694720
3	6	0	-2.426108	0.077334	0.726132
4	6	0	-1.211563	0.054556	1.476623
5	6	0	-1.193183	0.073521	2.883773
6	1	0	-2.149697	0.103512	3.391747
7	6	0	0.002478	0.053870	3.610389
8	6	0	1.199256	0.010619	2.876752
9	1	0	2.156751	-0.004230	3.387338
10	6	0	1.216310	-0.012485	1.474366
11	6	0	0.000137	0.010683	0.731735
12	6	0	0.046009	0.076638	5.148112
13	6	0	-1.362626	0.136248	5.768208
14	1	0	-1.906019	1.039142	5.466999
15	1	0	-1.278807	0.152941	6.859809
16	1	0	-1.968373	-0.736693	5.499571
17	6	0	0.839219	1.320513	5.616142

18	1	0	1.869006	1.317578	5.243425
19	1	0	0.884472	1.345383	6.710805
20	1	0	0.360416	2.245538	5.275841
21	6	0	0.749215	-1.205503	5.655034
22	1	0	0.204566	-2.103963	5.343842
23	1	0	0.795230	-1.199457	6.749988
24	1	0	1.775406	-1.287247	5.281515
25	6	0	-5.429258	-1.321392	0.023552
26	6	0	-5.750955	-2.009846	1.194066
27	6	0	-6.433970	-3.224391	1.196788
28	6	0	-6.832084	-3.787392	-0.011754
29	6	0	-6.550367	-3.124647	-1.203036
30	6	0	-5.865704	-1.913192	-1.163200
31	6	0	-5.504911	1.451881	0.011017
32	6	0	-6.900854	1.511090	0.031610
33	6	0	-7.610596	2.712327	0.021986
34	6	0	-6.919724	3.918664	-0.009134
35	6	0	-5.527229	3.911009	-0.029587
36	6	0	-4.859549	2.691826	-0.018926
37	9	0	-5.417471	-1.503707	2.397495
38	9	0	-6.711084	-3.850384	2.348893
39	9	0	-7.486044	-4.953239	-0.028742
40	9	0	-6.939927	-3.653935	-2.370780
41	9	0	-5.645866	-1.301346	-2.343828
42	9	0	-7.643805	0.390211	0.064280
43	9	0	-8.949192	2.711718	0.042816
44	9	0	-7.584461	5.077206	-0.018607
45	9	0	-4.851264	5.067264	-0.058685
46	9	0	-3.507528	2.743889	-0.037990
47	8	0	-3.642607	0.091071	-1.169612
48	8	0	-3.639185	0.117941	1.204049
49	5	0	4.633697	-0.086115	0.007657
50	6	0	2.428728	-0.057013	0.719497
51	6	0	2.426116	-0.078509	-0.701294
52	6	0	1.211327	-0.055361	-1.451673
53	6	0	1.192877	-0.075571	-2.858779
54	1	0	2.149274	-0.109261	-3.366772
55	6	0	-0.002687	-0.052856	-3.585467
56	6	0	-1.199352	-0.006431	-2.851842
57	1	0	-2.156721	0.011974	-3.362586
58	6	0	-1.216471	0.015516	-1.449465
59	6	0	-0.000333	-0.009536	-0.706840
60	6	0	-0.046254	-0.075629	-5.123200
61	6	0	1.362168	-0.139936	-5.743286

62	1	0	1.902755	-1.044378	-5.441708
63	1	0	1.278347	-0.156735	-6.834883
64	1	0	1.970639	0.731215	-5.474993
65	6	0	-0.843494	-1.316934	-5.591228
66	1	0	-1.873409	-1.310320	-5.218879
67	1	0	-0.888538	-1.341874	-6.685891
68	1	0	-0.367907	-2.243506	-5.250608
69	6	0	-0.745341	1.208724	-5.630233
70	1	0	-0.197802	2.105458	-5.319122
71	1	0	-0.791369	1.202737	-6.725189
72	1	0	-1.771248	1.293857	-5.256704
73	6	0	5.429431	1.321331	-0.029232
74	6	0	5.866640	1.878875	-1.232204
75	6	0	6.552451	3.088063	-1.306130
76	6	0	6.834262	3.784249	-0.134094
77	6	0	6.434970	3.256369	1.089782
78	6	0	5.751031	2.042744	1.121283
79	6	0	5.504335	-1.451314	0.031632
80	6	0	6.900300	-1.510367	0.051331
81	6	0	7.609769	-2.711645	0.070674
82	6	0	6.918579	-3.918200	0.071318
83	6	0	5.526050	-3.910687	0.053464
84	6	0	4.858648	-2.691452	0.034604
85	9	0	5.646436	1.233856	-2.394808
86	9	0	6.943195	3.583530	-2.488209
87	9	0	7.489347	4.948515	-0.184032
88	9	0	6.711775	3.914806	2.223752
89	9	0	5.416323	1.571794	2.338742
90	9	0	7.643565	-0.389221	0.054341
91	9	0	8.948401	-2.710851	0.089004
92	9	0	7.583041	-5.076788	0.089918
93	9	0	4.849790	-5.067137	0.055219
94	9	0	3.506574	-2.743645	0.020066
95	8	0	3.642513	-0.085262	1.194616
96	8	0	3.638875	-0.122143	-1.178889

3-T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	-4.628508	0.086613	0.020383
2	6	0	-2.423426	0.058898	-0.695301
3	6	0	-2.420670	0.076532	0.724724
4	6	0	-1.208751	0.054553	1.481955
5	6	0	-1.194375	0.074250	2.889662
6	1	0	-2.151665	0.103820	3.395511
7	6	0	0.001600	0.055709	3.615462
8	6	0	1.199272	0.013019	2.883833
9	1	0	2.157134	-0.000922	3.393050
10	6	0	1.213367	-0.010707	1.480462
11	6	0	0.000220	0.011187	0.738410
12	6	0	0.043656	0.079103	5.153188
13	6	0	-1.365276	0.137811	5.772752
14	1	0	-1.909172	1.040097	5.470752
15	1	0	-1.281999	0.154955	6.864434
16	1	0	-1.970115	-0.735657	5.503916
17	6	0	0.835499	1.323698	5.621544
18	1	0	1.865589	1.321087	5.249881
19	1	0	0.879183	1.349389	6.716298
20	1	0	0.356491	2.248137	5.279904
21	6	0	0.747485	-1.202232	5.661236
22	1	0	0.204017	-2.101183	5.349357
23	1	0	0.791990	-1.196085	6.756297
24	1	0	1.774043	-1.282955	5.288714
25	6	0	-5.423356	-1.321034	0.022918
26	6	0	-5.746915	-2.007136	1.194348
27	6	0	-6.431182	-3.220937	1.198197
28	6	0	-6.828506	-3.785362	-0.009985
29	6	0	-6.544872	-3.124861	-1.202093
30	6	0	-5.858989	-1.914065	-1.163566
31	6	0	-5.496832	1.452605	0.009412
32	6	0	-6.892789	1.513009	0.029398
33	6	0	-7.601177	2.715021	0.019663
34	6	0	-6.908988	3.920649	-0.010931
35	6	0	-5.516462	3.911693	-0.030768
36	6	0	-4.850057	2.691858	-0.020050
37	9	0	-5.414129	-1.499032	2.396998
38	9	0	-6.710257	-3.844726	2.350864
39	9	0	-7.483659	-4.950413	-0.025850
40	9	0	-6.933791	-3.655536	-2.369272
41	9	0	-5.637214	-1.304055	-2.344609
42	9	0	-7.636642	0.392862	0.061458
43	9	0	-8.939671	2.715789	0.039856
44	9	0	-7.572505	5.079737	-0.020496

45	9	0	-4.839361	5.067129	-0.059348
46	9	0	-3.497982	2.742160	-0.038519
47	8	0	-3.635815	0.089617	-1.170366
48	8	0	-3.632351	0.117068	1.202555
49	5	0	4.628293	-0.085943	0.009017
50	6	0	2.423050	-0.055417	0.719863
51	6	0	2.420694	-0.077982	-0.700096
52	6	0	1.208518	-0.055537	-1.457214
53	6	0	1.194085	-0.076529	-2.864871
54	1	0	2.151256	-0.109986	-3.370733
55	6	0	-0.001788	-0.054730	-3.590754
56	6	0	-1.199337	-0.008636	-2.859133
57	1	0	-2.157073	0.009032	-3.368508
58	6	0	-1.213479	0.013918	-1.455778
59	6	0	-0.000388	-0.010039	-0.713735
60	6	0	-0.043888	-0.078172	-5.128488
61	6	0	1.364820	-0.141942	-5.748034
62	1	0	1.905671	-1.045923	-5.445666
63	1	0	1.281544	-0.159167	-6.839711
64	1	0	1.972613	0.729578	-5.479533
65	6	0	-0.840072	-1.320022	-5.596792
66	1	0	-1.870284	-1.313478	-5.225478
67	1	0	-0.883576	-1.345802	-6.691544
68	1	0	-0.364497	-2.246116	-5.254822
69	6	0	-0.743289	1.205532	-5.636688
70	1	0	-0.196715	2.102640	-5.324915
71	1	0	-0.787799	1.199413	-6.731750
72	1	0	-1.769550	1.289901	-5.264170
73	6	0	5.423519	1.320983	-0.029482
74	6	0	5.861513	1.876617	-1.233099
75	6	0	6.548538	3.085022	-1.308017
76	6	0	6.830597	3.782141	-0.136548
77	6	0	6.430466	3.256056	1.087860
78	6	0	5.745301	2.043165	1.120548
79	6	0	5.496314	-1.451976	0.033610
80	6	0	6.892280	-1.512228	0.053420
81	6	0	7.600389	-2.714273	0.073474
82	6	0	6.907891	-3.920110	0.074687
83	6	0	5.515340	-3.911293	0.056698
84	6	0	4.849220	-2.691412	0.037139
85	9	0	5.640928	1.230255	-2.394738
86	9	0	6.940185	3.578788	-2.490364
87	9	0	7.486841	4.945563	-0.187571
88	9	0	6.707629	3.915339	2.221082

89	9	0	5.409681	1.573530	2.338089
90	9	0	7.636437	-0.391825	0.055887
91	9	0	8.938908	-2.714858	0.091915
92	9	0	7.571131	-5.079236	0.093942
93	9	0	4.837946	-5.066908	0.058943
94	9	0	3.497102	-2.741845	0.022378
95	8	0	3.635795	-0.083181	1.195136
96	8	0	3.632020	-0.121876	-1.177616

4-CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-4.594037	0.013736	0.033058
2	35	0	0.060986	-4.755294	2.644639
3	6	0	-2.394418	0.625262	-0.344764
4	6	0	-2.391518	-0.615239	0.364172
5	6	0	-1.174813	-1.261709	0.708401
6	6	0	-1.155707	-2.491115	1.392921
7	1	0	-2.095780	-2.961550	1.662386
8	6	0	0.056578	-3.098079	1.716635
9	6	0	1.266129	-2.499757	1.366826
10	1	0	2.207921	-2.974481	1.622202
11	6	0	1.280617	-1.272518	0.678882
12	6	0	0.051290	-0.619436	0.329392
13	6	0	-5.452539	0.656293	1.243946
14	6	0	-6.227437	-0.192754	2.037659
15	6	0	-7.023141	0.255775	3.086761
16	6	0	-7.061929	1.619089	3.370411
17	6	0	-6.309532	2.502955	2.603290
18	6	0	-5.522413	2.013554	1.560951
19	6	0	-5.485747	-0.621440	-1.157286
20	6	0	-6.253670	0.235714	-1.948928
21	6	0	-7.075573	-0.206888	-2.980240
22	6	0	-7.149964	-1.572205	-3.246499
23	6	0	-6.406762	-2.464078	-2.479626
24	6	0	-5.592669	-1.980566	-1.455483
25	9	0	-6.220747	-1.517871	1.789172
26	9	0	-7.744643	-0.601530	3.819886
27	9	0	-7.816442	2.074582	4.374732

28	9	0	-6.343462	3.814673	2.872969
29	9	0	-4.817444	2.925440	0.865760
30	9	0	-6.214278	1.563075	-1.715854
31	9	0	-7.788752	0.658118	-3.712571
32	9	0	-7.930069	-2.022122	-4.233658
33	9	0	-6.475650	-3.777847	-2.731978
34	9	0	-4.899980	-2.899854	-0.758105
35	8	0	-3.608693	1.035949	-0.570612
36	8	0	-3.603869	-1.017519	0.614584
37	5	0	4.703543	-0.006014	-0.045479
38	35	0	0.039062	4.754882	-2.663878
39	6	0	2.494663	-0.637165	0.306497
40	6	0	2.491383	0.610670	-0.392469
41	6	0	1.274725	1.256054	-0.736905
42	6	0	1.254818	2.486103	-1.419857
43	1	0	2.194595	2.957209	-1.688997
44	6	0	0.042549	3.093916	-1.742643
45	6	0	-1.167032	2.494085	-1.396084
46	1	0	-2.109163	2.971729	-1.644871
47	6	0	-1.180621	1.263381	-0.713826
48	6	0	0.048433	0.611424	-0.362157
49	6	0	5.563612	-0.674389	-1.242590
50	6	0	6.959329	-0.707977	-1.304543
51	6	0	7.658157	-1.299603	-2.357322
52	6	0	6.957023	-1.888834	-3.403832
53	6	0	5.564309	-1.880228	-3.387013
54	6	0	4.908267	-1.280166	-2.318875
55	6	0	5.504968	0.673727	1.181320
56	6	0	5.941481	-0.076068	2.275067
57	6	0	6.642209	0.475475	3.344041
58	6	0	6.938896	1.835745	3.335145
59	6	0	6.539492	2.618375	2.255958
60	6	0	5.840457	2.028217	1.205207
61	9	0	7.711636	-0.160188	-0.334130
62	9	0	8.996277	-1.303829	-2.367015
63	9	0	7.612254	-2.458287	-4.418058
64	9	0	4.877492	-2.443718	-4.389017
65	9	0	3.554274	-1.300028	-2.353328
66	9	0	5.706267	-1.402127	2.321306
67	9	0	7.033280	-0.286916	4.373498
68	9	0	7.608361	2.384366	4.353186
69	9	0	6.830688	3.925636	2.234146
70	9	0	5.504914	2.831512	0.176693
71	8	0	3.707325	-1.053138	0.523369

72	8	0	3.701991	1.017405	-0.637239

4-OS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	4.583130	0.002402	-0.031777
2	35	0	-0.073646	-5.135264	-1.798535
3	6	0	2.386408	0.669283	0.236529
4	6	0	2.380620	-0.665409	-0.245099
5	6	0	1.161578	-1.374961	-0.482383
6	6	0	1.149460	-2.698390	-0.950112
7	1	0	2.089194	-3.206645	-1.135847
8	6	0	-0.065585	-3.345006	-1.165859
9	6	0	-1.274953	-2.697317	-0.922668
10	1	0	-2.218737	-3.203441	-1.092860
11	6	0	-1.276751	-1.375110	-0.451663
12	6	0	-0.054482	-0.676770	-0.218297
13	6	0	5.436227	0.417142	-1.339153
14	6	0	6.195992	-0.566191	-1.977612
15	6	0	6.991227	-0.314177	-3.090593
16	6	0	7.045217	0.980216	-3.603074
17	6	0	6.309235	1.992728	-2.995452
18	6	0	5.522118	1.699822	-1.881897
19	6	0	5.471606	-0.411833	1.251678
20	6	0	6.241514	0.573448	1.874710
21	6	0	7.066632	0.321503	2.965742
22	6	0	7.141803	-0.974811	3.470645
23	6	0	6.397052	-1.989367	2.877242
24	6	0	5.579774	-1.696503	1.785653
25	9	0	6.175687	-1.827633	-1.502777
26	9	0	7.698236	-1.293273	-3.668371
27	9	0	7.799767	1.247235	-4.672619
28	9	0	6.358672	3.238127	-3.485324
29	9	0	4.835626	2.725706	-1.346600
30	9	0	6.201694	1.836652	1.405721
31	9	0	7.782260	1.302463	3.529628
32	9	0	7.925257	-1.241854	4.519192
33	9	0	6.467333	-3.236693	3.359534
34	9	0	4.887076	-2.724299	1.262399

35	8	0	3.599134	1.117722	0.384991
36	8	0	3.589413	-1.113980	-0.422493
37	5	0	-4.696548	0.014941	0.055261
38	35	0	-0.030409	5.144930	1.831665
39	6	0	-2.490262	-0.667152	-0.183909
40	6	0	-2.484144	0.671067	0.290715
41	6	0	-1.265074	1.380210	0.526879
42	6	0	-1.252230	2.704408	0.992200
43	1	0	-2.191878	3.213062	1.177025
44	6	0	-0.037390	3.352060	1.206454
45	6	0	1.172265	2.703870	0.966267
46	1	0	2.116183	3.212086	1.129521
47	6	0	1.173330	1.379405	0.501311
48	6	0	-0.048645	0.681087	0.266599
49	6	0	-5.562716	-0.431871	1.344673
50	6	0	-6.958339	-0.408978	1.415312
51	6	0	-7.666890	-0.803809	2.550506
52	6	0	-6.975857	-1.242877	3.674692
53	6	0	-5.583664	-1.281168	3.652966
54	6	0	-4.917223	-0.878821	2.501736
55	6	0	-5.481997	0.466318	-1.280591
56	6	0	-5.959633	-0.482125	-2.187366
57	6	0	-6.647181	-0.145125	-3.349417
58	6	0	-6.886967	1.196943	-3.633004
59	6	0	-6.445125	2.175558	-2.747851
60	6	0	-5.760759	1.797299	-1.594262
61	9	0	-7.699899	0.005547	0.373530
62	9	0	-9.004149	-0.762431	2.564860
63	9	0	-7.639860	-1.623903	4.768076
64	9	0	-4.907388	-1.699989	4.729842
65	9	0	-3.564733	-0.932171	2.535770
66	9	0	-5.778042	-1.794823	-1.944339
67	9	0	-7.078671	-1.093841	-4.190159
68	9	0	-7.542116	1.542069	-4.744956
69	9	0	-6.680752	3.467824	-3.008897
70	9	0	-5.381737	2.788959	-0.765089
71	8	0	-3.700914	-1.119390	-0.324065
72	8	0	-3.691535	1.120562	0.468679

4-T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	4.579282	0.003519	-0.032789
2	35	0	-0.068918	-5.180476	-1.684331
3	6	0	2.381779	0.675100	0.218181
4	6	0	2.377063	-0.669981	-0.232390
5	6	0	1.161008	-1.389772	-0.455228
6	6	0	1.152617	-2.724931	-0.892488
7	1	0	2.093250	-3.235407	-1.065427
8	6	0	-0.062297	-3.375947	-1.093038
9	6	0	-1.272505	-2.724955	-0.865455
10	1	0	-2.216423	-3.234108	-1.023597
11	6	0	-1.272581	-1.390917	-0.424912
12	6	0	-0.053230	-0.687588	-0.208225
13	6	0	5.432520	0.389489	-1.348206
14	6	0	6.192382	-0.607516	-1.964993
15	6	0	6.988636	-0.379421	-3.082395
16	6	0	7.043605	0.903853	-3.622085
17	6	0	6.307506	1.929327	-3.036697
18	6	0	5.519276	1.660440	-1.917916
19	6	0	5.464770	-0.381715	1.261163
20	6	0	6.233366	0.617291	1.863658
21	6	0	7.056366	0.389661	2.961609
22	6	0	7.130653	-0.895175	3.495237
23	6	0	6.387076	-1.922737	2.923075
24	6	0	5.571852	-1.654296	1.823726
25	9	0	6.170996	-1.858490	-1.463531
26	9	0	7.695636	-1.370851	-3.638562
27	9	0	7.799135	1.147962	-4.696289
28	9	0	6.357770	3.163975	-3.552755
29	9	0	4.832701	2.697492	-1.404987
30	9	0	6.194090	1.869711	1.366809
31	9	0	7.770681	1.383000	3.504915
32	9	0	7.912012	-1.138887	4.550888
33	9	0	6.456303	-3.158955	3.433081
34	9	0	4.880035	-2.693305	1.322132
35	8	0	3.593179	1.127560	0.356912
36	8	0	3.585254	-1.121742	-0.398648
37	5	0	-4.691269	0.010609	0.052294
38	35	0	-0.033666	5.189378	1.709204
39	6	0	-2.484105	-0.673722	-0.172090
40	6	0	-2.479138	0.675043	0.270108
41	6	0	-1.263046	1.394694	0.490854

42	6	0	-1.253910	2.730585	0.925739
43	1	0	-2.194464	3.241385	1.097906
44	6	0	-0.039224	3.382432	1.125320
45	6	0	1.171295	2.730797	0.901452
46	1	0	2.115324	3.241827	1.052902
47	6	0	1.170641	1.394666	0.466994
48	6	0	-0.048422	0.691569	0.248089
49	6	0	-5.553612	-0.406922	1.353440
50	6	0	-6.949347	-0.388881	1.424200
51	6	0	-7.655383	-0.757519	2.569710
52	6	0	-6.961642	-1.163885	3.704490
53	6	0	-5.569271	-1.196326	3.682893
54	6	0	-4.905348	-0.820884	2.521217
55	6	0	-5.478857	0.432317	-1.291350
56	6	0	-5.940290	-0.531378	-2.190343
57	6	0	-6.631322	-0.214508	-3.356165
58	6	0	-6.891739	1.121103	-3.651406
59	6	0	-6.466783	2.114175	-2.773947
60	6	0	-5.778329	1.756141	-1.616577
61	9	0	-7.693262	-0.005557	0.372299
62	9	0	-8.992744	-0.722230	2.583792
63	9	0	-7.623203	-1.519316	4.807826
64	9	0	-4.890545	-1.583876	4.769782
65	9	0	-3.552591	-0.867346	2.555468
66	9	0	-5.739342	-1.839110	-1.936631
67	9	0	-7.046831	-1.176806	-4.189386
68	9	0	-7.550663	1.446287	-4.767047
69	9	0	-6.722730	3.400205	-3.045917
70	9	0	-5.416545	2.759530	-0.793966
71	8	0	-3.693471	-1.130315	-0.300945
72	8	0	-3.685918	1.127615	0.437348

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