Supporting Information

Designing Indacenodithiophene Based Non-fullerene Acceptors with Donor-Acceptor Combined Bridge for Organic Solar Cells

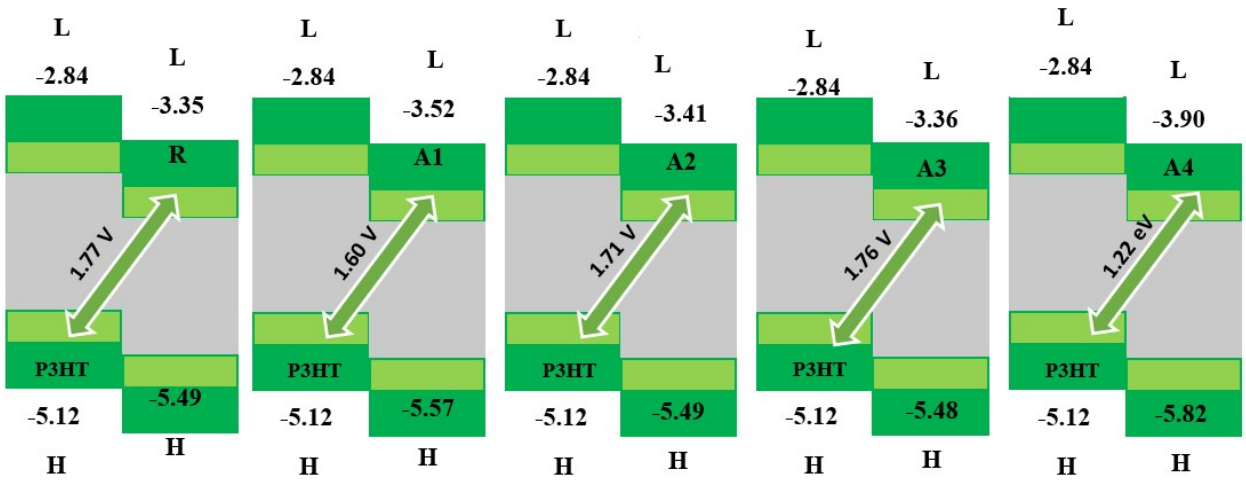

Figure S1. The open circuit voltages (V_{oc}) of reference **R** and designed molecules **A1, A2, A3** and **A4** with respect to donor material P3HTTh.

Mullikan Charges

Designed Molecule M1

Serial No	Symbol	Mullikan Charge
1	C	0.076
2	C	-0.161
3	C	0.043
4	C	0.075
5	C	-0.160
6	C	0.042
7	C	-0.227
8	C	0.056
9	C	-0.232
10	C	-0.227
11	C	-0.062
12	C	-0.231
13	C	-0.062
14	C	-0.297
15	S	-0.231
16	C	-0.062
17	C	-0.296
18	S	0.385

19	C	0.089
20	C	0.096
21	C	0.088
22	C	0.096
23	C	0.201
24	C	0.201
25	C	-0.242
26	C	0.332
27	C	0.092
28	C	0.183
29	C	0.186
30	C	-0.241
31	C	0.330
32	C	0.098
33	C	0.184
34	C	0.186
35	N	-0.601
36	S	0.635
37	N	-0.595
38	N	-0.603
39	S	0.636
40	N	-0.595
41	C	-0.143
42	C	-0.160
43	C	0.089
44	C	-0.159
45	C	-0.139
46	C	-0.144
47	C	-0.162
48	C	0.089
49	C	-0.159
50	C	-0.145
51	C	0.145
52	C	-0.158
53	C	0.089
54	C	-0.162
55	C	-0.144
56	C	-0.143
57	C	-0.160
58	C	0.089
59	C	-0.159
60	C	-0.139
61	C	-0.450
62	C	-0.450
63	C	-0.450

64	C	-0.450
65	C	-0.241
66	C	-0.245
67	C	-0.102
68	C	-0.102
69	C	-0.202
70	S	0.418
71	C	-0.119
72	C	-0.073
73	C	-0.253
74	S	0.412
75	C	-0.098
76	C	-0.116
77	H	0.149
78	H	0.148
79	H	0.146
80	H	0.146
81	H	0.157
82	H	0.157
83	H	0.133
84	H	0.124
85	H	0.123
86	H	0.132
87	H	0.136
88	H	0.123
89	H	0.123
90	H	0.136
91	H	0.136
92	H	0.123
93	H	0.124
94	H	0.136
95	H	0.133
96	H	0.124
97	H	0.123
98	H	0.132
99	H	0.157
100	H	0.147
101	H	0.144
102	H	0.147
103	H	0.143
104	H	0.158
105	H	0.157
106	H	0.144
107	H	0.145
108	H	0.157

109	H	0.145
110	H	0.145
111	H	0.163
112	H	0.156
113	H	0.162
114	H	0.199
115	H	0.178
116	F	-0.285
117	F	-0.287
118	C	0.002
119	C	0.093
120	C	0.030
121	C	-0.027
122	C	0.407
123	O	-0.504
124	C	0.036
125	C	0.328
126	N	-0.517
127	C	0.324
128	N	-0.510
129	C	-0.196
130	C	0.317
131	C	0.321
132	C	-0.187
133	H	0.198
134	H	0.184
135	C	-0.075
136	C	0.104
137	C	0.013
138	C	0.001
139	C	0.383
140	O	-0.484
141	C	-0.033
142	C	0.329
143	N	-0.511
144	C	0.330
145	N	-0.492
146	C	-0.199
147	C	0.319
148	C	0.320
149	C	-0.180
150	H	0.195
151	H	0.186
152	H	0.159
153	F	-0.272

154	F	-0.273
155	F	-0.272
156	F	-0.274

Designed Molecule M2

Serial No	Symbol	Mullikan Charge
1	C	0.075
2	C	-0.161
3	C	0.043
4	C	0.075
5	C	-0.161
6	C	0.043
7	C	0.227
8	C	0.055
9	C	-0.232
10	C	-0.227
11	C	0.056
12	C	-0.232
13	C	-0.063
14	C	-0.297
15	S	0.3835
16	C	-0.063
17	C	-0.296
18	S	0.0384
19	C	0.089
20	C	0.096
21	C	0.089
22	C	0.096
23	C	0.201
24	C	0.201
25	C	-0.242
26	C	0.330
27	C	0.093
28	C	0.181
29	C	0.186
30	C	-0.241
31	C	0.329
32	C	0.099
33	C	0.183
34	C	0.186

35	N	-0.600
36	S	0.633
37	N	0.596
38	N	-0.602
39	S	0.634
40	N	-0.596
41	C	-0.143
42	C	-0.160
43	C	0.089
44	C	-0.159
45	C	-0.139
46	C	-0.144
47	C	-0.162
48	C	0.089
49	C	-0.158
50	C	-0.145
51	C	-0.145
52	C	-0.159
53	C	0.089
54	C	-0.162
55	C	-0.144
56	C	-0.143
57	C	-0.160
58	C	0.089
59	C	-0.159
60	C	-0.139
61	C	-0.450
62	C	-0.450
63	C	-0.450
64	C	-0.450
65	C	-0.242
66	C	-0.246
67	C	-0.102
68	C	-0.103
69	C	-0.201
70	S	0.4175
71	C	-0.120
72	C	-0.074
73	C	-0.253
74	S	0.410
75	C	-0.099
76	C	-0.116
77	H	0.148
78	H	0.148
79	H	0.146

80	H	0.146
81	H	0.157
82	H	0.156
83	H	0.133
84	H	0.123
85	H	0.122
86	H	0.32
87	H	0.136
88	H	0.123
89	H	0.123
90	H	0.136
91	H	0.136
92	H	0.123
93	H	0.123
94	H	0.136
95	H	0.133
96	H	0.124
97	H	0.122
98	H	0.132
99	H	0.157
100	H	0.147
101	H	0.161
102	H	0.146
103	H	0.143
104	H	0.157
105	H	0.157
106	H	0.127
107	H	0.145
108	H	0.156
109	H	0.145
110	H	0.145
111	H	0.161
112	H	0.154
113	H	0.161
114	H	0.199
115	H	0.176
116	F	-0.286
117	F	-0.287
118	C	0.001
119	C	0.091
120	C	0.030
121	C	0.116
122	C	0.486
123	O	-0.506
124	C	0.033

125	C	0.328
126	N	-0.519
127	C	0.323
128	N	-0.513
129	C	-0.135
130	C	-0.134
131	C	-0.127
132	C	-0.126
133	H	0.177
134	H	0.149
135	H	0.146
136	H	0.161
137	C	-0.076
138	C	0.101
139	C	0.014
140	C	0.011
141	C	0.382
142	O	-0.487
143	C	0.032
144	C	0.329
145	N	-0.513
146	C	0.330
147	N	-0.449
148	C	-0.139
149	C	0.132
150	C	-0.127
151	C	-0.127
152	H	0.173
153	H	0.149
154	H	0.146
155	H	0.163
156	H	0.158

Designed Molecules M3

Serial No	Symbol	Mullikan Charge
1	C	0.075
2	C	-0.161
3	C	0.043
4	C	0.076
5	C	-0.161
6	C	0.043
7	C	-0.227
8	C	0.055
9	C	-0.232

10	**C**	**0.227**
11	**C**	**0.055**
12	**C**	**-0.232**
13	**C**	**-0.062**
14	**C**	**-0.296**
15	**S**	**0.3872**
16	**C**	**-0.063**
17	**C**	**-0.296**
18	**S**	**0.283**
19	**C**	**0.089**
20	**C**	**0.096**
21	**C**	**0.089**
22	**C**	**0.096**
23	**C**	**0.200**
24	**C**	**0.200**
25	**C**	**0.242**
26	**C**	**0.329**
27	**C**	**0.099**
28	**C**	**0.178**
29	**C**	**0.184**
30	**C**	**-0.242**
31	**C**	**0.329**
32	**C**	**0.094**
33	**C**	**0.184**
34	**C**	**0.186**
35	**N**	**-0.593**
36	**S**	**0.630**
37	**N**	**-0.597**
38	**N**	**-0.601**
39	**S**	**0.632**
40	**N**	**-0.596**
41	**C**	**-0.143**
42	**C**	**-0.160**
43	**C**	**0.089**
44	**C**	**-0.159**
45	**C**	**-0.138**
46	**C**	**-0.144**
47	**C**	**-0.162**
48	**C**	**-0.089**
49	**C**	**-0.158**
50	**C**	**-0.145**
51	**C**	**-0.145**
52	**C**	**-0.159**
53	**C**	**0.089**
54	**C**	**-0.162**

55	**C**	**-0.144**
56	**C**	**-0.143**
57	**C**	**-0.160**
58	**C**	**0.089**
59	**C**	**-0.159**
60	**C**	**-0.138**
61	**C**	**-0.450**
62	**C**	**-0.450**
63	**C**	**-0.450**
64	**C**	**-0.450**
65	**C**	**-0.271**
66	**C**	**-0.243**
67	**C**	**-0.119**
68	**C**	**-0.075**
69	**C**	**-0.252**
70	**S**	**0.407**
71	**C**	**-0.107**
72	**C**	**-0.117**
73	**C**	**-0.213**
74	**S**	**0.476**
75	**C**	**-0.121**
76	**C**	**-0.126**
77	**H**	**0.148**
78	**H**	**0.148**
79	**H**	**0.145**
80	**H**	**0.145**
81	**H**	**0.1569**
82	**H**	**0.156**
83	**H**	**0.133**
84	**H**	**0.123**
85	**H**	**0.122**
86	**H**	**0.132**
87	**H**	**0.136**
88	**H**	**0.123**
89	**H**	**0.123**
90	**H**	**0.136**
91	**H**	**0.136**
92	**H**	**0.123**
93	**H**	**0.123**
94	**H**	**0.136**
95	**H**	**0.133**
96	**H**	**0.123**
97	**H**	**0.122**
98	**H**	**0.132**
99	**H**	**0.157**

100	H	0.146
101	H	0.143
102	H	0.145
103	H	0.143
104	H	0.157
105	H	0.157
106	H	0.145
107	H	0.145
108	H	0.156
109	H	0.144
110	H	0.145
111	H	0.161
112	H	0.198
113	H	0.160
114	H	0.163
115	H	0.159
116	F	-0.287
117	F	-0.286
118	C	-0.028
119	C	0.114
120	C	0.015
121	C	-0.265
122	C	0.442
123	O	-0.485
124	C	0.038
125	C	0.322
126	N	-0.515
127	C	0.327
128	N	-0.516
129	C	-0.058
130	C	-0.357
131	S	0.378
132	H	0.119
133	H	0.187
134	C	0.02
135	C	0.105
136	C	0.021
137	C	-0.271
138	C	0.445
139	O	-0.499
140	C	0.3040
141	C	0.325
142	N	-0.516
143	C	0.324
144	N	-0.510

145	**C**	**-0.058**
146	**C**	**-0.375**
147	**S**	**0.378**
148	**H**	**0.190**
149	**H**	**0.188**
150	**H**	**0.159**

Designed Molecule M4

Serial No	Symbol	Mullikan Charge
1	**C**	**0.076**
2	**C**	**-0.159**
3	**C**	**0.044**
4	**C**	**0.075**
5	**C**	**-0.158**
6	**C**	**0.043**
7	**C**	**-0.226**
8	**C**	**0.057**
9	**C**	**-0.230**
10	**C**	**-0.226**
11	**C**	**0.056**
12	**C**	**-0.230**
13	**C**	**-0.061**
14	**C**	**-0.298**
15	**S**	**0.338**
16	**C**	**-0.061**
17	**C**	**-0.297**
18	**S**	**0.389**
19	**C**	**0.089**
20	**C**	**0.096**
21	**C**	**0.088**
22	**C**	**0.096**
23	**C**	**0.203**
24	**C**	**0.203**
25	**C**	**-0.242**
26	**C**	**0.336**
27	**C**	**0.089**
28	**C**	**0.185**
29	**C**	**0.127**
30	**C**	**-0.241**
31	**C**	**0.334**

32	C	0.0958
33	C	0.187
34	C	0.187
35	N	-0.603
36	S	0.639
37	N	-0.594
38	N	-0.6060.641
39	S	-0.595
40	N	-0.144
41	C	-0.159
42	C	0.089
43	C	0.159
44	C	-0.140
45	C	-0.3140
46	C	-0.144
47	C	-0.161
48	C	0.089
49	C	-0.159
50	C	-0.145
51	C	-0.145
52	C	-.158
53	C	0.88
54	C	-0.162
55	C	-0.145
56	C	-0.143
57	C	-0.160
58	C	0.089
59	C	-0.158
60	C	-0.140
61	C	-0.450
62	C	-0.450
63	C	-0.450
64	C	-0.450
65	C	-0.237
66	C	-0.242
67	C	-0.101
68	C	-0.199
69	C	-0.202
70	S	0.223
71	C	-0.118
72	C	-0.170
73	C	-0.255
74	S	0.419
75	C	-0.093
76	C	-0.168

77	**H**	**0.150**
78	**H**	**0.149**
79	**H**	**0.149**
80	**H**	**0.148**
81	**H**	**0.159**
82	**H**	**0.159**
83	**H**	**0.133**
84	**H**	**0.124**
85	**H**	**0.124**
86	**H**	**0.133**
87	**H**	**0.136**
88	**H**	**0.124**
89	**H**	**0.124**
90	**H**	**0.135**
91	**H**	**0.135**
92	**H**	**0.124**
93	**H**	**0.125**
94	**H**	**0.137**
95	**H**	**0.132**
96	**H**	**0.125**
97	**H**	**0.124**
98	**H**	**0.132**
99	**H**	**0.159**
100	**H**	**0.147**
101	**H**	**0.145**
102	**H**	**0.148**
103	**H**	**0.144**
104	**H**	**0.159**
105	**H**	**0.158**
106	**H**	**0.145**
107	**H**	**0.146**
108	**H**	**0.158**
109	**H**	**0.146**
110	**H**	**0.145**
111	**H**	**0.168**
112	**H**	**0.160**
113	**H**	**0.166**
114	**H**	**0.203**
115	**H**	**0.181**
116	**F**	**-0.283**
117	**F**	**-0.285**
118	**C**	**-0.082**
119	**C**	**0.093**
120	**C**	**0.033**
121	**C**	**-0.017**

122	C	0.411
123	O	-0.499
124	C	0.045
125	C	0.328
126	N	-0.503
127	C	0.327
128	N	-0.504
129	C	-0.117
130	C	0.094
131	C	0.104
132	C	-0.110
133	H	0.208
134	H	0.195
135	C	-0.081
136	C	0.105
137	C	0.016
138	C	0.009
139	C	0.388
140	O	-0.477
141	C	0.040
142	C	0.329
143	N	-0.502
144	C	0.332
145	N	-0.485
146	C	-0.121
147	C	0.096
148	C	0.102
149	C	-0.110
150	H	0.205
151	H	0.197
152	H	0.161
153	C	0.277
154	N	-0.469
155	C	0.276
156	N	-0.471
157	C	0.276
158	N	-0.471
159	C	0.274
160	N	-0.474

Reference Molecule R

Serial No	Symbol	Mullikan Charge
1	C	0.75
2	C	-0.159

3	**C**	**0.042**
4	**C**	**0.075**
5	**C**	**-0.159**
6	**C**	**0.042**
7	**C**	**-0.226**
8	**C**	**0.056**
9	**C**	**-0.232**
10	**C**	**-0.227**
11	**C**	**0.056**
12	**C**	**-0.32**
13	**C**	**-0.064**
14	**C**	**-0.297**
15	**S**	**0.383**
16	**C**	**-0.064**
17	**C**	**-0.297**
18	**S**	**0.383**
19	**C**	**0.089**
20	**C**	**0.095**
21	**C**	**0.089**
22	**C**	**0.095**
23	**C**	**0.200**
24	**C**	**0.200**
25	**C**	**-0.242**
26	**C**	**0.327**
27	**C**	**0.105**
28	**C**	**0.179**
29	**C**	**0.186**
30	**C**	**-0.242**
31	**C**	**0.327**
32	**C**	**0.105**
33	**C**	**0.179**
34	**C**	**0.186**
35	**N**	**-0.605**
36	**S**	**0.639**
37	**N**	**-0.595**
38	**N**	**-0.605**
39	**S**	**0.639**
40	**N**	**-0.595**
41	**C**	**-0.143**
42	**C**	**-0.159**
43	**C**	**0.089**
44	**C**	**-0.160**
45	**C**	**-0.140**
46	**C**	**-0.143**
47	**C**	**-0.161**

48	C	0.089
49	C	-0.160
50	C	-0.145
51	C	-0.145
52	C	-0.160
53	C	0.089
54	C	-0.161
55	C	-0.144
56	C	-0.143
57	C	-0.159
58	C	0.089
59	C	-0.160
60	C	-0.140
61	C	-0.450
62	C	-0.450
63	C	-0.450
64	C	-0.450
65	C	-0.270
66	C	-0.276
67	C	-0.110
68	C	-0.108
69	C	-0.245
70	S	0.427
71	C	-0.110
72	C	-0.108
73	C	-0.245
74	S	0.427
75	C	-0.058
76	C	-0.058
77	C	-0.322
78	C	-0.322
79	C	0.679
80	C	0.123
81	C	0.679
82	C	0.123
83	H	0.148
84	H	0.148
85	H	0.145
86	H	0.145
87	H	0.156
88	H	0.156
89	H	0.133
90	H	0.123
91	H	0.122
92	H	0.132

93	H	0.136
94	H	0.1247
95	H	0.123
96	H	0.136
97	H	0.136
98	H	0.123
99	H	0.124
100	H	0.136
101	H	0.133
102	H	0.123
103	H	0.122
104	H	0.132
105	H	0.158
106	H	0.144
107	H	0.144
108	H	0.144
109	H	0.144
110	H	0.158
111	H	0.156
112	H	0.147
113	H	0.143
114	H	0.156
115	H	0.147
116	H	0.143
117	H	0.161
118	H	0.151
119	H	0.161
120	H	0.151
121	H	0.187
122	H	0.187
123	F	-0.289
124	F	-0.289
125	O	-0.499
126	O	-0.499
127	N	-0.588
128	N	-0.588
129	C	-0.276
130	C	-0.276
131	H	0.188
132	H	0.196
133	H	0.188
134	H	0.196
135	H	0.188
136	H	0.188
137	C	0.130

138	C	0.130
139	C	0.301
140	N	0.496
141	C	0.331
142	N	-0.508
143	C	0.331
144	N	-0.509
145	C	0.301
146	N	-0.496
147	S	0.410
148	S	0.410

Cartesian coordinates

Reference R

Symbol	X	Y	Z
C	1.3701840	-0.1386610	-0.0570230
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C	-0.5388700	1.2845030	-0.0626110
C	-1.3701830	0.1386970	-0.0573790
C	-0.8373950	-1.1538910	-0.0549640
C	0.5388690	-1.2844670	-0.0625410
C	1.3683960	-2.5783110	-0.0300410
C	2.7719220	-1.9933530	-0.0012870
C	2.7315310	-0.6149080	-0.0326970
C	-1.3684040	2.5783390	-0.0302370
C	-2.7719420	1.9933800	-0.0018060
C	-2.7315360	0.6149380	-0.0333210
C	-4.0775730	2.4973680	0.0090780
C	-5.0406330	1.4956360	-0.0063070
S	-4.2910400	-0.0946930	-0.0430850
C	4.0775430	-2.4973610	0.0097220
C	5.0406160	-1.4956390	-0.0054530
S	4.2910460	0.0947040	-0.0422190

C	1.2299290	-3.4281330	-1.2998590
C	1.0061240	-3.3572490	1.2400910
C	-1.2296400	3.4282490	-1.2999600
C	-1.0064190	3.3572440	1.2400010
C	-6.4734210	1.6841410	0.0014100
C	6.4734020	-1.6841600	0.0024470
C	-7.0528520	2.9416980	0.0144290
C	-8.4411280	3.1460780	0.0224880
C	-9.4100250	2.1534800	0.0184410
C	-8.8433000	0.8359520	0.0044500
C	-7.4159750	0.6010080	-0.0040010
C	7.0528140	-2.9417210	0.0158390
C	8.4410870	-3.1461190	0.0239760
C	9.4099980	-2.1535350	0.0196810
C	8.8432920	-0.8360020	0.0053450
C	7.4159710	-0.6010410	-0.0031970
N	-9.5511990	-0.2893040	-0.0021220
S	-8.4937840	-1.5270810	-0.0178870
N	-7.1005110	-0.6897630	-0.0166720
N	9.5512060	0.2892420	-0.0014970
S	8.4938090	1.5270290	-0.0175950
N	7.1005240	0.6897310	-0.0161970
C	0.7222050	-2.9087960	-2.4903140
C	0.6918290	-3.6784990	-3.6493080
C	1.1667900	-4.9897810	-3.6638880
C	1.6822210	-5.5042110	-2.4712830
C	1.7136750	-4.7405940	-1.3119910
C	-0.0684360	-4.2521990	1.2412460
C	-0.4553780	-4.9018460	2.4064280

C	0.2146670	-4.6866010	3.6133350
C	1.2820400	-3.7882220	3.6088440
C	1.6719770	-3.1331120	2.4452670
C	-1.6723860	3.1328890	2.4450740
C	-1.2827240	3.7879920	3.6087470
C	-0.2155250	4.6865780	3.6134360
C	0.4546360	4.9020350	2.4066320
C	0.0679700	4.2523950	1.2413530
C	-0.7210010	2.9093250	-2.4901380
C	-0.6902980	3.6792460	-3.6490510
C	-1.1658540	4.9902450	-3.6637460
C	-1.6822260	5.5043120	-2.4713180
C	-1.7139810	4.7405500	-1.3121990
C	1.1016350	-5.8305160	-4.9081970
C	-1.1006340	5.8313810	-4.9077780
C	0.1845850	5.4185510	4.8638550
C	-0.1857410	-5.4185820	4.8636540
C	-10.8359300	2.4044930	0.0268470
C	10.8359000	-2.4045660	0.0281370
C	11.4941100	-3.6308560	0.0397180
C	12.8866500	-3.5177770	0.0454500
C	13.3352410	-2.2056070	0.0386800
S	11.9924580	-1.1016100	0.0245490
C	-11.4941580	3.6307780	0.0379090
C	-12.8866960	3.5176810	0.0438210
C	-13.3352670	2.2055000	0.0377150
S	-11.9924680	1.1015180	0.0239530
C	14.7016980	-1.8098950	0.0424630
C	-14.7017180	1.8097700	0.0418270

C	15.2648660	-0.5762260	0.0379580
C	-15.2648670	0.5760890	0.0379750
C	16.7237670	-0.4270740	0.0434830
C	16.0282100	1.8121420	0.0285980
C	-16.7237650	0.4269170	0.0437500
C	-16.0281760	-1.8122950	0.0298670
H	1.4835290	2.0246460	-0.0349420
H	-1.4835370	-2.0246100	-0.0354770
H	-4.3188960	3.5517870	0.0238260
H	4.3188370	-3.5517890	0.0243480
H	-6.4477850	3.8386460	0.0173200
H	6.4477350	-3.8386600	0.0189840
H	0.3481950	-1.8917710	-2.5189890
H	0.2891350	-3.2467180	-4.5608700
H	2.0635810	-6.5210010	-2.4486230
H	2.1079270	-5.1745220	-0.3988100
H	-0.6007910	-4.4540650	0.3177080
H	-1.2934430	-5.5921050	2.3761090
H	1.8201920	-3.5942500	4.5320180
H	2.5020180	-2.4359970	2.4798150
H	-2.5022990	2.4356140	2.4794600
H	-1.8209560	3.5938540	4.5318390
H	1.2925720	5.5924580	2.3764710
H	0.6004100	4.4544160	0.3178980
H	-0.3464750	1.8924900	-2.5187550
H	-0.2868320	3.2477970	-4.5604220
H	-2.0640620	6.5209310	-2.4487280
H	-2.1088890	5.1741770	-0.3991580
H	0.1765340	-6.4159510	-4.9401230

H	1.9338380	-6.5366160	-4.9569470
H	1.1276910	-5.2136090	-5.8090720
H	-1.9403530	6.5281010	-4.9630740
H	-1.1129380	5.2140600	-5.8086230
H	-0.1820500	6.4273130	-4.9327210
H	-0.2554160	6.4211030	4.8917840
H	1.2687640	5.5396730	4.9260300
H	-0.1487320	4.8903070	5.7595920
H	0.2542610	-6.4211320	4.8916840
H	-1.2699330	-5.5397090	4.9255690
H	0.1473610	-4.8903420	5.7594740
H	10.9722350	-4.5739240	0.0436540
H	13.5620370	-4.3644890	0.0543180
H	-10.9722980	4.5738560	0.0413460
H	-13.5620950	4.3643860	0.0523520
H	15.4283350	-2.6197720	0.0503570
H	-15.4283670	2.6196380	0.0494180
F	-8.8129690	4.4343350	0.0348310
F	8.8129110	-4.4343760	0.0366630
O	17.5482760	-1.3164710	0.0518910
O	-17.5482870	1.3163060	0.0518270
N	17.0690210	0.9391130	0.0376250
N	-17.0689990	-0.9392770	0.0386020
C	-18.4774310	-1.3064580	0.0430580
C	18.4774600	1.3062740	0.0416830
H	18.7211350	1.8890490	0.9294590
H	19.0314830	0.3689690	0.0486540
H	18.7285210	1.8802120	-0.8497790
H	-19.0314670	-0.3691580	0.0497120

H	-18.7286380	-1.8807910	-0.8481080
H	-18.7209440	-1.8888480	0.9311320
C	-16.0672530	-3.1932550	0.0235770
C	16.0673080	3.1930990	0.0216310
C	14.8329070	3.9008900	0.0127450
N	13.8137770	4.4604460	0.0056240
C	17.2505100	3.9793780	0.0227370
N	18.1910970	4.6629910	0.0233450
C	-17.2504420	-3.9795520	0.0251840
N	-18.1910190	-4.6631790	0.0262150
C	-14.8328420	-3.9010320	0.0149020
N	-13.8137040	-4.4605750	0.0079420
S	14.4762190	0.9890910	0.0260910
S	-14.4761970	-0.9892210	0.0267630

Molecule A1

Symbol	X	Y	Z
C	1.7231660	0.5451660	0.0064040
C	1.0934560	-0.7025090	0.0477150
C	-0.2888740	-0.7275230	0.0493410
C	-1.0295490	0.4774420	-0.0111970
C	-0.3999050	1.7247570	-0.0602550
C	0.9820770	1.7505140	-0.0406290
C	1.9076590	2.9759070	-0.1037230
C	3.2628750	2.2854110	-0.0912060
C	3.1168340	0.9153550	-0.0150450
C	-1.2149050	-1.9539260	0.0734710
C	-2.5695700	-1.2650810	0.0070390
C	-2.4228990	0.1068000	-0.0245670
C	-3.9098640	-1.6657070	0.0130030

C	-4.7927550	-0.5925200	-0.0215730
S	-3.9221580	0.9351950	-0.0518300
C	4.6028830	2.6874230	-0.0983100
C	5.4862830	1.6162730	-0.0346310
S	4.6168790	0.0895500	0.0407200
C	1.8175820	3.8770150	1.1344530
C	1.6234970	3.7350540	-1.4055910
C	-1.1461270	-2.7481440	1.3844370
C	-0.9114190	-2.8216080	-1.1540430
C	-6.2346290	-0.6716930	-0.0306890
C	6.9284600	1.6969440	-0.0198900
C	-6.9086990	-1.8816180	-0.0224010
C	-8.3082820	-1.9795730	-0.0259290
C	-9.1993770	-0.9149920	-0.0394610
C	-8.5330050	0.3559060	-0.0508550
C	-7.0919130	0.4805420	-0.0468160
C	7.6009350	2.9073310	-0.0386520
C	9.0002510	3.0065030	-0.0228060
C	9.8923910	1.9437400	0.0149850
C	9.2279160	0.6718760	0.0297280
C	7.7867570	0.5462400	0.0153490
N	-9.1520280	1.5319400	-0.0661580
S	-8.0018630	2.6843110	-0.0746500
N	-6.6769220	1.7424620	-0.0592650
N	9.8470950	-0.5041240	0.0578380
S	8.6971460	-1.6566330	0.0713670
N	7.3723280	-0.7158180	0.0360930
C	1.2407720	3.4473440	2.3286830
C	1.2551820	4.2576300	3.4606250

C	1.8449960	5.5208090	3.4426830
C	2.4281720	5.9457880	2.2454180
C	2.4153110	5.1421280	1.1137430
C	0.6332840	4.7202870	-1.4527130
C	0.3135330	5.3544830	-2.6472540
C	0.9696040	5.0326980	-3.8372590
C	1.9534360	4.0438760	-3.7865130
C	2.2755130	3.4046360	-2.5945280
C	-1.5401170	-2.5912190	-2.3786770
C	-1.1992420	-3.3301720	-3.5059230
C	-0.2189600	-4.3226500	-3.4542800
C	0.4133700	-4.5446430	-2.2292680
C	0.0745250	-3.8106350	-1.0987800
C	-0.5757060	-2.2262510	2.5442770
C	-0.6074390	-2.9404800	3.7390520
C	-1.2087490	-4.1955280	3.8201300
C	-1.7858480	-4.7129880	2.6565640
C	-1.7554160	-4.0056640	1.4628610
C	1.8337130	6.4074190	4.6563790
C	-1.2158560	-4.9795580	5.1025220
C	0.1232200	-5.1424170	-4.6668350
C	0.6475920	5.7462760	-5.1204450
C	-10.6398200	-1.0533740	-0.0418950
C	11.3318490	2.0891830	0.0489070
C	12.0719330	3.2718630	0.0586060
C	13.4482510	3.0592660	0.0752600
C	13.8070090	1.7154360	0.1121080
S	12.3891250	0.7116440	0.0848260
C	-11.3855680	-2.2364940	-0.0312340

C	-12.7633850	-2.0406630	-0.0358890
C	-13.1253340	-0.6947260	-0.0504470
S	-11.6958860	0.3162750	-0.0586100
C	15.1485950	1.2582440	0.0264930
C	-14.3645520	-0.0041010	-0.0603170
H	1.6709070	-1.6201540	0.0702510
H	-0.9771600	2.6408820	-0.1197660
H	-4.2340800	-2.6970760	0.0480290
H	4.9257160	3.7187580	-0.1447530
H	-6.3749090	-2.8226860	-0.0124470
H	7.0662280	3.8476680	-0.0608740
H	0.7765580	2.4693240	2.3830880
H	0.7968920	3.8956740	4.3762250
H	2.8985960	6.9236890	2.1978870
H	2.8646090	5.5072790	0.1958240
H	0.1149510	5.0053020	-0.5432690
H	-0.4599280	6.1169380	-2.6530270
H	2.4784610	3.7660440	-4.6957660
H	3.0408770	2.6362370	-2.5926680
H	-2.3016120	-1.8229070	-2.4562520
H	-1.7061460	-3.1288060	-4.4451130
H	1.1831190	-5.3073530	-2.1559990
H	0.5743160	-4.0194720	-0.1588470
H	-0.1019080	-1.2516360	2.5217580
H	-0.1526700	-2.5088070	4.6257240
H	-2.2647040	-5.6875320	2.6852520
H	-2.1987650	-4.4420490	0.5735890
H	1.0244320	7.1431250	4.5998950
H	2.7695260	6.9632930	4.7533000

H	1.6873260	5.8298680	5.5714160
H	-2.1676570	-5.4961690	5.2492680
H	-1.0449510	-4.3338260	5.9662530
H	-0.4302260	-5.7424630	5.1023640
H	-0.5183340	-6.0272650	-4.7382140
H	1.1572860	-5.4925710	-4.6333460
H	-0.0108220	-4.5692850	-5.5870520
H	1.2761700	6.6344200	-5.2457890
H	-0.3926160	6.0788950	-5.1421300
H	0.8160200	5.1040140	-5.9877710
H	11.6174820	4.2486810	0.0466260
H	14.1835610	3.8545450	0.0673840
H	-10.9288220	-3.2127170	-0.0202170
H	-13.5016410	-2.8288080	-0.0289170
H	15.8518630	2.0334220	-0.2806690
F	-8.7736530	-3.2355620	-0.0157410
F	9.4652760	4.2630050	-0.0440160
C	-15.6748690	-0.4266830	-0.0539380
C	-16.8435440	0.4574100	-0.0660230
C	-18.0496480	-0.3989610	-0.0383570
C	-17.6479080	-1.7382890	-0.0168060
C	-16.1737730	-1.8229920	-0.0270880
O	-15.5453650	-2.8677670	-0.0141380
C	-16.8794400	1.8349930	-0.1003620
C	-18.0939560	2.5811460	-0.1084450
N	-19.0610360	3.2261050	-0.1159550
C	-15.7310850	2.6785160	-0.1334590
N	-14.8276870	3.4101150	-0.1616630
C	-19.4133210	-0.0945550	-0.0317810

C	-20.3091650	-1.1498520	-0.0040890
C	-19.8880780	-2.4845610	0.0165990
C	-18.5417500	-2.7964430	0.0104490
H	-19.8089920	0.9110710	-0.0466220
H	-18.2006410	-3.8244480	0.0264430
C	15.7423960	0.0286390	0.1072500
C	15.3247520	-1.2866180	0.5582700
C	16.1935660	-2.2731880	-0.1193640
C	17.2543290	-1.5890500	-0.7323510
C	17.0694610	-0.1303160	-0.5586210
O	17.8130510	0.7518990	-0.9375780
C	14.4723700	-1.5663180	1.6024020
C	14.1301760	-2.8971700	1.9783870
N	13.8257650	-3.9772300	2.2815460
C	13.9775620	-0.5558030	2.4753920
N	13.6091390	0.2398000	3.2380630
C	16.1397750	-3.6656460	-0.1814000
C	17.1534460	-4.3165380	-0.8651150
C	18.2121680	-3.6226460	-1.4629280
C	18.2767200	-2.2428010	-1.4016640
H	15.3511600	-4.2560760	0.2650730
H	19.0935410	-1.6988530	-1.8603710
H	-14.2335020	1.0725360	-0.0746340
F	17.1391900	-5.6421490	-0.9684780
F	-20.8129580	-3.4391820	0.0423760
F	-21.6169750	-0.9084750	0.0035450
F	19.1489800	-4.3241150	-2.0943580

Molecule A2

Symbol	X	Y	Z

C	-1.6611590	0.3801140	0.0657840
C	-1.0197760	-0.8617320	0.0980410
C	0.3625180	-0.8746450	0.0725040
C	1.0923410	0.3377150	0.0371570
C	0.4510380	1.5798780	0.0132030
C	-0.9313720	1.5922440	0.0167320
C	-1.8684920	2.8103750	0.0086830
C	-3.2167050	2.1086510	0.0700010
C	-3.0580070	0.7382730	0.0863900
C	1.2997440	-2.0920570	0.1158530
C	2.6487000	-1.3891040	0.1065600
C	2.4894190	-0.0197120	0.0485340
C	3.9926300	-1.7783070	0.1051140
C	4.8657010	-0.6981410	0.0530790
S	3.9813880	0.8210310	-0.0001510
C	-4.5607890	2.4980930	0.0672480
C	-5.4341040	1.4174280	0.0889140
S	-4.5507160	-0.1029140	0.1028940
C	-1.8101630	3.6199760	-1.2932740
C	-1.5695620	3.6668140	1.2450880
C	1.2119760	-2.9785190	-1.1329910
C	1.0287710	-2.8710470	1.4088610
C	6.3086190	-0.7643260	0.0362240
C	-6.8775190	1.4844170	0.0938030
C	6.9933730	-1.9679090	0.0338230
C	8.3940320	-2.0534540	0.0225230
C	9.2755750	-0.9813250	0.0104070
C	8.5976370	0.2836120	0.0089450
C	7.1553640	0.3954130	0.0211680

C	-7.5607690	2.6885130	0.1019040
C	-8.9612280	2.7751840	0.0933460
C	-9.8440910	1.7045670	0.0775340
C	-9.1680640	0.4386260	0.0808120
C	-7.7255350	0.3259010	0.0869090
N	9.2059200	1.4653430	-0.0035720
S	8.0455940	2.6072390	-0.0004570
N	6.7289500	1.6536730	0.0173710
N	-9.7768010	-0.7431930	0.0785890
S	-8.6168260	-1.8854000	0.0783010
N	-7.2998850	-0.9326790	0.0863670
C	-1.2431800	3.1139920	-2.4618520
C	-1.2859000	3.8407230	-3.6487050
C	-1.8950360	5.0929690	-3.7129090
C	-2.4682990	5.5946020	-2.5406150
C	-2.4270940	4.8746850	-1.3547600
C	-0.5892200	4.6619930	1.1998040
C	-0.2539290	5.3861160	2.3376110
C	-0.8845840	5.1479370	3.5605140
C	-1.8594310	4.1497710	3.6021140
C	-2.1966730	3.4205370	2.4673620
C	1.6806010	-2.5478390	2.5999090
C	1.3699190	-3.2058160	3.7846650
C	0.3979180	-4.2067270	3.8258650
C	-0.2579150	-4.5214450	2.6338890
C	0.0506740	-3.8686410	1.4464250
C	0.6163730	-2.5442200	-2.3162020
C	0.6313110	-3.3414410	-3.4575240
C	1.2401940	-4.5955620	-3.4601220

C	1.8422220	-5.0251930	-2.2738110
C	1.8288160	-4.2347130	-1.1330020
C	-1.9149380	5.8902370	-4.9870090
C	1.2292750	-5.4687080	-4.6835880
C	0.0881750	-4.9398540	5.1010590
C	-0.5461060	5.9571080	4.7812350
C	10.7176120	-1.1070070	0.0008410
C	-11.2853410	1.8370840	0.0474940
C	-12.0351830	3.0127840	0.0302640
C	-13.4102820	2.7881950	0.0152870
C	-13.7572840	1.4418140	-0.0125880
S	-12.3315320	0.4504370	0.0222220
C	11.4737890	-2.2827840	-0.0061460
C	12.8505010	-2.0743730	-0.0123280
C	13.1999100	-0.7257650	-0.0100790
S	11.7619250	0.2721580	-0.0002280
C	-15.0967220	0.9738730	0.0726270
C	14.4338940	-0.0229500	-0.0092040
H	-1.5884420	-1.7837630	0.1486540
H	1.0200940	2.5029350	-0.0008030
H	4.3258060	-2.8068650	0.1390140
H	-4.8937060	3.5269420	0.0411980
H	6.4678590	-2.9137030	0.0376780
H	-7.0345000	3.6338360	0.1118980
H	-0.7640400	2.1417590	-2.4524770
H	-0.8342160	3.4209800	-4.5426620
H	-2.9532880	6.5664140	-2.5562460
H	-2.8685850	5.2986310	-0.4585890
H	-0.0911170	4.8833170	0.2618180

H	0.5116660	6.1537150	2.2720650
H	-2.3649260	3.9360290	4.5393380
H	-2.9540580	2.6474210	2.5369050
H	2.4367230	-1.7703770	2.6054170
H	1.8944930	-2.9332280	4.6957660
H	-1.0223390	-5.2930000	2.6323640
H	-0.4668950	-4.1482940	0.5349040
H	0.1361580	-1.5731980	-2.3543450
H	0.1575080	-2.9764660	-4.3639830
H	2.3275860	-5.9964330	-2.2422190
H	2.2924750	-4.6036570	-0.2237450
H	-1.1361710	6.6601660	-4.9826110
H	-2.8720330	6.3996870	-5.1240840
H	-1.7425330	5.2549610	-5.8581730
H	2.1745840	-6.0044730	-4.8001210
H	1.0580290	-4.8840760	-5.5897810
H	0.4358440	-6.2212270	-4.6240400
H	0.7277390	-5.8218250	5.2139440
H	-0.9479180	-5.2852130	5.1214040
H	0.2512980	-4.3062220	5.9757330
H	-1.1859680	6.8428380	4.8569690
H	0.4888780	6.3052770	4.7551640
H	-0.6853270	5.3767880	5.6961460
H	-11.5893390	3.9936300	0.0355560
H	-14.1524050	3.5771390	0.0179220
H	11.0260610	-3.2632710	-0.0064700
H	13.5967570	-2.8550580	-0.0187690
H	-15.8065360	1.7455490	0.3738780
F	8.8701740	-3.3057060	0.0234370

F	-9.4366430	4.0282500	0.0995360
C	15.7469830	-0.4332650	-0.0270480
C	16.9087300	0.4611240	-0.0201930
C	18.1224040	-0.3831710	-0.0976470
C	17.7327630	-1.7274760	-0.1281950
C	16.2602180	-1.8256120	-0.0799200
O	15.6365040	-2.8736620	-0.0879220
C	16.9296210	1.8375040	0.0569900
C	18.1324190	2.6031040	0.0558200
N	19.0833540	3.2717390	0.0577610
C	15.7730550	2.6652060	0.1535910
N	14.8631440	3.3848150	0.2349030
C	19.4827980	-0.0706900	-0.1392920
C	20.4021590	-1.1156860	-0.2087930
C	19.9959830	-2.4514010	-0.2362850
C	18.6420650	-2.7692630	-0.1957700
H	19.8404290	0.9487110	-0.1205410
H	21.4600820	-0.8795480	-0.2422540
H	20.7399440	-3.2385780	-0.2897730
H	18.2869120	-3.7933850	-0.2159350
C	-15.6815000	-0.2588100	-0.0039640
C	-15.2546370	-1.5767070	-0.4405910
C	-16.1186760	-2.5626130	0.2457570
C	-17.1910100	-1.8791970	0.8429720
C	-17.0149820	-0.4213610	0.6531000
O	-17.7645520	0.4641390	1.0131650
C	-14.4018210	-1.8576970	-1.4839900
C	-14.0541290	-3.1878520	-1.8588360
N	-13.7411650	-4.2638380	-2.1676650

C	-13.9115820	-0.8491160	-2.3621940
N	-13.5456950	-0.0560040	-3.1287580
C	-16.0535580	-3.9521860	0.3361230
C	-17.0683450	-4.6176320	1.0222160
C	-18.1379890	-3.9286920	1.5981330
C	-18.2075420	-2.5410570	1.5109430
H	-15.2394290	-4.5146910	-0.1006300
H	-17.0231420	-5.6978260	1.1074720
H	-18.9138740	-4.4804460	2.1172720
H	-19.0233220	-1.9768500	1.9485730
H	14.2921240	1.0523110	0.0062930

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Symbol	X	Y	Z
C	-1.2650710	0.2600760	0.0107670
C	-0.6004760	1.4900950	0.0055620
C	0.7819530	1.4765030	0.0174190
C	1.4891110	0.2502230	0.0108080
C	0.8245010	-0.9797640	0.0083300
C	-0.5579960	-0.9661510	0.0201190
C	-1.5177760	-2.1664850	0.0071690
C	-2.8531230	-1.4385510	-0.0237900
C	-2.6685910	-0.0714380	-0.0063130
C	1.7417580	2.6767500	0.0015630
C	3.0770470	1.9486620	-0.0274960
C	2.8926830	0.5816970	-0.0069650
C	4.4283810	2.3128830	-0.0284190
C	5.2812680	1.2159950	-0.0161170
S	4.3694130	-0.2873740	0.0057520
C	-4.2043380	-1.8026130	-0.0236680

C	-5.0572500	-0.7055510	-0.0136850
S	-4.1451030	0.7977600	0.0049590
C	-1.4617610	-3.0090580	1.2880630
C	-1.2466600	-2.9976220	-1.2526870
C	1.6854400	3.5227010	1.2802020
C	1.4706760	3.5045120	-1.2605600
C	6.7259620	1.2552650	-0.0176580
C	-6.5016700	-0.7446990	-0.0153350
C	7.4322320	2.4454190	-0.0301290
C	8.8345840	2.5051670	-0.0307220
C	9.6987460	1.4189460	-0.0197050
C	8.9967930	0.1660280	-0.0068570
C	7.5517630	0.0810570	-0.0056680
C	-7.2082980	-1.9351350	-0.0285420
C	-8.6105830	-1.9950700	-0.0288010
C	-9.4722990	-0.9074790	-0.0169000
C	-8.7714070	0.3446820	-0.0034140
C	-7.3271080	0.4301440	-0.0025210
N	9.5814220	-1.0275520	0.0052280
S	8.4003910	-2.1463760	0.0170920
N	7.1008930	-1.1686310	0.0072630
N	-9.3580650	1.5374050	0.0095510
S	-8.1770330	2.6577880	0.0218000
N	-6.8778050	1.6804120	0.0110600
C	-0.8678650	-2.5459720	2.4611460
C	-0.9112900	-3.3015520	3.6298040
C	-1.5475950	-4.5412390	3.6706450
C	-2.1476610	-4.9997780	2.4941800
C	-2.1060390	-4.2508730	1.3263670

C	-0.2856740	-4.0123980	-1.2413050
C	0.0257620	-4.7136930	-2.3999720
C	-0.6106860	-4.4325220	-3.6107210
C	-1.5663850	-3.4152640	-3.6182770
C	-1.8795040	-2.7085280	-2.4625470
C	2.1038900	3.2124240	-2.4694750
C	1.7908920	3.9161410	-3.6271170
C	0.8349940	4.9331970	-3.6224450
C	0.1981380	5.2173490	-2.4125640
C	0.5094290	4.5191100	-1.2520440
C	1.0918420	3.0625030	2.4545800
C	1.1347020	3.8213680	3.6211160
C	1.7701690	5.0616090	3.6584950
C	2.3700960	5.5171570	2.4808090
C	2.3290340	4.7649570	1.3150880
C	-1.5672010	-5.3704650	4.9242290
C	1.7888990	5.8944880	4.9096560
C	0.5224240	5.7144430	-4.8680240
C	-0.2979710	-5.2168360	-4.8543420
C	11.1446550	1.5248990	-0.0208910
C	-10.9169610	-1.0074310	-0.0177440
C	-11.6941740	-2.1679470	-0.0293890
C	-13.0679680	-1.9337220	-0.0270530
C	-13.3914710	-0.5803960	-0.0133330
S	-11.9368400	0.3907290	-0.0034140
C	11.9036200	2.6960480	-0.0292650
C	13.2716510	2.4505710	-0.0283450
C	13.6080720	1.0963160	-0.0193380
S	12.1661210	0.1155730	-0.0115380

C	-14.6163390	0.1432300	-0.0056990
C	14.9743570	0.7039140	-0.0174520
H	-1.1520290	2.4236430	-0.0141470
H	1.3760910	-1.9133280	-0.0092680
H	4.7804480	3.3356720	-0.0329520
H	-4.5564360	-2.8254090	-0.0255820
H	6.9244060	3.4008140	-0.0392520
H	-6.7002090	-2.8903600	-0.0386770
H	-0.3664520	-1.5850210	2.4694870
H	-0.4382090	-2.9149010	4.5276360
H	-2.6540480	-5.9607450	2.4920200
H	-2.5689000	-4.6419940	0.4260250
H	0.2161790	-4.2665840	-0.3136920
H	0.7769950	-5.4971310	-2.3607830
H	-2.0757470	-3.1682920	-4.5451660
H	-2.6221790	-1.9193950	-2.5058360
H	2.8468520	2.4234380	-2.5105040
H	2.3006310	3.6669900	-4.5532160
H	-0.5532020	6.0007850	-2.3755550
H	0.0073770	4.7757060	-0.3251970
H	0.5910620	2.1012420	2.4656280
H	0.6617620	3.4369780	4.5199950
H	2.8758360	6.4784460	2.4759690
H	2.7917420	5.1538530	0.4137090
H	-0.7918010	-6.1434010	4.8979350
H	-2.5260670	-5.8789920	5.0516210
H	-1.3888130	-4.7582610	5.8106470
H	2.7467710	6.4053900	5.0349230
H	1.6123310	5.2845090	5.7979750

H	1.0118670	6.6657150	4.8816090
H	1.1689030	6.5944010	-4.9541170
H	-0.5106630	6.0693120	-4.8679660
H	0.6733550	5.1112820	-5.7660940
H	-0.9484260	-6.0937690	-4.9414560
H	0.7334120	-5.5765800	-4.8506300
H	-0.4432210	-4.6140590	-5.7536210
H	-11.2652390	-3.1567660	-0.0391930
H	-13.8263150	-2.7025890	-0.0348430
H	11.4738190	3.6839550	-0.0354810
H	14.0260270	3.2286260	-0.0339300
H	15.6174190	1.5777690	-0.0240440
F	9.3297010	3.7506580	-0.0437080
F	-9.1092760	-3.2386060	-0.0423610
C	15.6223890	-0.5022060	-0.0093290
C	17.0747400	-0.6977900	-0.0088050
C	17.3088400	-2.1467930	0.0018030
C	16.0924080	-2.7960180	0.0072440
C	14.9766420	-1.8442150	0.0008150
O	13.7862400	-2.0968280	0.0032560
C	18.0867270	0.2353700	-0.0164410
C	19.4572000	-0.1563140	-0.0142970
N	20.5772680	-0.4663100	-0.0126010
C	17.8836150	1.6450020	-0.0270220
N	17.7474490	2.7996600	-0.0357590
C	18.4086630	-3.0476750	0.0079590
C	17.9712660	-4.3446120	0.0179010
S	16.2470400	-4.4907920	0.0198990
H	19.4534390	-2.7731880	0.0053680

H	18.5785960	-5.2385880	0.0242810
C	-15.9331130	-0.2422850	-0.0100360
C	-17.0729670	0.6850640	0.0002340
C	-18.2927740	-0.1299810	-0.0085880
C	-17.9357720	-1.4602520	-0.0235000
C	-16.4803250	-1.6346950	-0.0255230
O	-15.8818850	-2.6950690	-0.0374160
C	-17.0894680	2.0614280	0.0153400
C	-18.3171950	2.7864400	0.0236590
N	-19.3109380	3.3889390	0.0305770
C	-15.9338270	2.8941090	0.0239670
N	-15.0171190	3.6091970	0.0313350
C	-19.7025160	0.0565290	-0.0062260
C	-20.3492850	-1.1496790	-0.0195530
S	-19.2772720	-2.5078060	-0.0349360
H	-20.2175610	1.0058140	0.0045230
H	-21.4169270	-1.3177540	-0.0211990
H	-14.4602380	1.2172960	0.0059770

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Symbol	X	Y	Z
C	1.7609040	0.6443140	0.0238040
C	1.1380060	-0.6055050	0.0964020
C	-0.2438840	-0.6384130	0.0839990
C	-0.9898010	0.5606550	-0.0209330
C	-0.3668520	1.8096710	-0.1032920
C	1.0144600	1.8439590	-0.0701170
C	1.9339370	3.0720090	-0.1627060
C	3.2921760	2.3901770	-0.1053550
C	3.1522780	1.0213550	0.0105180

C	-1.1635550	-1.8686050	0.1367650
C	-2.5208850	-1.1888070	0.0405430
C	-2.3806580	0.1829830	-0.0331780
C	-3.8585110	-1.5948880	0.0505600
C	-4.7464580	-0.5265930	-0.0230610
S	-3.8824620	1.0036020	-0.0967360
C	4.6291950	2.7986390	-0.1048250
C	5.5173020	1.7337850	0.0043100
S	4.6545010	0.2050020	0.1103760
C	1.8189710	4.0175510	1.0397310
C	1.6663440	3.7804010	-1.4965960
C	-1.1000830	-2.6244040	1.4706060
C	-0.8470940	-2.7680960	-1.0644860
C	-6.1862910	-0.6128150	-0.0360590
C	6.9568010	1.8233270	0.0434950
C	-6.8554020	-1.8256240	0.0153910
C	-8.2534960	-1.9293520	0.0089960
C	-9.1490570	-0.8682470	-0.0488470
C	-8.4884160	0.4043620	-0.1055890
C	-7.0485560	0.5348750	-0.1000050
C	7.6224590	3.0388010	0.0319060
C	9.0196790	3.1456250	0.0690020
C	9.9172830	2.0864430	0.1248310
C	9.2604940	0.8105130	0.1337310
C	7.8211940	0.6770780	0.0972130
N	-9.1123540	1.5759070	-0.1682690
S	-7.9666800	2.7324900	-0.2157010
N	-6.6387480	1.7969000	-0.1586690
N	9.8857960	-0.3615380	0.1760560

S	8.7418530	-1.5209230	0.1760150
N	7.4135280	-0.5869320	0.1163790
C	1.2305960	3.6259830	2.2415620
C	1.2219010	4.4772900	3.3427700
C	1.7996750	5.7451230	3.2857100
C	2.3949750	6.1314520	2.0814640
C	2.4049510	5.2867030	0.9798910
C	0.6666150	4.7521650	-1.5970000
C	0.3626170	5.3397730	-2.8189690
C	1.0442440	4.9833930	-3.9847330
C	2.0372530	4.0082340	-3.8806210
C	2.3438060	3.4153450	-2.6607480
C	-1.4669990	-2.5731190	-2.2997140
C	-1.1141620	-3.3402580	-3.4041380
C	-0.1302020	-4.3268170	-3.3183700
C	0.4932780	-4.5132330	-2.0829220
C	0.1426540	-3.7507800	-0.9750300
C	-0.5452060	-2.0633390	2.6195960
C	-0.5811250	-2.7425570	3.8344500
C	-1.1717250	-4.0002720	3.9470160
C	-1.7338590	-4.5567840	2.7940730
C	-1.6991200	-3.8845450	1.5804050
C	1.7617740	6.6756240	4.4654270
C	-1.1836990	-4.7465980	5.2515800
C	0.2247980	-5.1768880	-4.5059960
C	0.7382820	5.6474930	-5.2979650
C	-10.5871090	-1.0113390	-0.0517700
C	11.3532650	2.2392230	0.1817550
C	12.0878320	3.4283730	0.2091110

C	13.4618920	3.2235860	0.2449540
C	13.8290450	1.8784530	0.2778350
S	12.4148580	0.8669070	0.2259740
C	-11.3295910	-2.1987080	-0.0004830
C	-12.7052580	-2.0090100	-0.0165190
C	-13.0735460	-0.6628980	-0.0813980
S	-11.6456110	0.3529980	-0.1225850
C	15.1695270	1.4344760	0.2062720
C	-14.3103350	0.0191470	-0.1206320
H	1.7201090	-1.5186230	0.1541100
H	-0.9484890	2.7200910	-0.1970680
H	-4.1780590	-2.6262520	0.1154040
H	4.9474050	3.8297050	-0.1800920
H	-6.3175910	-2.7630490	0.0647930
H	7.0822920	3.9756730	0.0012420
H	0.7755190	2.6458200	2.3261970
H	0.7550680	4.1445320	4.2650960
H	2.8563220	7.1117220	2.0040580
H	2.8628100	5.6222820	0.0549500
H	0.1283640	5.0640330	-0.7081220
H	-0.4184850	6.0929450	-2.8658700
H	2.5822380	3.7042480	-4.7694880
H	3.1174000	2.6563990	-2.6181900
H	-2.2310270	-1.8105060	-2.4042380
H	-1.6144480	-3.1661410	-4.3522500
H	1.2653490	-5.2705140	-1.9831530
H	0.6359980	-3.9326350	-0.0261220
H	-0.0801830	-1.0853780	2.5728650
H	-0.1381990	-2.2810570	4.7120080

H	-2.2038130	-5.5346020	2.8470730
H	-2.1300790	-4.3510540	0.7003850
H	0.9229810	7.3755510	4.3883580
H	2.6750210	7.2715890	4.5334180
H	1.6447090	6.1277410	5.4026960
H	-2.1381330	-5.2541470	5.4123090
H	-1.0103310	-4.0769830	6.0963340
H	-0.4020240	-5.5131280	5.2739180
H	-0.4158390	-6.0635010	-4.5612610
H	1.2584640	-5.5256170	-4.4529990
H	0.0999180	-4.6274960	-5.4418170
H	1.3405500	6.5525020	-5.4312690
H	-0.3111650	5.9440810	-5.3605030
H	0.9542610	4.9861280	-6.1398920
H	11.6274250	4.4023140	0.1963430
H	14.1932060	4.0225610	0.2527720
H	-10.8685270	-3.1717100	0.0472180
H	-13.4397480	-2.7999420	0.0171260
H	15.8749110	2.2234590	-0.0572790
F	-8.7151650	-3.1844650	0.0648710
F	9.4794920	4.4031090	0.0512870
C	-15.6243080	-0.4093290	-0.0974160
C	-16.7924110	0.4683950	-0.1469120
C	-17.9996620	-0.3911890	-0.0660980
C	-17.5904280	-1.7256580	0.0142480
C	-16.1102640	-1.8014150	-0.0049680
O	-15.4832200	-2.8451630	0.0505290
C	-16.8393800	1.8415270	-0.2564180
C	-18.0569300	2.5815090	-0.2938380

N	**-19.0257870**	**3.2227070**	**-0.3273830**
C	**-15.6944050**	**2.6853850**	**-0.3488150**
N	**-14.7917260**	**3.4139160**	**-0.4275740**
C	**-19.3616590**	**-0.0978910**	**-0.0586600**
C	**-20.2767920**	**-1.1537600**	**0.0284080**
C	**-19.8422450**	**-2.4976730**	**0.1070590**
C	**-18.4748480**	**-2.7818800**	**0.0994090**
H	**-19.7442400**	**0.9109910**	**-0.1163360**
H	**-18.1105970**	**-3.8004400**	**0.1590830**
C	**15.7695340**	**0.1997030**	**0.2524760**
C	**15.3515410**	**-1.1239540**	**0.6652590**
C	**16.2364230**	**-2.0944670**	**-0.0233590**
C	**17.3008200**	**-1.3900560**	**-0.6055570**
C	**17.1001570**	**0.0690320**	**-0.3999400**
O	**17.8466950**	**0.9581030**	**-0.7543120**
C	**14.4917000**	**-1.4383460**	**1.6938430**
C	**14.1474100**	**-2.7793500**	**2.0283650**
N	**13.8407000**	**-3.8675330**	**2.2979190**
C	**13.9878530**	**-0.4519190**	**2.5884630**
N	**13.6135820**	**0.3274400**	**3.3648560**
C	**16.1874190**	**-3.4801790**	**-0.1330420**
C	**17.2114860**	**-4.1331980**	**-0.8300340**
C	**18.2877900**	**-3.4112630**	**-1.3972190**
C	**18.3292090**	**-2.0190130**	**-1.2779270**
H	**15.3851000**	**-4.0688460**	**0.2903710**
H	**19.1418720**	**-1.4441640**	**-1.7056060**
H	**-14.1852070**	**1.0950480**	**-0.1777020**
C	**-21.6749960**	**-0.8537670**	**0.0375190**
N	**-22.8056910**	**-0.5951570**	**0.0440900**

C	**-20.7866970**	**-3.5662260**	**0.1949470**
N	**-21.5296360**	**-4.4542790**	**0.2671580**
C	**19.3304330**	**-4.0912170**	**-2.0987620**
N	**20.1897800**	**-4.6165320**	**-2.6744170**
C	**17.1526560**	**-5.5553870**	**-0.9673210**
N	**17.0855850**	**-6.7085950**	**-1.0723560**