Quantum Chemical modification of indaceno dithiophene-based small acceptor molecules with enhanced Photovoltaic aspects for highly efficient organic solar cells

Supporting information, Cartesian coordinates of internally optimized geometries of all molecules (reference **IDSTR**, and investigated molecules **IDST1, IDST2, IDST3, IDST4, IDST5, IDST6** and **IDST7** along X, Y and Z axis at MPW1PW91/6-31G (d, p) level of density functional theory (DFT).

Cartesian coordinates of Reference Molecule IDSTR

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.064387	-0.284287	0.165203
2	6	0	-0.606803	-1.585701	-0.107777
3	6	0	-1.447211	-2.693408	-0.209805
4	6	0	-2.790185	-2.454278	0.082721
5	6	0	-3.285415	-1.161676	0.340288
6	6	0	-2.429285	-0.034957	0.464318
7	1	0	-1.083512	-3.664365	-0.470971
8	1	0	-2.791413	0.934990	0.737189
9	6	0	0.156056	0.699301	0.063680
10	6	0	0.243696	1.704937	1.232732
11	6	0	0.089831	1.497267	-1.245526
12	6	0	-3.943831	-3.483315	0.180472
13	6	0	-3.940282	-4.510661	-0.963844
14	6	0	-3.858784	-4.243434	1.516072
15	6	0	0.904753	-1.517025	-0.228205
16	6	0	1.340440	-0.291165	-0.003803
17	6	0	2.880389	-0.211099	0.134057

18	6	0	3.424216	-1.464634	-0.053376
19	16	0	2.189881	-2.672283	-0.531389
20	1	0	3.441296	0.676996	0.346701
21	6	0	-4.826836	-1.312246	0.400509
22	6	0	-5.172880	-2.571527	0.183265
23	6	0	-6.685685	-2.793030	-0.022013
24	6	0	-7.356737	-1.601072	0.106497
25	16	0	-6.238596	-0.279270	0.627929
26	1	0	-7.143800	-3.734408	-0.244035
27	6	0	4.907299	-1.820681	0.111111
28	6	0	5.360158	-3.094524	0.195333
29	16	0	6.217561	-0.651035	0.206542
30	6	0	6.934774	-3.144651	-0.019107
31	6	0	7.487767	-1.849274	-0.038479
32	1	0	7.500070	-4.048268	-0.133541
33	6	0	8.985089	-1.387051	-0.211083
34	6	0	10.663985	0.681467	-0.169693
35	6	0	9.278042	-0.028684	-0.152316
36	6	0	8.251585	1.116289	-0.053089
37	6	0	11.883982	0.083884	-0.231836
38	6	0	11.982161	-1.448284	-0.283719
39	6	0	13.178224	0.927195	-0.253988
40	8	0	7.004447	0.991470	0.001293
41	7	0	12.055361	-2.590054	-0.322383
42	7	0	14.145089	1.545682	-0.270883
43	6	0	10.818002	4.589647	0.018991
44	6	0	11.321666	3.268488	-0.057815
45	6	0	10.400770	2.210976	-0.080716

46	6	0	9.034223	2.449253	-0.020856
47	6	0	8.516723	3.742906	0.050146
48	6	0	9.419969	4.823951	0.069968
49	1	0	12.374882	3.086789	-0.096718
50	1	0	7.460059	3.910764	0.091525
51	9	0	8.951926	6.089440	0.137623
52	9	0	11.671580	5.637060	0.045149
53	6	0	-8.871231	-1.409114	-0.146747
54	6	0	-10.805258	0.360720	-0.215242
55	6	0	-9.351848	-0.150916	-0.104593
56	6	0	-8.474459	1.081368	0.077250
57	6	0	-11.941176	-0.376988	-0.359875
58	6	0	-11.879296	-1.914042	-0.438831
59	6	0	-13.311871	0.323673	-0.441729
60	8	0	-7.225437	1.089651	0.223691
61	7	0	-11.842126	-3.058435	-0.498380
62	7	0	-14.334870	0.840359	-0.503261
63	6	0	-11.400475	4.212182	-0.091774
64	6	0	-11.747244	2.845181	-0.194091
65	6	0	-10.719174	1.905686	-0.127969
66	6	0	-9.396674	2.301519	0.037100
67	6	0	-9.031039	3.633847	0.143092
68	6	0	-10.045861	4.602789	0.075791
69	1	0	-12.766230	2.542830	-0.318476
70	1	0	-8.005891	3.912823	0.270757
71	9	0	-9.726687	5.910483	0.171817
72	9	0	-12.362612	5.156350	-0.154253
73	1	0	-9.510719	-2.242627	-0.358682

74	1	0	9.771320	-2.095203	-0.360941
75	1	0	-3.037270	-5.082184	-0.928948
76	1	0	-4.780918	-5.163218	-0.861413
77	1	0	-4.000585	-3.996460	-1.902020
78	1	0	-3.859939	-3.543787	2.325206
79	1	0	-4.701748	-4.896057	1.606923
80	1	0	-2.957394	-4.818381	1.541970
81	1	0	1.121085	2.308028	1.121031
82	1	0	-0.622870	2.331164	1.228984
83	1	0	0.295026	1.171642	2.160074
84	1	0	0.971132	2.098498	-1.340348
85	1	0	0.030942	0.820259	-2.071847
86	1	0	-0.772845	2.126624	-1.235863
87	16	0	4.125597	-4.383203	0.538764
88	6	0	4.288884	-6.019043	-0.148076
89	1	0	5.167121	-6.487494	0.236631
90	1	0	3.424915	-6.607973	0.123119
91	1	0	4.349504	-5.954701	-1.210109

Cartesian coordinates of Designed Molecule IDST1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.033345	-1.286346	0.214335
2	6	0	-0.569640	-2.623920	0.180051
3	6	0	-1.466177	-3.696157	-0.009614
4	6	0	-2.784451	-3.356668	-0.194264
5	6	0	-3.249044	-2.016472	-0.116682

6	6	0	-2.346276	-0.941708	0.015762
7	1	0	-1.138487	-4.715509	-0.025184
8	1	0	-2.668205	0.079205	-0.017253
9	6	0	0.174832	-0.372152	0.515802
10	6	0	0.106396	0.123451	1.971912
11	6	0	0.281449	0.852105	-0.406873
12	6	0	-3.987833	-4.286026	-0.500572
13	6	0	-3.964671	-4.786555	-1.957411
14	6	0	-4.028714	-5.517474	0.422502
15	6	0	0.859060	-2.609040	0.333157
16	6	0	1.329493	-1.360896	0.370367
17	6	0	2.736532	-1.214959	0.267436
18	6	0	3.397284	-2.476147	0.266285
19	16	0	2.177347	-3.791061	0.455389
20	1	0	3.240277	-0.274531	0.205273
21	6	0	-4.681437	-2.034369	-0.149212
22	6	0	-5.158269	-3.308896	-0.325845
23	6	0	-6.565073	-3.446620	-0.314852
24	6	0	-7.230069	-2.186721	-0.181516
25	16	0	-6.016305	-0.874654	0.069301
26	1	0	-7.075860	-4.382646	-0.420153
27	6	0	4.812675	-2.634911	0.144978
28	6	0	5.520526	-3.853259	0.301255
29	16	0	5.972381	-1.317559	-0.198061
30	6	0	6.932314	-3.697955	0.262502
31	6	0	7.373673	-2.371278	0.086888
32	1	0	7.608663	-4.520930	0.366669
33	6	0	8.757873	-2.046687	0.144896

34	6	0	10.837825	-0.552531	-0.030935
35	6	0	9.318995	-0.798662	0.050069
36	6	0	8.675374	0.597041	0.006072
37	6	0	11.788157	-1.512461	0.019551
38	6	0	11.403318	-2.854563	0.141595
39	6	0	13.144491	-1.169586	-0.039185
40	8	0	7.447711	0.865028	0.052105
41	7	0	11.078903	-3.948916	0.241289
42	7	0	14.255626	-0.891507	-0.087078
43	6	0	12.188838	3.045789	-0.284438
44	6	0	12.263860	1.677205	-0.322300
45	6	0	11.063850	0.967509	-0.166713
46	6	0	9.840901	1.619909	-0.099104
47	6	0	9.768486	2.960909	-0.125740
48	6	0	10.918859	3.683241	-0.236168
49	1	0	13.201480	1.169641	-0.450466
50	1	0	8.825957	3.458125	-0.062542
51	6	0	-8.655028	-2.083397	-0.276556
52	6	0	-10.940862	-0.857926	-0.209601
53	6	0	-9.397746	-0.937376	-0.105716
54	6	0	-8.933293	0.489370	0.208415
55	6	0	-11.754984	-1.921434	-0.447562
56	6	0	-11.174611	-3.178650	-0.656555
57	6	0	-13.152138	-1.786889	-0.490528
58	8	0	-7.752981	0.864652	0.418633
59	7	0	-10.688132	-4.202883	-0.826228
60	7	0	-14.295019	-1.693420	-0.528741
61	6	0	-12.655118	2.605457	0.050033

62	6	0	-12.615265	1.232189	-0.020287
63	6	0	-11.344145	0.627525	-0.003222
64	6	0	-10.197147	1.385822	0.208516
65	6	0	-10.254902	2.718238	0.366282
66	6	0	-11.457251	3.342595	0.219729
67	1	0	-13.512915	0.651342	-0.097213
68	1	0	-9.373608	3.280458	0.586759
69	1	0	-9.194975	-2.979260	-0.503470
70	1	0	9.435085	-2.864471	0.272301
71	1	0	-3.098736	-5.395270	-2.112501
72	1	0	-4.846838	-5.364036	-2.144390
73	1	0	-3.936120	-3.951203	-2.624291
74	1	0	-4.046005	-5.191916	1.443819
75	1	0	-4.902229	-6.094492	0.217511
76	1	0	-3.156596	-6.115606	0.255391
77	1	0	0.991232	0.679615	2.200709
78	1	0	-0.751529	0.749568	2.095944
79	1	0	0.032960	-0.716317	2.632495
80	1	0	1.163908	1.405944	-0.163338
81	1	0	0.334101	0.524953	-1.424122
82	1	0	-0.577864	1.474605	-0.275413
83	16	0	4.761914	-5.444273	0.556619
84	6	0	5.983867	-6.722690	0.308968
85	1	0	6.769615	-6.606771	1.029182
86	1	0	5.527676	-7.682828	0.433253
87	1	0	6.391070	-6.646007	-0.676483
88	6	0	-11.499491	4.880867	0.219242
89	6	0	-13.978365	3.398078	-0.069558

90	6	0	-12.592909	6.924942	0.430136
91	6	0	-15.107611	5.459859	0.322461
92	8	0	-10.443244	5.533032	0.417342
93	8	0	-15.088560	2.805059	-0.109100
94	8	0	-13.910583	4.832866	-0.148786
95	8	0	-12.725845	5.575715	-0.020460
96	1	0	-11.787015	7.394343	-0.096666
97	1	0	-13.501031	7.457134	0.239026
98	1	0	-12.387074	6.934848	1.478795
99	1	0	-15.015558	6.522411	0.215635
100	1	0	-15.941674	5.115865	-0.252263
101	1	0	-15.259031	5.217652	1.352295
102	6	0	10.792677	5.217565	-0.323833
103	6	0	13.454601	3.932642	-0.258961
104	6	0	11.672425	7.357339	-0.100417
105	6	0	14.306541	6.185330	-0.273383
106	8	0	9.671766	5.745196	-0.112765
107	8	0	14.586138	3.477059	-0.575530
108	8	0	11.901681	6.058041	-0.654814
109	1	0	10.699979	7.700691	-0.390517
110	1	0	11.728672	7.304355	0.965317
111	1	0	12.412754	8.039550	-0.464099
112	1	0	14.122863	7.155592	0.140047
113	1	0	15.261711	5.833493	0.057546
114	1	0	14.296210	6.243230	-1.338587
115	8	0	13.284698	5.294030	0.172719

Cartesian coordinates of Designed Molecule IDST2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.055448	-0.947397	0.207256
2	6	0	-0.587483	-2.283610	0.178168
3	6	0	-1.480881	-3.359574	-0.005084
4	6	0	-2.800568	-3.025173	-0.188925
5	6	0	-3.269353	-1.686146	-0.116549
6	6	0	-2.369833	-0.607891	0.009461
7	1	0	-1.149926	-4.377925	-0.016649
8	1	0	-2.695117	0.411819	-0.027576
9	6	0	0.150296	-0.027963	0.502468
10	6	0	0.082816	0.473970	1.956452
11	6	0	0.251334	1.192463	-0.425893
12	6	0	-4.001476	-3.959776	-0.488918
13	6	0	-3.979255	-4.466785	-1.943529
14	6	0	-4.036755	-5.187180	0.439758
15	6	0	0.841428	-2.263433	0.328675
16	6	0	1.307889	-1.013624	0.359437
17	6	0	2.714266	-0.863616	0.253358
18	6	0	3.379088	-2.122659	0.256711
19	16	0	2.163741	-3.440635	0.453888
20	1	0	3.214859	0.078141	0.186074
21	6	0	-4.701736	-1.708808	-0.146462
22	6	0	-5.174755	-2.985648	-0.316515
23	6	0	-6.581086	-3.127856	-0.302411

24	6	0	-7.249915	-1.869520	-0.173566
25	16	0	-6.039959	-0.552431	0.069197
26	1	0	-7.089028	-4.065990	-0.402596
27	6	0	4.794769	-2.277404	0.133612
28	6	0	5.506828	-3.492747	0.294114
29	16	0	5.949608	-0.957878	-0.217402
30	6	0	6.918037	-3.333068	0.252163
31	6	0	7.354796	-2.005779	0.069802
32	1	0	7.597224	-4.153380	0.358833
33	6	0	8.738039	-1.676469	0.123898
34	6	0	10.812839	-0.176421	-0.062336
35	6	0	9.294957	-0.427081	0.022464
36	6	0	8.646752	0.966328	-0.026671
37	6	0	11.766356	-1.133045	-0.009216
38	6	0	11.386072	-2.475817	0.119545
39	6	0	13.121469	-0.786067	-0.071896
40	8	0	7.418312	1.230560	0.020330
41	7	0	11.065372	-3.570751	0.224735
42	7	0	14.231614	-0.504625	-0.123006
43	6	0	12.151767	3.425058	-0.334415
44	6	0	12.231145	2.056566	-0.366253
45	6	0	11.033710	1.343713	-0.205350
46	6	0	9.808780	1.992464	-0.138511
47	6	0	9.731985	3.333090	-0.171051
48	6	0	10.879820	4.058623	-0.286764
49	1	0	13.170175	1.551456	-0.493795
50	1	0	8.787966	3.827544	-0.108420
51	6	0	-8.675366	-1.771221	-0.266546

52	6	0	-10.965027	-0.552837	-0.201056
53	6	0	-9.421482	-0.626842	-0.099548
54	6	0	-8.961093	0.802794	0.207339
55	6	0	-11.776124	-1.620026	-0.432789
56	6	0	-11.192058	-2.876292	-0.637152
57	6	0	-13.173780	-1.490181	-0.473885
58	8	0	-7.781633	1.182823	0.413776
59	7	0	-10.702571	-3.899705	-0.803077
60	7	0	-14.317022	-1.400571	-0.510493
61	6	0	-12.690010	2.906135	0.046032
62	6	0	-12.645843	1.532700	-0.018181
63	6	0	-11.372746	0.932221	-0.000647
64	6	0	-10.227835	1.695157	0.205646
65	6	0	-10.289620	3.028077	0.357519
66	6	0	-11.494236	3.647888	0.210288
67	1	0	-13.541744	0.948621	-0.090903
68	1	0	-9.409761	3.594124	0.573904
69	1	0	-9.212812	-2.669832	-0.488471
70	1	0	9.418114	-2.491482	0.253781
71	1	0	-3.111631	-5.073397	-2.097412
72	1	0	-4.859879	-5.047943	-2.126346
73	1	0	-3.954576	-3.634357	-2.614209
74	1	0	-4.053304	-4.857083	1.459629
75	1	0	-4.908760	-5.767929	0.238912
76	1	0	-3.163003	-5.783243	0.273795
77	1	0	0.966250	1.034009	2.181178
78	1	0	-0.776910	1.097869	2.079185
79	1	0	0.013255	-0.363047	2.620935

80	1	0	1.132424	1.750236	-0.186414
81	1	0	0.303257	0.860904	-1.441751
82	1	0	-0.609754	1.812775	-0.295713
83	16	0	4.753813	-5.085032	0.557976
84	6	0	5.979454	-6.360606	0.313914
85	1	0	6.766087	-6.238911	1.032207
86	1	0	5.526588	-7.321639	0.443325
87	1	0	6.384676	-6.287049	-0.672592
88	6	0	-11.541448	5.185998	0.202957
89	6	0	-14.016020	3.693938	-0.074780
90	6	0	-12.641096	7.227466	0.406590
91	8	0	-10.486968	5.842451	0.396250
92	8	0	-12.770461	5.875802	-0.037696
93	1	0	-11.837650	7.697085	-0.123745
94	1	0	-13.551268	7.755861	0.214697
95	1	0	-12.433452	7.242759	1.454827
96	6	0	10.748526	5.592121	-0.381106
97	6	0	13.414700	4.316094	-0.315169
98	6	0	11.621745	7.735705	-0.168876
99	8	0	9.626288	6.117081	-0.170429
100	8	0	11.854225	6.434670	-0.717828
101	1	0	10.647686	8.074610	-0.458795
102	1	0	11.680035	7.687704	0.896984
103	1	0	12.359225	8.418655	-0.536934
104	7	0	-14.961397	4.183352	0.304216
105	7	0	14.468774	4.634801	-0.061689

Cartesian coordinates of Designed Molecule IDST3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.990871	-0.346246	-0.099808
2	6	0	0.561688	-1.695032	0.009102
3	6	0	1.471429	-2.750087	0.136239
4	6	0	2.819072	-2.439769	0.151896
5	6	0	3.247369	-1.093556	0.040223
6	6	0	2.335755	-0.037038	-0.086031
7	1	0	1.125671	-3.775110	0.220371
8	1	0	2.682639	0.987699	-0.170329
9	6	0	-0.195318	0.607667	-0.227152
10	6	0	-0.162130	1.364272	-1.564389
11	6	0	-0.245977	1.596756	0.948393
12	6	0	4.003366	-3.395815	0.281669
13	6	0	3.968697	-4.149266	1.620469
14	6	0	4.051303	-4.388022	-0.891411
15	6	0	-0.876915	-1.668249	-0.040877
16	6	0	-1.345252	-0.374547	-0.173516
17	6	0	-2.739401	-0.303425	-0.235180
18	6	0	-3.347314	-1.555322	-0.145241
19	16	0	-2.140144	-2.824705	0.014358
20	1	0	-3.308022	0.610564	-0.352708
21	6	0	4.684445	-1.110138	0.086819
22	6	0	5.153790	-2.413798	0.224739
23	6	0	6.537130	-2.466240	0.273226

24	6	0	7.144794	-1.198507	0.169339
25	16	0	5.922420	0.066625	0.011638
26	1	0	7.134005	-3.364789	0.378005
27	6	0	-4.757727	-1.805288	-0.152251
28	6	0	-5.474899	-3.014771	-0.242110
29	16	0	-5.825176	-0.437396	-0.038921
30	6	0	-6.853858	-2.794643	-0.230965
31	6	0	-7.237487	-1.454010	-0.130640
32	1	0	-7.596382	-3.578554	-0.299812
33	6	0	-8.606609	-1.112742	-0.111431
34	6	0	-10.732832	0.265121	-0.022596
35	6	0	-9.285389	0.084244	-0.026384
36	6	0	-8.659739	1.409979	0.077654
37	6	0	-11.719218	-0.694062	-0.101334
38	6	0	-11.457831	-2.091038	-0.202335
39	6	0	-13.110571	-0.388967	-0.088814
40	8	0	-7.470874	1.681809	0.105278
41	7	0	-11.271521	-3.235689	-0.285542
42	7	0	-14.253294	-0.176729	-0.081433
43	6	0	-12.088991	3.855744	0.237523
44	6	0	-12.171330	2.461461	0.131747
45	6	0	-10.991284	1.723607	0.084747
46	6	0	-9.763842	2.394545	0.143658
47	6	0	-9.660072	3.766272	0.248354
48	6	0	-10.838950	4.515097	0.296333
49	1	0	-13.149712	2.004473	0.089453
50	1	0	-8.689105	4.244644	0.291860
51	6	0	8.549184	-1.087025	0.195738

52	6	0	10.884231	-0.101689	0.149397
53	6	0	9.428489	-0.026258	0.110139
54	6	0	9.048933	1.384018	-0.046869
55	6	0	11.685836	-1.213852	0.290960
56	6	0	11.183471	-2.539802	0.429654
57	6	0	13.108880	-1.155450	0.313794
58	8	0	7.928699	1.861821	-0.115581
59	7	0	10.800820	-3.631783	0.544736
60	7	0	14.270871	-1.146345	0.336785
61	6	0	12.915753	3.258344	-0.189848
62	6	0	12.691331	1.802115	-0.030572
63	6	0	11.398966	1.284496	0.006207
64	6	0	10.310869	2.157463	-0.107668
65	6	0	10.452576	3.521395	-0.257389
66	6	0	11.689203	4.027347	-0.294159
67	1	0	13.572599	1.182639	0.053499
68	1	0	9.581777	4.160444	-0.341693
69	1	0	9.002825	-2.064941	0.305974
70	1	0	-9.222139	-2.001809	-0.178715
71	1	0	3.091096	-4.798462	1.671439
72	1	0	4.857117	-4.776375	1.727505
73	1	0	3.932972	-3.455301	2.462246
74	1	0	4.072835	-3.865308	-1.849599
75	1	0	4.942016	-5.017340	-0.822120
76	1	0	3.176170	-5.042461	-0.876072
77	1	0	-1.053197	1.987712	-1.671415
78	1	0	0.712326	2.017775	-1.612733
79	1	0	-0.122377	0.672027	-2.407385

80	1	0	-1.140015	2.221840	0.882029
81	1	0	-0.263885	1.071362	1.905105
82	1	0	0.625691	2.255785	0.933438
83	16	0	-4.705530	-4.590927	-0.382413
84	6	0	-6.124133	-5.711762	-0.368743
85	1	0	-6.767057	-5.557933	-1.237180
86	1	0	-5.700004	-6.714228	-0.421169
87	1	0	-6.696123	-5.620039	0.556233
88	6	0	12.024881	5.445430	-0.445498
89	6	0	14.242175	3.790418	-0.228444
90	6	0	-10.768030	5.937817	0.405084
91	6	0	-13.299696	4.614750	0.285045
92	7	0	15.324729	4.206355	-0.259551
93	7	0	-14.290547	5.216482	0.323052
94	7	0	12.252730	6.576326	-0.566811
95	7	0	-10.677729	7.091018	0.493428

Cartesian coordinates of Designed Molecule IDST4

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	6	0	-1.079015	-0.500271	0.248328
2	6	0	-0.616956	-1.837973	0.200582
3	6	0	-1.516461	-2.910927	0.017701
4	6	0	-2.833826	-2.567367	-0.166155
5	6	0	-3.294927	-1.226620	-0.082195
6	6	0	-2.392044	-0.153502	0.057543
7	1	0	-1.190518	-3.930132	0.006990

8	1	0	-2.713304	0.866769	0.038773
9	6	0	0.130897	0.409601	0.556151
10	6	0	0.080392	0.877261	2.020497
11	6	0	0.224376	1.653210	-0.344722
12	6	0	-4.041182	-3.488542	-0.480077
13	6	0	-4.020697	-3.946782	-1.949962
14	6	0	-4.089492	-4.746221	0.407221
15	6	0	0.813344	-1.823045	0.334159
16	6	0	1.283935	-0.575759	0.379458
17	6	0	2.689003	-0.427902	0.253898
18	6	0	3.349000	-1.689899	0.227091
19	16	0	2.132387	-3.006448	0.422644
20	1	0	3.192158	0.513644	0.192476
21	6	0	-4.726524	-1.239554	-0.115425
22	6	0	-5.204849	-2.515701	-0.265676
23	6	0	-6.606522	-2.659527	-0.194669
24	6	0	-7.266198	-1.400678	-0.072851
25	16	0	-6.054394	-0.072364	0.088361
26	1	0	-7.118306	-3.597709	-0.249039
27	6	0	4.761558	-1.851731	0.078479
28	6	0	5.464395	-3.076313	0.202825
29	16	0	5.924204	-0.536867	-0.263380
30	6	0	6.876090	-2.929518	0.145436
31	6	0	7.322774	-1.603930	-0.016362
32	1	0	7.547898	-3.758431	0.228265
33	6	0	8.709475	-1.286696	0.025678
34	6	0	10.785588	0.230936	-0.139407
35	6	0	9.267356	-0.035125	-0.057845

36	6	0	8.605569	1.352025	-0.083610
37	6	0	11.744678	-0.732500	-0.130359
38	6	0	11.356797	-2.077837	-0.033697
39	6	0	13.102798	-0.393871	-0.208780
40	8	0	7.375143	1.600814	-0.034317
41	7	0	11.039794	-3.178049	0.045343
42	7	0	14.214414	-0.124046	-0.272605
43	6	0	12.067669	3.879331	-0.245098
44	6	0	12.171142	2.509633	-0.320206
45	6	0	10.985564	1.764685	-0.222760
46	6	0	9.750052	2.397828	-0.169179
47	6	0	9.645298	3.739937	-0.189964
48	6	0	10.785529	4.492095	-0.209943
49	1	0	13.120989	2.027714	-0.445782
50	1	0	8.686779	4.210717	-0.178048
51	6	0	-8.686775	-1.307448	-0.106287
52	6	0	-10.950544	-0.084930	-0.028193
53	6	0	-9.411985	-0.165251	0.071308
54	6	0	-8.936112	1.260809	0.385099
55	6	0	-11.789900	-1.122478	-0.265552
56	6	0	-11.233744	-2.380032	-0.499269
57	6	0	-13.188969	-0.964242	-0.288746
58	8	0	-7.756601	1.633049	0.615882
59	7	0	-10.768505	-3.406937	-0.690305
60	7	0	-14.331979	-0.848762	-0.310463
61	6	0	-12.659461	3.292569	0.060764
62	6	0	-12.600340	1.948295	0.146382
63	6	0	-11.335450	1.382625	0.160281

64	6	0	-10.198958	2.153537	0.337913
65	6	0	-10.277067	3.488712	0.415911
66	6	0	-11.478007	4.063207	0.110523
67	1	0	-13.488513	1.354522	0.185499
68	1	0	-9.430458	4.081322	0.690411
69	1	0	-9.238014	-2.204215	-0.293355
70	1	0	9.386654	-2.109454	0.129173
71	1	0	-3.158566	-4.555165	-2.122775
72	1	0	-4.905624	-4.515628	-2.154906
73	1	0	-3.990147	-3.092686	-2.591987
74	1	0	-4.105686	-4.452428	1.437242
75	1	0	-4.969116	-5.310779	0.184014
76	1	0	-3.223110	-5.346148	0.221733
77	1	0	0.967913	1.430345	2.247965
78	1	0	-0.775932	1.500297	2.166915
79	1	0	0.016602	0.025030	2.664700
80	1	0	1.109639	2.203036	-0.102413
81	1	0	0.264226	1.347175	-1.369973
82	1	0	-0.633773	2.271728	-0.190296
83	16	0	4.702257	-4.667347	0.444199
84	6	0	5.913349	-5.942538	0.136067
85	1	0	6.720498	-5.841302	0.834296
86	1	0	5.459141	-6.904011	0.255527
87	1	0	6.291169	-5.847711	-0.859747
88	6	0	-11.544867	5.430954	-0.170187
89	6	0	-12.789785	6.066969	-0.195431
90	6	0	-13.966081	5.310267	-0.118153
91	6	0	-13.896540	3.917492	-0.087048

92	6	0	13.222256	4.691809	-0.185249
93	6	0	13.094978	6.091118	-0.111309
94	6	0	11.826673	6.687530	-0.132305
95	6	0	10.679353	5.888586	-0.192645
96	1	0	14.196906	4.247334	-0.191494
97	1	0	13.967445	6.708073	-0.037950
98	1	0	11.733993	7.753678	-0.100837
99	1	0	9.714286	6.350307	-0.220229
100	1	0	-12.840378	7.129209	-0.272944
101	1	0	-10.647705	5.985574	-0.366634
102	1	0	-14.917566	5.794484	-0.086612
103	1	0	-14.784903	3.329046	-0.174303

Cartesian coordinates of Designed Molecule IDST5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.103161	-1.464092	0.206422
2	6	0	-0.637743	-2.801431	0.200475
3	6	0	-1.534637	-3.881104	0.048961
4	6	0	-2.854097	-3.546888	-0.139108
5	6	0	-3.319114	-2.205916	-0.094334
6	6	0	-2.418091	-1.126763	0.008749
7	1	0	-1.205454	-4.899149	0.063403
8	1	0	-2.741968	-0.108355	-0.041223
9	6	0	0.105206	-0.541586	0.480241
10	6	0	0.052626	-0.020171	1.925988
11	6	0	0.197627	0.667489	-0.466591

12	6	0	-4.058895	-4.482777	-0.416925
13	6	0	-4.042238	-5.001383	-1.866766
14	6	0	-4.096636	-5.702693	0.522042
15	6	0	0.792590	-2.779346	0.335145
16	6	0	1.260459	-1.530389	0.339420
17	6	0	2.665452	-1.383631	0.213130
18	6	0	3.328699	-2.643795	0.230784
19	16	0	2.114452	-3.956368	0.464935
20	1	0	3.166714	-0.443554	0.122132
21	6	0	-4.751523	-2.224460	-0.122108
22	6	0	-5.227186	-3.504842	-0.243311
23	6	0	-6.631774	-3.647364	-0.189660
24	6	0	-7.296844	-2.383750	-0.099687
25	16	0	-6.083731	-1.056538	0.057588
26	1	0	-7.140742	-4.587702	-0.234723
27	6	0	4.742446	-2.804682	0.092725
28	6	0	5.451209	-4.020659	0.262601
29	16	0	5.899015	-1.496126	-0.291107
30	6	0	6.862012	-3.868132	0.204320
31	6	0	7.301658	-2.547257	-0.002516
32	1	0	7.538886	-4.689609	0.316582
33	6	0	8.685871	-2.224112	0.025079
34	6	0	10.759075	-0.724212	-0.213309
35	6	0	9.242118	-0.977814	-0.116503
36	6	0	8.589000	0.419735	-0.183328
37	6	0	11.719238	-1.677450	-0.154481
38	6	0	11.338384	-3.017979	0.003510
39	6	0	13.078096	-1.336539	-0.230863

40	8	0	7.359987	0.673973	-0.125049
41	7	0	11.011493	-4.111253	0.132261
42	7	0	14.188016	-1.058053	-0.293255
43	6	0	12.067344	2.854063	-0.316616
44	6	0	12.162665	1.503628	-0.481806
45	6	0	10.968307	0.799483	-0.353119
46	6	0	9.742768	1.456214	-0.302813
47	6	0	9.653946	2.810727	-0.336836
48	6	0	10.826924	3.528937	-0.280009
49	1	0	13.099644	1.014152	-0.675965
50	1	0	8.709099	3.304935	-0.386570
51	6	0	-8.722786	-2.289316	-0.159001
52	6	0	-11.012950	-1.060676	-0.102047
53	6	0	-9.463856	-1.141049	-0.008479
54	6	0	-8.993313	0.288739	0.266383
55	6	0	-11.831051	-2.122042	-0.307005
56	6	0	-11.253085	-3.387667	-0.501099
57	6	0	-13.224348	-1.986561	-0.341132
58	8	0	-7.808876	0.673423	0.447484
59	7	0	-10.770784	-4.416576	-0.658245
60	7	0	-14.366585	-1.887543	-0.370918
61	6	0	-12.604610	2.490720	0.079332
62	6	0	-12.667637	1.081078	0.061576
63	6	0	-11.409321	0.438107	0.074388
64	6	0	-10.244135	1.185115	0.254809
65	6	0	-10.249430	2.521058	0.372941
66	6	0	-11.374652	3.148811	0.182431
67	1	0	-13.592676	0.498642	0.021414

68	1	0	-9.397340	3.079727	0.598523
69	1	0	-9.264539	-3.194008	-0.341703
70	1	0	9.365858	-3.037672	0.169344
71	1	0	-3.178512	-5.613118	-2.018178
72	1	0	-4.925964	-5.582182	-2.043318
73	1	0	-4.018431	-4.175132	-2.544103
74	1	0	-4.109413	-5.365548	1.539011
75	1	0	-4.973506	-6.281075	0.327533
76	1	0	-3.227281	-6.304853	0.357695
77	1	0	0.938896	0.542522	2.133612
78	1	0	-0.805005	0.606395	2.048269
79	1	0	-0.010447	-0.847984	2.601268
80	1	0	1.081788	1.227421	-0.244243
81	1	0	0.239219	0.323051	-1.479652
82	1	0	-0.661573	1.289896	-0.336577
83	16	0	4.695832	-5.605833	0.559064
84	6	0	5.913899	-6.887509	0.309947
85	1	0	6.713982	-6.757689	1.011572
86	1	0	5.461471	-7.845491	0.460815
87	1	0	6.300976	-6.828571	-0.685046
88	6	0	13.237080	3.829577	-0.110844
89	6	0	12.857566	5.140994	-0.036822
90	16	0	11.084995	5.273530	-0.069273
91	1	0	14.241076	3.484781	-0.042490
92	6	0	-13.194661	4.888216	0.004141
93	6	0	-13.693371	3.614357	-0.009352
94	16	0	-11.442712	4.894362	0.027425
95	1	0	-14.731061	3.389270	-0.066734

96	35	0	-14.201477	6.521884	0.004883
97	35	0	14.082909	6.625579	0.053073

Cartesian coordinates of Designed Molecule IDST6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.048066	-0.929193	0.252205
2	6	0	-0.588097	-2.267379	0.198226
3	6	0	-1.489373	-3.338130	0.011199
4	6	0	-2.806330	-2.991736	-0.170251
5	6	0	-3.265311	-1.650668	-0.080046
6	6	0	-2.360686	-0.579567	0.063837
7	1	0	-1.165006	-4.357777	-0.004243
8	1	0	-2.680388	0.441269	0.049801
9	6	0	0.163449	-0.022553	0.563243
10	6	0	0.114635	0.438694	2.029679
11	6	0	0.258245	1.224889	-0.332177
12	6	0	-4.015309	-3.909656	-0.487440
13	6	0	-3.996505	-4.361413	-1.959353
14	6	0	-4.064966	-5.171177	0.394312
15	6	0	0.842312	-2.255239	0.330910
16	6	0	1.314852	-1.008891	0.381416
17	6	0	2.720063	-0.862637	0.255571
18	6	0	3.378099	-2.125515	0.222734
19	16	0	2.159591	-3.441047	0.413270
20	1	0	3.224625	0.078398	0.197982
21	6	0	-4.696948	-1.661255	-0.112374

22	6	0	-5.177336	-2.935988	-0.267954
23	6	0	-6.579181	-3.077975	-0.196646
24	6	0	-7.236838	-1.818666	-0.068813
25	16	0	-6.022885	-0.492941	0.097468
26	1	0	-7.092444	-4.015120	-0.254827
27	6	0	4.790307	-2.288857	0.072460
28	6	0	5.491341	-3.515055	0.190911
29	16	0	5.954748	-0.974278	-0.264352
30	6	0	6.903222	-3.370176	0.133227
31	6	0	7.351838	-2.044572	-0.022999
32	1	0	7.573809	-4.200478	0.211935
33	6	0	8.739053	-1.729657	0.019516
34	6	0	10.817389	-0.214499	-0.140238
35	6	0	9.298804	-0.478587	-0.058838
36	6	0	8.639136	0.909678	-0.078017
37	6	0	11.775001	-1.179438	-0.136099
38	6	0	11.385115	-2.524593	-0.045136
39	6	0	13.133588	-0.842551	-0.213929
40	8	0	7.409126	1.160136	-0.026798
41	7	0	11.066471	-3.624655	0.029244
42	7	0	14.245575	-0.574153	-0.277304
43	6	0	12.105012	3.432354	-0.230632
44	6	0	12.206327	2.062846	-0.311874
45	6	0	11.019669	1.319295	-0.216932
46	6	0	9.785169	1.954091	-0.159721
47	6	0	9.682467	3.296438	-0.174492
48	6	0	10.823840	4.046925	-0.191905
49	1	0	13.155349	1.580029	-0.440219

50	1	0	8.724681	3.768633	-0.159850
51	6	0	-8.657292	-1.723107	-0.100883
52	6	0	-10.919125	-0.497472	-0.015860
53	6	0	-9.380626	-0.580595	0.082254
54	6	0	-8.902351	0.843329	0.402037
55	6	0	-11.760233	-1.532667	-0.257249
56	6	0	-11.206168	-2.790027	-0.496905
57	6	0	-13.159072	-1.372182	-0.278804
58	8	0	-7.722115	1.212731	0.633676
59	7	0	-10.742637	-3.816788	-0.692797
60	7	0	-14.301918	-1.254852	-0.299243
61	6	0	-12.622783	2.882221	0.089196
62	6	0	-12.565674	1.537492	0.168822
63	6	0	-11.301647	0.969824	0.179368
64	6	0	-10.163852	1.738195	0.359650
65	6	0	-10.239855	3.073130	0.443612
66	6	0	-11.440112	3.650816	0.141576
67	1	0	-13.454734	0.944916	0.205904
68	1	0	-9.392154	3.663218	0.720167
69	1	0	-9.210034	-2.618189	-0.291551
70	1	0	9.415034	-2.553905	0.118913
71	1	0	-3.135426	-4.970347	-2.135437
72	1	0	-4.882441	-4.927985	-2.166222
73	1	0	-3.965067	-3.504529	-2.597610
74	1	0	-4.080025	-4.881925	1.425634
75	1	0	-4.945606	-5.733389	0.169197
76	1	0	-3.199632	-5.771607	0.205589
77	1	0	1.003157	0.989401	2.259000

78	1	0	-0.740632	1.062389	2.179428
79	1	0	0.049961	-0.416284	2.670145
80	1	0	1.144513	1.772276	-0.088029
81	1	0	0.296943	0.923337	-1.358799
82	1	0	-0.598849	1.844034	-0.174439
83	16	0	4.726916	-5.105971	0.425748
84	6	0	5.935840	-6.381643	0.111162
85	1	0	6.743606	-6.284740	0.809290
86	1	0	5.480232	-7.342936	0.226667
87	1	0	6.313145	-6.282986	-0.884476
88	6	0	-11.505053	5.019893	-0.133030
89	6	0	-12.749008	5.657926	-0.154623
90	6	0	-13.926415	4.902696	-0.079909
91	6	0	-13.858997	3.509692	-0.055018
92	6	0	13.260887	4.242785	-0.167959
93	6	0	13.135811	5.641947	-0.087739
94	6	0	11.868412	6.240393	-0.105243
95	6	0	10.719824	5.443488	-0.168351
96	1	0	14.234848	3.796846	-0.176825
97	1	0	9.755451	5.906808	-0.193245
98	1	0	-10.607169	5.574000	-0.327620
99	1	0	-14.748322	2.923003	-0.144282
100	9	0	-12.811059	7.003347	-0.246763
101	9	0	-15.128081	5.516389	-0.036526
102	9	0	14.236734	6.417455	0.007429
103	9	0	11.753644	7.584729	-0.059534

Cartesian coordinates of Designed Molecule IDST7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109207	-0.259575	0.201722
2	6	0	-0.639690	-1.595349	0.182304
3	6	0	-1.532531	-2.675335	0.011543
4	6	0	-2.852561	-2.342811	-0.176300
5	6	0	-3.322315	-1.004065	-0.115893
6	6	0	-2.424673	0.076480	0.002793
7	1	0	-1.200139	-3.692532	0.013339
8	1	0	-2.751177	1.094311	-0.036103
9	6	0	0.095274	0.663239	0.491907
10	6	0	0.033483	1.169852	1.941950
11	6	0	0.189437	1.881899	-0.442880
12	6	0	-4.052620	-3.280038	-0.469196
13	6	0	-4.029401	-3.786117	-1.922859
14	6	0	-4.088741	-4.507736	0.459910
15	6	0	0.789971	-1.570876	0.325950
16	6	0	1.254035	-0.320713	0.345739
17	6	0	2.659232	-0.168853	0.227869
18	6	0	3.326565	-1.426803	0.236090
19	16	0	2.114642	-2.745574	0.448485
20	1	0	3.158460	0.773970	0.153829
21	6	0	-4.754895	-1.028229	-0.148727
22	6	0	-5.224598	-2.308954	-0.292353
23	6	0	-6.627760	-2.458378	-0.255062

24	6	0	-7.296452	-1.203919	-0.148876
25	16	0	-6.093709	0.128733	0.046078
26	1	0	-7.135058	-3.397559	-0.324170
27	6	0	4.741883	-1.580847	0.105231
28	6	0	5.454476	-2.795988	0.265223
29	16	0	5.897393	-0.264183	-0.254473
30	6	0	6.865736	-2.637282	0.219761
31	6	0	7.302545	-1.312556	0.033790
32	1	0	7.544595	-3.457949	0.320868
33	6	0	8.688924	-0.982940	0.098795
34	6	0	10.778383	0.539542	-0.045654
35	6	0	9.236607	0.273628	0.010450
36	6	0	8.519745	1.652515	-0.052154
37	6	0	11.734748	-0.412451	-0.026052
38	6	0	11.349374	-1.754048	0.078008
39	6	0	13.085426	-0.062192	-0.124724
40	8	0	7.288169	1.885473	-0.000692
41	7	0	11.016975	-2.846078	0.163676
42	7	0	14.193112	0.225062	-0.205653
43	6	0	-8.718154	-1.114960	-0.219647
44	6	0	-10.997697	0.121842	-0.139493
45	6	0	-9.435363	0.037666	-0.061412
46	6	0	-8.882080	1.462149	0.216531
47	6	0	-11.825884	-0.938939	-0.369353
48	6	0	-11.251536	-2.202295	-0.577612
49	6	0	-13.225803	-0.806867	-0.409600
50	8	0	-7.687077	1.786084	0.408807
51	7	0	-10.765326	-3.227359	-0.745667

52	7	0	-14.370213	-0.722873	-0.446932
53	1	0	-9.264988	-2.012080	-0.415769
54	1	0	9.369951	-1.797893	0.210079
55	1	0	-3.163211	-4.393448	-2.076861
56	1	0	-4.910717	-4.368494	-2.107158
57	1	0	-4.006575	-2.954213	-2.593483
58	1	0	-4.106176	-4.178899	1.479329
59	1	0	-4.962548	-5.088172	0.257696
60	1	0	-3.216392	-5.104942	0.293131
61	1	0	0.917058	1.732824	2.159944
62	1	0	-0.826530	1.792824	2.065814
63	1	0	-0.030930	0.335100	2.608412
64	1	0	1.070843	2.441951	-0.210299
65	1	0	0.237465	1.547597	-1.459169
66	1	0	-0.672146	2.500642	-0.311504
67	16	0	4.702993	-4.387061	0.541010
68	6	0	5.927290	-5.662415	0.290261
69	1	0	6.721094	-5.537192	1.000228
70	1	0	5.476712	-6.623327	0.428329
71	1	0	6.322332	-5.592337	-0.700376
72	6	0	-12.479279	2.357633	0.174208
73	6	0	-11.355114	1.609195	0.072269
74	6	0	-10.087301	2.406282	0.210391
75	6	0	-10.262214	3.743447	0.285516
76	16	0	-12.012532	4.082686	0.247495
77	1	0	-13.476759	1.992463	0.209866
78	17	0	-8.998351	4.961632	0.339767
79	6	0	12.007139	2.942641	-0.218747

80	6	0	10.972710	2.060793	-0.156922
81	6	0	9.620696	2.704762	-0.202113
82	6	0	9.634835	4.035917	-0.352537
83	16	0	11.330485	4.572752	-0.504834
84	1	0	13.045853	2.717000	-0.121219
85	17	0	8.218594	5.066092	-0.410831

Atomic coordinates of TD-DFT for all molecules (reference **IDSTR**, and investigated molecules **IDST1, IDST2, IDST3, IDST4, IDST5, IDST6** and **IDST7** along X, Y and Z axis at MPW1PW91/6-31G (d, p) level.

Atomic coordinates of Designed Molecule IDSTR

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	6	0	-1.018145	-0.137158	0.248365
2	6	0	-0.583730	-1.468807	0.021219
3	6	0	-1.489207	-2.506705	-0.219099
4	6	0	-2.837540	-2.196872	-0.230490
5	6	0	-3.271062	-0.867380	-0.003495
6	6	0	-2.363889	0.171650	0.237520
7	1	0	-1.140458	-3.519902	-0.391718
8	1	0	-2.713838	1.184611	0.409607
9	6	0	0.163577	0.800580	0.484758
10	6	0	0.107936	1.423612	1.888286
11	6	0	0.229661	1.899645	-0.586910
12	6	0	-4.017500	-3.136401	-0.469651
13	6	0	-3.954897	-3.764069	-1.870704
14	6	0	-4.087167	-4.232126	0.605211
15	6	0	0.855624	-1.444522	0.095239

16	6	0	1.317567	-0.169009	0.355443
17	6	0	2.712597	-0.102597	0.447912
18	6	0	3.323325	-1.337710	0.253428
19	16	0	2.124426	-2.588720	-0.045234
20	1	0	3.279579	0.794030	0.666694
21	6	0	-4.709038	-0.880734	-0.081023
22	6	0	-5.170894	-2.164765	-0.347157
23	6	0	-6.555561	-2.213010	-0.429718
24	6	0	-7.167062	-0.962977	-0.226612
25	16	0	-5.953399	0.282385	0.072465
26	1	0	-7.147815	-3.098908	-0.628390
27	6	0	4.737404	-1.586096	0.241207
28	6	0	5.456965	-2.785337	0.371002
29	16	0	5.796789	-0.221640	0.050014
30	6	0	6.837170	-2.561391	0.334395
31	6	0	7.213152	-1.226866	0.173932
32	1	0	7.583646	-3.338830	0.431075
33	6	0	8.585132	-0.879834	0.126105
34	6	0	10.705036	0.498272	-0.040447
35	6	0	9.256834	0.310273	-0.016106
36	6	0	8.627107	1.633686	-0.176563
37	6	0	11.693002	-0.455554	0.078608
38	6	0	11.439353	-1.846810	0.253280
39	6	0	13.083322	-0.146618	0.039668
40	8	0	7.435199	1.893182	-0.207834
41	7	0	11.262954	-2.987280	0.396514
42	7	0	14.225040	0.069943	0.012193
43	6	0	12.032588	4.053089	-0.482479

44	6	0	12.138022	2.682438	-0.313215
45	6	0	10.955118	1.946177	-0.219387
46	6	0	9.725019	2.611556	-0.298493
47	6	0	9.617171	3.982037	-0.468098
48	6	0	10.794432	4.701105	-0.559650
49	1	0	13.126291	2.247327	-0.262115
50	1	0	8.653093	4.472291	-0.527553
51	9	0	10.780013	6.019907	-0.722935
52	9	0	13.131571	4.794817	-0.577184
53	6	0	-8.574861	-0.847252	-0.279747
54	6	0	-10.911854	0.128522	-0.218253
55	6	0	-9.456422	0.198291	-0.128339
56	6	0	-9.088323	1.596255	0.157797
57	6	0	-11.703162	-0.971364	-0.474032
58	6	0	-11.195743	-2.283014	-0.702653
59	6	0	-13.125138	-0.910524	-0.537795
60	8	0	-7.969355	2.060543	0.303315
61	7	0	-10.813649	-3.364774	-0.892987
62	7	0	-14.286039	-0.897523	-0.597045
63	6	0	-12.885824	3.358022	0.307689
64	6	0	-12.731163	2.005256	0.053315
65	6	0	-11.431762	1.494630	0.019218
66	6	0	-10.350624	2.356740	0.239902
67	6	0	-10.502552	3.709705	0.493750
68	6	0	-11.793069	4.204622	0.525623
69	1	0	-13.618907	1.409412	-0.106321
70	1	0	-9.648445	4.354633	0.660834
71	9	0	-12.026971	5.491580	0.762873

72	9	0	-14.104366	3.888827	0.349945
73	1	0	-9.022109	-1.813137	-0.486099
74	1	0	9.203533	-1.764662	0.224754
75	1	0	-3.073648	-4.403838	-1.966398
76	1	0	-4.838955	-4.380835	-2.052359
77	1	0	-3.906841	-2.995387	-2.644619
78	1	0	-4.130254	-3.799354	1.606725
79	1	0	-4.975502	-4.852330	0.459867
80	1	0	-3.210663	-4.883136	0.549388
81	1	0	0.994490	2.037252	2.068898
82	1	0	-0.771023	2.065603	1.989385
83	1	0	0.060648	0.652186	2.659490
84	1	0	1.120560	2.517053	-0.444995
85	1	0	0.266083	1.469719	-1.589880
86	1	0	-0.644779	2.552710	-0.524013
87	16	0	4.689529	-4.354338	0.597840
88	6	0	6.110192	-5.471659	0.614552
89	1	0	6.766631	-5.276340	1.463760
90	1	0	5.689354	-6.471842	0.721543
91	1	0	6.667944	-5.423879	-0.321624

Atomic coordinates of Designed Molecule IDST1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.921211	-1.102663	-0.236327
2	6	0	0.490282	-2.437131	-0.018337
3	6	0	1.397154	-3.470764	0.234974

4	6	0	2.743387	-3.153856	0.268937
5	6	0	3.173511	-1.821674	0.050819
6	6	0	2.264901	-0.786897	-0.203367
7	1	0	1.050907	-4.485994	0.400570
8	1	0	2.612329	0.228192	-0.367818
9	6	0	-0.261541	-0.170450	-0.488904
10	6	0	-0.187802	0.456459	-1.889874
11	6	0	-0.349896	0.925477	0.584381
12	6	0	3.924030	-4.087587	0.526660
13	6	0	3.840900	-4.718662	1.925070
14	6	0	4.018087	-5.180378	-0.549283
15	6	0	-0.947657	-2.420293	-0.114750
16	6	0	-1.412189	-1.146446	-0.379525
17	6	0	-2.805749	-1.086913	-0.492255
18	6	0	-3.413209	-2.325610	-0.308660
19	16	0	-2.212394	-3.571204	0.005164
20	1	0	-3.373805	-0.192484	-0.717208
21	6	0	4.609803	-1.827062	0.152930
22	6	0	5.073982	-3.109429	0.425945
23	6	0	6.456477	-3.149857	0.534339
24	6	0	7.064813	-1.895576	0.343524
25	16	0	5.849673	-0.656771	0.022117
26	1	0	7.050122	-4.031980	0.745279
27	6	0	-4.825841	-2.580214	-0.318124
28	6	0	-5.538372	-3.784165	-0.450562
29	16	0	-5.893550	-1.218944	-0.154297
30	6	0	-6.919331	-3.565960	-0.437678
31	6	0	-7.303739	-2.231381	-0.293119

32	1	0	-7.661088	-4.346975	-0.541311
33	6	0	-8.676957	-1.890283	-0.272455
34	6	0	-10.804328	-0.516288	-0.157529
35	6	0	-9.356005	-0.700684	-0.150736
36	6	0	-8.730973	0.623272	0.017721
37	6	0	-11.786888	-1.468406	-0.320749
38	6	0	-11.522255	-2.856567	-0.506727
39	6	0	-13.180099	-1.168913	-0.334003
40	8	0	-7.539971	0.882720	0.068808
41	7	0	-11.336166	-3.994284	-0.659271
42	7	0	-14.325972	-0.976200	-0.359035
43	6	0	-12.164278	3.054568	0.286889
44	6	0	-12.239609	1.669236	0.116377
45	6	0	-11.061075	0.931740	0.031024
46	6	0	-9.834050	1.600512	0.124736
47	6	0	-9.745072	2.965555	0.312363
48	6	0	-10.923644	3.704809	0.413815
49	1	0	-13.220712	1.219081	0.050140
50	1	0	-8.782036	3.455656	0.394461
51	6	0	8.469321	-1.771858	0.429669
52	6	0	10.801092	-0.779775	0.427549
53	6	0	9.348934	-0.720674	0.296303
54	6	0	8.977705	0.670068	-0.016678
55	6	0	11.589668	-1.862993	0.750959
56	6	0	11.078560	-3.167710	1.011188
57	6	0	13.007745	-1.796574	0.875279
58	8	0	7.858557	1.122792	-0.192064
59	7	0	10.692715	-4.243115	1.228085

60	7	0	14.163811	-1.794536	0.995602
61	6	0	12.791293	2.464377	-0.137028
62	6	0	12.611697	1.105307	0.135947
63	6	0	11.320198	0.584304	0.163412
64	6	0	10.239202	1.437566	-0.089214
65	6	0	10.402860	2.777639	-0.378460
66	6	0	11.695937	3.299090	-0.422843
67	1	0	13.491708	0.505455	0.323808
68	1	0	9.548455	3.412350	-0.582256
69	1	0	8.916949	-2.734914	0.647876
70	1	0	-9.290020	-2.778356	-0.374869
71	1	0	2.961996	-5.363919	2.004157
72	1	0	4.725393	-5.330539	2.120610
73	1	0	3.774947	-3.952005	2.699666
74	1	0	4.076514	-4.744971	-1.548867
75	1	0	4.906836	-5.796450	-0.389710
76	1	0	3.143998	-5.835836	-0.510199
77	1	0	-1.074914	1.065617	-2.082351
78	1	0	0.688892	1.103721	-1.975719
79	1	0	-0.124337	-0.312631	-2.662263
80	1	0	-1.241578	1.538692	0.430097
81	1	0	-0.399627	0.492775	1.585577
82	1	0	0.522026	1.583122	0.536535
83	16	0	-4.760803	-5.351384	-0.653035
84	6	0	-6.176041	-6.475418	-0.678214
85	1	0	-6.821250	-6.291949	-1.538599
86	1	0	-5.749295	-7.474721	-0.768729
87	1	0	-6.747139	-6.420239	0.249474

88	6	0	11.816383	4.727106	-0.846214
89	6	0	14.201778	2.958176	-0.044343
90	6	0	13.031588	6.268964	-2.106145
91	6	0	15.600527	4.626475	0.788988
92	8	0	11.008149	5.579550	-0.563998
93	8	0	15.156446	2.349557	-0.461684
94	8	0	14.278234	4.107769	0.637357
95	8	0	12.870360	4.926530	-1.645995
96	1	0	13.187593	6.945041	-1.263926
97	1	0	13.904680	6.254612	-2.754802
98	1	0	12.147646	6.591639	-2.658029
99	1	0	15.494410	5.535555	1.376958
100	1	0	16.235921	3.905887	1.305722
101	1	0	16.038431	4.846636	-0.186030
102	6	0	-10.765069	5.158587	0.722224
103	6	0	-13.475092	3.778420	0.266433
104	6	0	-11.584440	6.971541	1.940773
105	6	0	-14.647454	5.601115	-0.592809
106	8	0	-9.855093	5.835164	0.305589
107	8	0	-14.472948	3.377124	0.813202
108	8	0	-11.692729	5.592944	1.582505
109	1	0	-10.607391	7.175147	2.380984
110	1	0	-11.714899	7.605405	1.062137
111	1	0	-12.376458	7.150278	2.664612
112	1	0	-14.450329	6.425407	-1.274751
113	1	0	-15.444917	4.964569	-0.978450
114	1	0	-14.938909	5.975110	0.390074
115	8	0	-13.422856	4.870386	-0.505672

Atomic coordinates of Designed Molecule IDST2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.948248	-0.823016	-0.204453
2	6	0	0.513317	-2.159957	-0.008317
3	6	0	1.417141	-3.202532	0.218562
4	6	0	2.764977	-2.892410	0.247720
5	6	0	3.198837	-1.557836	0.051334
6	6	0	2.293288	-0.513943	-0.175978
7	1	0	1.067330	-4.219088	0.367338
8	1	0	2.644304	0.502355	-0.324255
9	6	0	-0.231833	0.118871	-0.431374
10	6	0	-0.164764	0.771952	-1.820741
11	6	0	-0.308496	1.194579	0.663210
12	6	0	3.943504	-3.836067	0.477351
13	6	0	3.870476	-4.491938	1.864960
14	6	0	4.022674	-4.909614	-0.619079
15	6	0	-0.924775	-2.135510	-0.094658
16	6	0	-1.385620	-0.854385	-0.332671
17	6	0	-2.778854	-0.787001	-0.433968
18	6	0	-3.390772	-2.026940	-0.268750
19	16	0	-2.192950	-3.283202	0.012951
20	1	0	-3.343998	0.114396	-0.637425
21	6	0	4.635201	-1.571024	0.139582
22	6	0	5.096946	-2.861233	0.383565

23	6	0	6.479374	-2.909274	0.474770
24	6	0	7.091431	-1.652914	0.300244
25	16	0	5.877069	-0.402948	0.017676
26	1	0	7.071804	-3.798007	0.659755
27	6	0	-4.803671	-2.274490	-0.275377
28	6	0	-5.522602	-3.476959	-0.402897
29	16	0	-5.864586	-0.907906	-0.113763
30	6	0	-6.901432	-3.252520	-0.386859
31	6	0	-7.280046	-1.914854	-0.244927
32	1	0	-7.646944	-4.030687	-0.484955
33	6	0	-8.649687	-1.568385	-0.218495
34	6	0	-10.769961	-0.185709	-0.094449
35	6	0	-9.323883	-0.373585	-0.097871
36	6	0	-8.691740	0.947409	0.055033
37	6	0	-11.759836	-1.136918	-0.214786
38	6	0	-11.504504	-2.530430	-0.369689
39	6	0	-13.150758	-0.828774	-0.197930
40	8	0	-7.500211	1.204250	0.098876
41	7	0	-11.324213	-3.672084	-0.496986
42	7	0	-14.294079	-0.619950	-0.189054
43	6	0	-12.112383	3.406313	0.293312
44	6	0	-12.193212	2.011886	0.136130
45	6	0	-11.020089	1.268542	0.064984
46	6	0	-9.790508	1.932716	0.151712
47	6	0	-9.695216	3.300297	0.305867
48	6	0	-10.862597	4.059929	0.379082
49	1	0	-13.173071	1.559832	0.075617
50	1	0	-8.733343	3.794791	0.371651

51	6	0	8.495903	-1.537661	0.364021
52	6	0	10.831470	-0.555679	0.331850
53	6	0	9.378654	-0.485765	0.236378
54	6	0	9.005291	0.913292	-0.026594
55	6	0	11.626611	-1.655265	0.574459
56	6	0	11.119443	-2.970853	0.781261
57	6	0	13.048254	-1.595396	0.646398
58	8	0	7.885819	1.376171	-0.167724
59	7	0	10.734962	-4.054715	0.953305
60	7	0	14.208670	-1.590272	0.713002
61	6	0	12.820219	2.713099	-0.140782
62	6	0	12.639628	1.338839	0.092753
63	6	0	11.349876	0.819098	0.117303
64	6	0	10.267818	1.681957	-0.092311
65	6	0	10.428844	3.032482	-0.322110
66	6	0	11.715721	3.569423	-0.349392
67	1	0	13.516823	0.726344	0.246284
68	1	0	9.576739	3.682420	-0.481923
69	1	0	8.943763	-2.506461	0.554637
70	1	0	-9.267724	-2.453626	-0.315215
71	1	0	2.989666	-5.134980	1.940040
72	1	0	4.753971	-5.110978	2.041234
73	1	0	3.814647	-3.739460	2.654114
74	1	0	4.073324	-4.456847	-1.611337
75	1	0	4.910081	-5.532314	-0.479188
76	1	0	3.146250	-5.562035	-0.583042
77	1	0	-1.050844	1.387716	-1.995870
78	1	0	0.713461	1.417940	-1.899607

79	1	0	-0.108764	0.017748	-2.608229
80	1	0	-1.198645	1.814165	0.526808
81	1	0	-0.352928	0.743501	1.656506
82	1	0	0.565552	1.849725	0.621366
83	16	0	-4.752647	-5.047688	-0.601084
84	6	0	-6.172413	-6.166081	-0.619364
85	1	0	-6.818399	-5.982842	-1.479187
86	1	0	-5.749595	-7.167231	-0.707583
87	1	0	-6.740955	-6.105695	0.309552
88	6	0	11.798350	5.041152	-0.604987
89	6	0	14.182829	3.159165	-0.150509
90	6	0	13.197819	6.897949	-0.844384
91	8	0	10.820504	5.729694	-0.789541
92	8	0	13.046696	5.496976	-0.604764
93	1	0	12.679443	7.471355	-0.074737
94	1	0	14.268534	7.083159	-0.810041
95	1	0	12.789131	7.161049	-1.820881
96	6	0	-10.667372	5.533973	0.546986
97	6	0	-13.371378	4.089351	0.356426
98	6	0	-11.700998	7.617423	0.784618
99	8	0	-9.572871	6.046529	0.606541
100	8	0	-11.813620	6.201548	0.622743
101	1	0	-11.170638	7.851223	1.708676
102	1	0	-11.160611	8.052705	-0.056960
103	1	0	-12.723061	7.986142	0.821065
104	7	0	15.315516	3.409522	-0.138051
105	7	0	-14.441210	4.536295	0.394536

Atomic coordinates of Designed Molecule IDST3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.995616	-0.353332	-0.216114
2	6	0	0.563239	-1.690853	-0.016436
3	6	0	1.468856	-2.733446	0.203060
4	6	0	2.816648	-2.422968	0.221257
5	6	0	3.248162	-1.087918	0.021079
6	6	0	2.340581	-0.043913	-0.198857
7	1	0	1.120467	-3.750002	0.354772
8	1	0	2.690088	0.972442	-0.350049
9	6	0	-0.186770	0.588001	-0.433056
10	6	0	-0.131860	1.240829	-1.823155
11	6	0	-0.254785	1.663758	0.662134
12	6	0	3.996789	-3.366482	0.441781
13	6	0	3.934827	-4.021959	1.830197
14	6	0	4.067780	-4.440197	-0.655172
15	6	0	-0.875166	-1.667496	-0.090838
16	6	0	-1.338989	-0.386085	-0.324446
17	6	0	-2.732641	-0.320174	-0.412952
18	6	0	-3.341851	-1.561460	-0.242979
19	16	0	-2.140395	-2.816686	0.027085
20	1	0	-3.300374	0.580759	-0.611178
21	6	0	4.684656	-1.100568	0.097752
22	6	0	5.149051	-2.391420	0.338671
23	6	0	6.531169	-2.439117	0.419111

24	6	0	7.142046	-1.181812	0.239236
25	16	0	5.924550	0.067898	-0.034502
26	1	0	7.125218	-3.327617	0.599929
27	6	0	-4.753706	-1.810613	-0.237760
28	6	0	-5.471611	-3.015982	-0.357456
29	16	0	-5.815557	-0.446089	-0.069503
30	6	0	-6.849779	-2.794300	-0.330735
31	6	0	-7.230547	-1.456361	-0.187738
32	1	0	-7.594435	-3.574150	-0.421798
33	6	0	-8.598867	-1.113190	-0.150739
34	6	0	-10.721631	0.265696	-0.011208
35	6	0	-9.275627	0.081699	-0.025585
36	6	0	-8.645899	1.401189	0.121926
37	6	0	-11.710885	-0.687019	-0.123882
38	6	0	-11.453785	-2.079930	-0.280647
39	6	0	-13.101610	-0.379323	-0.096079
40	8	0	-7.456336	1.668776	0.157053
41	7	0	-11.270628	-3.220884	-0.409207
42	7	0	-14.243828	-0.165332	-0.077519
43	6	0	-12.068591	3.847197	0.384353
44	6	0	-12.154576	2.457989	0.229100
45	6	0	-10.976725	1.719422	0.149866
46	6	0	-9.747133	2.385290	0.227416
47	6	0	-9.640088	3.752455	0.380822
48	6	0	-10.816926	4.501323	0.460878
49	1	0	-13.134282	2.004693	0.176093
50	1	0	-8.667737	4.226702	0.437531
51	6	0	8.545109	-1.066377	0.292488

52	6	0	10.880835	-0.083884	0.243495
53	6	0	9.427898	-0.013249	0.157846
54	6	0	9.052876	1.382810	-0.102970
55	6	0	11.678246	-1.183044	0.479974
56	6	0	11.172624	-2.498732	0.689568
57	6	0	13.100176	-1.120705	0.541270
58	8	0	7.935614	1.852895	-0.238354
59	7	0	10.788183	-3.582183	0.863571
60	7	0	14.261013	-1.108070	0.598139
61	6	0	12.864842	3.177033	-0.240040
62	6	0	12.693364	1.807092	-0.005287
63	6	0	11.400598	1.290334	0.025974
64	6	0	10.316294	2.152456	-0.177164
65	6	0	10.462747	3.504722	-0.409156
66	6	0	11.756251	4.031686	-0.442559
67	1	0	13.571930	1.195518	0.143686
68	1	0	9.594942	4.135169	-0.560996
69	1	0	8.995365	-2.034552	0.480385
70	1	0	-9.216509	-1.999296	-0.241539
71	1	0	3.054583	-4.664817	1.912153
72	1	0	4.819407	-4.641321	1.999393
73	1	0	3.885357	-3.269572	2.619846
74	1	0	4.110530	-3.987981	-1.648046
75	1	0	4.956238	-5.062765	-0.521880
76	1	0	3.191899	-5.092808	-0.611947
77	1	0	-1.019429	1.856471	-1.990715
78	1	0	0.745365	1.887135	-1.909462
79	1	0	-0.082361	0.486764	-2.611191

80	1	0	-1.146344	2.282842	0.533083
81	1	0	-0.290382	1.213130	1.655982
82	1	0	0.618259	2.319625	0.612571
83	16	0	-4.699493	-4.584479	-0.558902
84	6	0	-6.116720	-5.706136	-0.571714
85	1	0	-6.767004	-5.523129	-1.428313
86	1	0	-5.691677	-6.705986	-0.663625
87	1	0	-6.680472	-5.648771	0.360285
88	6	0	11.944608	5.427747	-0.681091
89	6	0	14.191772	3.709068	-0.273085
90	6	0	-10.742513	5.919281	0.619483
91	6	0	-13.277399	4.606762	0.465779
92	7	0	15.273819	4.126149	-0.297083
93	7	0	-14.266570	5.208995	0.530346
94	7	0	12.065258	6.564776	-0.876991
95	7	0	-10.649307	7.068421	0.748011

Atomic coordinates of Designed Molecule IDST4

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	6	0	0.990201	-0.409548	-0.228619
2	6	0	0.556560	-1.742313	-0.006826
3	6	0	1.462923	-2.778675	0.237269
4	6	0	2.810592	-2.466166	0.257653
5	6	0	3.243208	-1.135500	0.036059
6	6	0	2.335220	-0.098056	-0.208566
7	1	0	1.115205	-3.792974	0.405649

8	1	0	2.684278	0.915922	-0.376554
9	6	0	-0.191635	0.526476	-0.470942
10	6	0	-0.127817	1.152645	-1.872654
11	6	0	-0.266799	1.623066	0.602575
12	6	0	3.991277	-3.403716	0.501674
13	6	0	3.922156	-4.034233	1.901087
14	6	0	4.069103	-4.497243	-0.574761
15	6	0	-0.882438	-1.720339	-0.090243
16	6	0	-1.344770	-0.445292	-0.351352
17	6	0	-2.739265	-0.380544	-0.453603
18	6	0	-3.349914	-1.616519	-0.265348
19	16	0	-2.151131	-2.866419	0.039533
20	1	0	-3.306097	0.515605	-0.674612
21	6	0	4.680825	-1.145713	0.121600
22	6	0	5.143449	-2.429495	0.387466
23	6	0	6.527796	-2.475207	0.476719
24	6	0	7.138135	-1.223564	0.278893
25	16	0	5.923591	0.020541	-0.023122
26	1	0	7.121260	-3.360111	0.676215
27	6	0	-4.764047	-1.865737	-0.263630
28	6	0	-5.482103	-3.064996	-0.399388
29	16	0	-5.825123	-0.501124	-0.080050
30	6	0	-6.862595	-2.841329	-0.373471
31	6	0	-7.240191	-1.506834	-0.215555
32	1	0	-7.608581	-3.618422	-0.476289
33	6	0	-8.613398	-1.161664	-0.180007
34	6	0	-10.737673	0.213182	-0.034551
35	6	0	-9.287979	0.028037	-0.043790

36	6	0	-8.654472	1.350335	0.124299
37	6	0	-11.719156	-0.749266	-0.166913
38	6	0	-11.456475	-2.138147	-0.340784
39	6	0	-13.111463	-0.450479	-0.144138
40	8	0	-7.458024	1.594647	0.165827
41	7	0	-11.272326	-3.277853	-0.483758
42	7	0	-14.255818	-0.245063	-0.130466
43	6	0	-12.094890	3.792833	0.402545
44	6	0	-12.159324	2.385912	0.226050
45	6	0	-10.993710	1.657669	0.143606
46	6	0	-9.745757	2.332258	0.237310
47	6	0	-9.644526	3.683467	0.407701
48	6	0	-10.828706	4.455819	0.495144
49	1	0	-13.135493	1.924297	0.161371
50	1	0	-8.668003	4.152009	0.474899
51	6	0	8.545977	-1.107781	0.337209
52	6	0	10.884511	-0.134221	0.280760
53	6	0	9.428497	-0.061823	0.189109
54	6	0	9.054531	1.336049	-0.097250
55	6	0	11.669161	-1.240573	0.542951
56	6	0	11.155097	-2.547905	0.776535
57	6	0	13.090823	-1.189582	0.609579
58	8	0	7.927770	1.786467	-0.239294
59	7	0	10.766981	-3.627212	0.971121
60	7	0	14.251966	-1.187824	0.671892
61	6	0	12.888350	3.113035	-0.262343
62	6	0	12.688244	1.732352	-0.000276
63	6	0	11.407956	1.227393	0.039640

64	6	0	10.310008	2.101921	-0.183297
65	6	0	10.463146	3.434954	-0.436297
66	6	0	11.769863	3.979862	-0.482789
67	1	0	13.559945	1.112495	0.161212
68	1	0	9.592092	4.061294	-0.599637
69	1	0	8.991582	-2.074393	0.543422
70	1	0	-9.228841	-2.047782	-0.284718
71	1	0	3.041860	-4.676272	1.990771
72	1	0	4.806799	-4.649041	2.086622
73	1	0	3.868012	-3.266976	2.676025
74	1	0	4.116757	-4.062240	-1.575107
75	1	0	4.958148	-5.115614	-0.425863
76	1	0	3.193727	-5.150346	-0.525087
77	1	0	-1.014499	1.764760	-2.057986
78	1	0	0.750634	1.796482	-1.966660
79	1	0	-0.073877	0.382789	-2.644998
80	1	0	-1.157998	2.239064	0.456250
81	1	0	-0.309117	1.190592	1.604220
82	1	0	0.606981	2.277752	0.547064
83	16	0	-4.712801	-4.634148	-0.620562
84	6	0	-6.133177	-5.751747	-0.644039
85	1	0	-6.784473	-5.558024	-1.497564
86	1	0	-5.711855	-6.752244	-0.746220
87	1	0	-6.697043	-5.701613	0.288345
88	6	0	12.003352	5.350820	-0.741334
89	6	0	13.283005	5.848245	-0.782558
90	6	0	14.386998	4.995552	-0.566164
91	6	0	14.193999	3.659928	-0.311836

92	6	0	-13.277452	4.567397	0.490311
93	6	0	-13.214398	5.928525	0.661232
94	6	0	-11.965387	6.579889	0.752498
95	6	0	-10.799002	5.859062	0.671305
96	1	0	-14.236423	4.064594	0.419697
97	1	0	-14.127780	6.509276	0.726866
98	1	0	-11.930425	7.655301	0.887711
99	1	0	-9.837123	6.356451	0.741520
100	1	0	13.450009	6.901051	-0.982019
101	1	0	11.152223	6.003179	-0.907411
102	1	0	15.392190	5.400833	-0.601555
103	1	0	15.041075	3.002602	-0.144883

Atomic coordinates of Designed Molecule IDST5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.908711	-1.279595	-0.195349
2	6	0	0.478551	-2.616021	0.010572
3	6	0	1.386478	-3.650609	0.256150
4	6	0	2.732462	-3.332693	0.293928
5	6	0	3.161768	-1.998438	0.087973
6	6	0	2.252137	-0.962704	-0.157918
7	1	0	1.041219	-4.667708	0.412222
8	1	0	2.598668	0.054093	-0.313657
9	6	0	-0.274576	-0.346610	-0.442816
10	6	0	-0.197628	0.293138	-1.837683
11	6	0	-0.367031	0.739319	0.640164

12	6	0	3.914155	-4.267584	0.542892
13	6	0	3.832441	-4.910676	1.935877
14	6	0	4.008156	-5.351219	-0.542230
15	6	0	-0.959367	-2.599768	-0.089256
16	6	0	-1.424574	-1.324726	-0.345420
17	6	0	-2.817982	-1.265819	-0.463664
18	6	0	-3.424966	-2.506249	-0.292498
19	16	0	-2.223742	-3.752754	0.016668
20	1	0	-3.386134	-0.370259	-0.683733
21	6	0	4.598460	-2.003875	0.189079
22	6	0	5.063418	-3.287773	0.449611
23	6	0	6.446977	-3.328905	0.553914
24	6	0	7.054398	-2.073619	0.372709
25	16	0	5.838485	-0.832064	0.066818
26	1	0	7.041400	-4.213196	0.753293
27	6	0	-4.837445	-2.763212	-0.311868
28	6	0	-5.546963	-3.967334	-0.450132
29	16	0	-5.909448	-1.403484	-0.155117
30	6	0	-6.929041	-3.751385	-0.446177
31	6	0	-7.316476	-2.418329	-0.303525
32	1	0	-7.668832	-4.533683	-0.553917
33	6	0	-8.691948	-2.080397	-0.290593
34	6	0	-10.825073	-0.715570	-0.188473
35	6	0	-9.375067	-0.893974	-0.174853
36	6	0	-8.755501	0.434471	-0.011569
37	6	0	-11.799729	-1.683369	-0.321652
38	6	0	-11.527924	-3.073644	-0.472951
39	6	0	-13.194288	-1.392844	-0.322528

40	8	0	-7.563311	0.694227	0.046973
41	7	0	-11.338251	-4.214362	-0.597943
42	7	0	-14.339774	-1.194008	-0.327820
43	6	0	-12.203809	2.843488	0.180104
44	6	0	-12.277879	1.449608	0.021848
45	6	0	-11.092156	0.731520	-0.031982
46	6	0	-9.856561	1.408529	0.072259
47	6	0	-9.748606	2.774076	0.229000
48	6	0	-10.943024	3.489291	0.281675
49	1	0	-13.248330	0.979201	-0.052888
50	1	0	-8.773848	3.242052	0.305081
51	6	0	8.461018	-1.951915	0.448933
52	6	0	10.794861	-0.965340	0.429794
53	6	0	9.340212	-0.901393	0.319254
54	6	0	8.967213	0.496347	0.035993
55	6	0	11.582455	-2.067426	0.695605
56	6	0	11.072938	-3.379584	0.914445
57	6	0	13.003126	-2.010043	0.782021
58	8	0	7.843813	0.949784	-0.120029
59	7	0	10.690435	-4.462700	1.097480
60	7	0	14.163186	-2.002739	0.860200
61	6	0	12.781093	2.279095	-0.061133
62	6	0	12.607224	0.907568	0.188450
63	6	0	11.315285	0.402300	0.204080
64	6	0	10.222025	1.265660	-0.027840
65	6	0	10.357162	2.615105	-0.274778
66	6	0	11.657082	3.116177	-0.289323
67	1	0	13.477314	0.289217	0.359425

68	1	0	9.482049	3.231324	-0.446056
69	1	0	8.908642	-2.917834	0.653874
70	1	0	-9.301092	-2.970641	-0.396713
71	1	0	2.954341	-5.557672	2.009995
72	1	0	4.717862	-5.523002	2.125847
73	1	0	3.765970	-4.150616	2.716921
74	1	0	4.065010	-4.907216	-1.538120
75	1	0	4.897861	-5.967560	-0.388990
76	1	0	3.134847	-6.008020	-0.507760
77	1	0	-1.085311	0.902383	-2.027559
78	1	0	0.678306	0.942566	-1.915193
79	1	0	-0.130540	-0.468951	-2.616669
80	1	0	-1.259149	1.352878	0.489387
81	1	0	-0.418911	0.297132	1.637098
82	1	0	0.504370	1.398297	0.600794
83	16	0	-4.766961	-5.534289	-0.647802
84	6	0	-6.180840	-6.659995	-0.677146
85	1	0	-6.822282	-6.479373	-1.540942
86	1	0	-5.752589	-7.659063	-0.763179
87	1	0	-6.756590	-6.603107	0.247551
88	6	0	-13.291885	3.772292	0.258963
89	6	0	-12.858042	5.047299	0.412013
90	16	0	-11.124596	5.209133	0.470707
91	1	0	-14.336217	3.497090	0.203305
92	6	0	13.814039	4.320506	-0.385201
93	6	0	14.014526	3.005967	-0.123187
94	16	0	12.139899	4.763706	-0.572183
95	1	0	14.991603	2.565577	0.020664

96	35	0	15.120909	5.635920	-0.555304
97	35	0	-13.912650	6.574137	0.556793

Atomic coordinates of Designed Molecule IDST6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.950959	-0.819808	-0.204609
2	6	0	0.518701	-2.155443	0.003138
3	6	0	1.425442	-3.192458	0.243276
4	6	0	2.772381	-2.877841	0.273798
5	6	0	3.203552	-1.544378	0.066053
6	6	0	2.295173	-0.506208	-0.174448
7	1	0	1.078522	-4.208747	0.400822
8	1	0	2.643410	0.509761	-0.331674
9	6	0	-0.231141	0.116261	-0.445271
10	6	0	-0.160484	0.755678	-1.840661
11	6	0	-0.314695	1.202507	0.638145
12	6	0	3.953372	-3.815479	0.515943
13	6	0	3.878059	-4.458487	1.909356
14	6	0	4.038945	-4.899216	-0.569805
15	6	0	-0.919642	-2.135535	-0.088544
16	6	0	-1.382940	-0.858868	-0.341319
17	6	0	-2.776590	-0.795987	-0.450834
18	6	0	-3.386058	-2.034998	-0.276600
19	16	0	-2.186454	-3.285146	0.024197
20	1	0	-3.343599	0.101235	-0.666998
21	6	0	4.640406	-1.552679	0.158959

22	6	0	5.104317	-2.838173	0.416331
23	6	0	6.487868	-2.881937	0.512084
24	6	0	7.096944	-1.627092	0.327557
25	16	0	5.881111	-0.382815	0.029976
26	1	0	7.082071	-3.767333	0.707142
27	6	0	-4.799244	-2.286805	-0.286819
28	6	0	-5.514012	-3.488696	-0.423642
29	16	0	-5.864726	-0.923657	-0.118771
30	6	0	-6.894694	-3.267815	-0.410195
31	6	0	-7.276651	-1.933159	-0.261156
32	1	0	-7.638145	-4.046968	-0.515632
33	6	0	-8.649954	-1.590945	-0.238346
34	6	0	-10.778336	-0.220552	-0.117384
35	6	0	-9.328704	-0.401499	-0.113614
36	6	0	-8.700258	0.922526	0.051954
37	6	0	-11.757138	-1.185201	-0.250937
38	6	0	-11.490548	-2.574815	-0.413030
39	6	0	-13.149711	-0.887138	-0.241121
40	8	0	-7.505688	1.173018	0.102858
41	7	0	-11.302486	-3.714938	-0.546599
42	7	0	-14.293586	-0.678822	-0.237442
43	6	0	-12.148208	3.357576	0.284450
44	6	0	-12.208634	1.950532	0.116813
45	6	0	-11.039935	1.225095	0.049316
46	6	0	-9.795932	1.902661	0.149331
47	6	0	-9.697829	3.255375	0.311802
48	6	0	-10.883738	4.024378	0.383696
49	1	0	-13.182829	1.486181	0.046672

50	1	0	-8.722978	3.725911	0.384278
51	6	0	8.503433	-1.508914	0.393447
52	6	0	10.839917	-0.529371	0.354758
53	6	0	9.384712	-0.459346	0.257067
54	6	0	9.009029	0.938640	-0.021579
55	6	0	11.626908	-1.634391	0.613953
56	6	0	11.115542	-2.944474	0.838093
57	6	0	13.048033	-1.577813	0.686562
58	8	0	7.883295	1.390333	-0.165729
59	7	0	10.728832	-4.025573	1.024840
60	7	0	14.208880	-1.567898	0.752797
61	6	0	12.838382	2.724953	-0.160815
62	6	0	12.641739	1.343199	0.092179
63	6	0	11.361921	0.835465	0.123921
64	6	0	10.264093	1.707808	-0.097844
65	6	0	10.413351	3.043078	-0.342554
66	6	0	11.717891	3.590480	-0.380669
67	1	0	13.514043	0.724570	0.253374
68	1	0	9.541157	3.667430	-0.505401
69	1	0	8.950643	-2.475905	0.594362
70	1	0	-9.263044	-2.478610	-0.343645
71	1	0	2.998838	-5.103353	1.988338
72	1	0	4.763032	-5.072983	2.094207
73	1	0	3.817855	-3.698414	2.690892
74	1	0	4.091084	-4.455379	-1.566028
75	1	0	4.928187	-5.517429	-0.421609
76	1	0	3.164504	-5.554213	-0.530387
77	1	0	-1.047547	1.367350	-2.025491

78	1	0	0.716769	1.402675	-1.923222
79	1	0	-0.099949	-0.006608	-2.619987
80	1	0	-1.206154	1.818230	0.492411
81	1	0	-0.361915	0.760632	1.635449
82	1	0	0.558042	1.859378	0.593681
83	16	0	-4.740037	-5.057093	-0.630750
84	6	0	-6.157621	-6.178158	-0.657839
85	1	0	-6.802953	-5.991225	-1.517374
86	1	0	-5.733060	-7.178161	-0.750899
87	1	0	-6.728199	-6.123798	0.270202
88	6	0	11.941508	4.965238	-0.630945
89	6	0	13.217026	5.452426	-0.661610
90	6	0	14.323590	4.600943	-0.445613
91	6	0	14.146129	3.269447	-0.200479
92	6	0	-13.337740	4.124255	0.355960
93	6	0	-13.267699	5.478313	0.517474
94	6	0	-12.019764	6.133635	0.615278
95	6	0	-10.851361	5.429317	0.550895
96	1	0	-14.308075	3.647334	0.283523
97	1	0	-9.908029	5.956560	0.629080
98	1	0	11.110674	5.639843	-0.799949
99	1	0	15.012390	2.639045	-0.037886
100	9	0	13.458731	6.740572	-0.894827
101	9	0	15.539956	5.140199	-0.488899
102	9	0	-14.367750	6.223931	0.587963
103	9	0	-12.021578	7.455248	0.771902

Atomic coordinates of Designed Molecule IDST7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.015403	-0.162185	0.244535
2	6	0	-0.576426	-1.495663	0.036788
3	6	0	-1.478164	-2.541262	-0.183532
4	6	0	-2.827688	-2.237377	-0.194918
5	6	0	-3.266049	-0.906062	0.012269
6	6	0	-2.362431	0.140671	0.233671
7	1	0	-1.125513	-3.555513	-0.341321
8	1	0	-2.716334	1.154683	0.390691
9	6	0	0.163509	0.783858	0.461518
10	6	0	0.110808	1.428918	1.855179
11	6	0	0.221164	1.866008	-0.627791
12	6	0	-4.004136	-3.185701	-0.415147
13	6	0	-3.942923	-3.836384	-1.805688
14	6	0	-4.066101	-4.263604	0.678121
15	6	0	0.862662	-1.464626	0.104573
16	6	0	1.320917	-0.183192	0.342906
17	6	0	2.715776	-0.110082	0.426869
18	6	0	3.330601	-1.346056	0.247792
19	16	0	2.134651	-2.606028	-0.025121
20	1	0	3.280102	0.792458	0.627581
21	6	0	-4.703897	-0.926163	-0.060898
22	6	0	-5.161133	-2.216991	-0.305385
23	6	0	-6.544950	-2.272280	-0.384095
24	6	0	-7.161240	-1.020743	-0.200056
25	16	0	-5.952005	0.234478	0.076524

26	1	0	-7.134196	-3.163520	-0.567145
27	6	0	4.744848	-1.589752	0.233051
28	6	0	5.467853	-2.788860	0.356469
29	16	0	5.800692	-0.222011	0.045593
30	6	0	6.846626	-2.562084	0.315552
31	6	0	7.219325	-1.225524	0.159033
32	1	0	7.595332	-3.338192	0.405203
33	6	0	8.589024	-0.876349	0.104419
34	6	0	10.716141	0.470686	-0.066716
35	6	0	9.264108	0.313625	-0.035284
36	6	0	8.628976	1.647051	-0.179595
37	6	0	11.708395	-0.482550	0.030820
38	6	0	11.470397	-1.875802	0.189971
39	6	0	13.081185	-0.111410	-0.024638
40	8	0	7.434716	1.889785	-0.198278
41	7	0	11.289452	-3.017368	0.320412
42	7	0	14.199157	0.204263	-0.071590
43	6	0	-8.568161	-0.911378	-0.254362
44	6	0	-10.911747	0.023143	-0.220620
45	6	0	-9.458886	0.130886	-0.123205
46	6	0	-9.094002	1.544641	0.137690
47	6	0	-11.702523	-1.083778	-0.451712
48	6	0	-11.204146	-2.401444	-0.647289
49	6	0	-13.119516	-0.965874	-0.510196
50	8	0	-7.971704	1.998631	0.277054
51	7	0	-10.812564	-3.484746	-0.809018
52	7	0	-14.276282	-0.857649	-0.556021
53	1	0	-9.014083	-1.882087	-0.443974

54	1	0	9.211374	-1.760200	0.194092
55	1	0	-3.059683	-4.474622	-1.892940
56	1	0	-4.825281	-4.459112	-1.974766
57	1	0	-3.899531	-3.080596	-2.592472
58	1	0	-4.107954	-3.814323	1.672388
59	1	0	-4.952259	-4.889869	0.546024
60	1	0	-3.187028	-4.911795	0.630395
61	1	0	0.995922	2.048254	2.022751
62	1	0	-0.769932	2.069527	1.949097
63	1	0	0.068836	0.669784	2.638803
64	1	0	1.110236	2.488975	-0.499486
65	1	0	0.255094	1.420376	-1.623971
66	1	0	-0.655502	2.516659	-0.571526
67	16	0	4.705622	-4.360769	0.578905
68	6	0	6.129334	-5.474280	0.585529
69	1	0	6.788208	-5.280727	1.433242
70	1	0	5.711546	-6.476038	0.689646
71	1	0	6.683568	-5.420712	-0.352417
72	6	0	-12.675337	1.977413	0.013712
73	6	0	-11.448107	1.373912	-0.020939
74	6	0	-10.368073	2.281645	0.192633
75	6	0	-10.779214	3.564151	0.387355
76	16	0	-12.512350	3.668973	0.309210
77	1	0	-13.659322	1.551466	-0.112726
78	17	0	-9.831365	4.950484	0.674859
79	6	0	12.070692	2.723135	-0.332212
80	6	0	10.979869	1.903866	-0.229592
81	6	0	9.739394	2.606580	-0.296516

82	6	0	9.895037	3.950154	-0.449295
83	16	0	11.580941	4.366902	-0.512176
84	1	0	13.122451	2.479677	-0.315263
85	17	0	8.692680	5.150374	-0.573693

Input script of IDSTR molecule for Geometry Optimization

IDSTR

%nprocshared=22

%mem=22GB

%chk=IDSTR.chk

opt rmpw1pw91/6-31g(d,p) geom=connectivity

IDSTR

0 1

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100

C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400

N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300

H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

1 2 1.5 6 2.0 9 1.0

2 3 1.5 15 1.5

3 4 2.0 7 1.0

4 5 1.5 12 1.0

5 6 1.5 21 1.5

6 8 1.0

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9 10 1.0 11 1.0 16 1.0

10 81 1.0 82 1.0 83 1.0

11 84 1.0 85 1.0 86 1.0

12 13 1.0 14 1.0 22 1.0

13 75 1.0 76 1.0 77 1.0

14 78 1.0 79 1.0 80 1.0

15 16 2.0 19 1.0

16 17 1.5

17 18 1.5 20 1.0

18 19 1.0 27 1.5

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21 22 1.5 25 1.0

22 23 1.5

23 24 1.5 26 1.0

24 25 1.0 53 1.5

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27 28 1.5 29 1.0

28 30 1.5 87 1.0

29 31 1.0

30 31 1.5 32 1.0

31 33 1.5

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33 35 2.0 74 1.0

34 35 1.0 37 2.0 45 1.0

35 36 1.0

36 40 2.0 46 1.0

37 38 1.5 39 1.5

38 41 3.0

39 42 3.0

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43 44 2.0 48 1.5 52 1.0

44 45 1.5 49 1.0

45 46 1.5

46 47 2.0

47 48 2.0 50 1.0

48 51 1.0

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53 55 2.0 73 1.0

54 55 1.0 57 2.0 65 1.0

55 56 1.0

56 60 2.0 66 1.0

57 58 1.5 59 1.5

58 61 3.0

59 62 3.0

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63 64 2.0 68 1.5 72 1.0

64 65 1.5 69 1.0

65 66 1.5

66 67 2.0

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91

Input script of IDSTR molecule for TD-DFT.

IDSTR

%nprocshared=22

%mem=22GB

td=(nstates=10) rmpw1pw91/6-31g(d,p) scrf=(iefpcm,solvent=chloroform)

geom=connectivity

IDSTRes

0 1

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900

C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900

C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300

F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

1 2 1.5 6 2.0 9 1.0

2 3 1.5 15 1.5

3 4 2.0 7 1.0

4 5 1.5 12 1.0

5 6 1.5 21 1.5

6 8 1.0

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9 10 1.0 11 1.0 16 1.0

10 81 1.0 82 1.0 83 1.0

11 84 1.0 85 1.0 86 1.0

12 13 1.0 14 1.0 22 1.0

13 75 1.0 76 1.0 77 1.0

14 78 1.0 79 1.0 80 1.0

15 16 2.0 19 1.0

16 17 1.5

17 18 1.5 20 1.0

18 19 1.0 27 1.5

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21 22 1.5 25 1.0

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23 24 1.5 26 1.0

24 25 1.0 53 1.5

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27 28 1.5 29 1.0

28 30 1.5 87 1.0

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31 33 1.5

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33 35 2.0 74 1.0

34 35 1.0 37 2.0 45 1.0

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37 38 1.5 39 1.5

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43 44 2.0 48 1.5 52 1.0

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53 55 2.0 73 1.0

54 55 1.0 57 2.0 65 1.0

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56 60 2.0 66 1.0

57 58 1.5 59 1.5

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59 62 3.0

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63 64 2.0 68 1.5 72 1.0

64 65 1.5 69 1.0

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66 67 2.0

67 68 2.0 70 1.0

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91

Input Script of IDSTR molecule for Transition Density Matrix (TDM).

IDSTR

%chk=IDSTRtdm.chk

%nprocshared=11

%mem=11GB

td=(nstates=10) rmpw1pw91/6-31g(d,p) density=transition=1

geom=connectivity iop(6/8=3)

IDSTRtdm

0 1

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200

C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700

C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900

H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

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10 81 1.0 82 1.0 83 1.0

11 84 1.0 85 1.0 86 1.0

12 13 1.0 14 1.0 22 1.0

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15 16 2.0 19 1.0

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Input Script of Density of states (DOS) for IDSTR

IDSTR

%nprocshared=22

%mem=22GB

rmpw1pw91/6-31g(d,p) pop=full geom=connectivity iop(3/33=1,3/36=-1)

IDSTRdos

0 1

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300

C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500

H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900

H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

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Input Script of Cation ground state energy taken from ground state neutral optimized geometry of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTRe+

1 2

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000

C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300

C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500

H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

1 2 1.5 6 2.0 9 1.0

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12 13 1.0 14 1.0 22 1.0

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15 16 2.0 19 1.0

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Input Script of Anion ground state energy taken from ground state neutral optimized geometry of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTRe-

-1 2

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900

C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700
C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200

H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300
C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500

O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500
C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000

C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

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Input Script of neutral ground state energy taken from ground state neutral optimized geometry of IDSTR

%nprocshared=3

%mem=2GB

rmpw1pw91/6-31g(d,p) geom=connectivity

IDSTRe0

0 1

C	-1.01814500	-0.13715800	0.24836500
C	-0.58373000	-1.46880700	0.02121900
C	-1.48920700	-2.50670500	-0.21909900
C	-2.83754000	-2.19687200	-0.23049000
C	-3.27106200	-0.86738000	-0.00349500
C	-2.36388900	0.17165000	0.23752000
H	-1.14045800	-3.51990200	-0.39171800
H	-2.71383800	1.18461100	0.40960700

C	0.16357700	0.80058000	0.48475800
C	0.10793600	1.42361200	1.88828600
C	0.22966100	1.89964500	-0.58691000
C	-4.01750000	-3.13640100	-0.46965100
C	-3.95489700	-3.76406900	-1.87070400
C	-4.08716700	-4.23212600	0.60521100
C	0.85562400	-1.44452200	0.09523900
C	1.31756700	-0.16900900	0.35544300
C	2.71259700	-0.10259700	0.44791200
C	3.32332500	-1.33771000	0.25342800
S	2.12442600	-2.58872000	-0.04523400
H	3.27957900	0.79403000	0.66669400
C	-4.70903800	-0.88073400	-0.08102300
C	-5.17089400	-2.16476500	-0.34715700
C	-6.55556100	-2.21301000	-0.42971800
C	-7.16706200	-0.96297700	-0.22661200
S	-5.95339900	0.28238500	0.07246500
H	-7.14781500	-3.09890800	-0.62839000
C	4.73740400	-1.58609600	0.24120700
C	5.45696500	-2.78533700	0.37100200
S	5.79678900	-0.22164000	0.05001400
C	6.83717000	-2.56139100	0.33439500
C	7.21315200	-1.22686600	0.17393200
H	7.58364600	-3.33883000	0.43107500
C	8.58513200	-0.87983400	0.12610500
C	10.70503600	0.49827200	-0.04044700
C	9.25683400	0.31027300	-0.01610600
C	8.62710700	1.63368600	-0.17656300

C	11.69300200	-0.45555400	0.07860800
C	11.43935300	-1.84681000	0.25328000
C	13.08332200	-0.14661800	0.03966800
O	7.43519900	1.89318200	-0.20783400
N	11.26295400	-2.98728000	0.39651400
N	14.22504000	0.06994300	0.01219300
C	12.03258800	4.05308900	-0.48247900
C	12.13802200	2.68243800	-0.31321500
C	10.95511800	1.94617700	-0.21938700
C	9.72501900	2.61155600	-0.29849300
C	9.61717100	3.98203700	-0.46809800
C	10.79443200	4.70110500	-0.55965000
H	13.12629100	2.24732700	-0.26211500
H	8.65309300	4.47229100	-0.52755300
F	10.78001300	6.01990700	-0.72293500
F	13.13157100	4.79481700	-0.57718400
C	-8.57486100	-0.84725200	-0.27974700
C	-10.91185400	0.12852200	-0.21825300
C	-9.45642200	0.19829100	-0.12833900
C	-9.08832300	1.59625500	0.15779700
C	-11.70316200	-0.97136400	-0.47403200
C	-11.19574300	-2.28301400	-0.70265300
C	-13.12513800	-0.91052400	-0.53779500
O	-7.96935500	2.06054300	0.30331500
N	-10.81364900	-3.36477400	-0.89298700
N	-14.28603900	-0.89752300	-0.59704500
C	-12.88582400	3.35802200	0.30768900
C	-12.73116300	2.00525600	0.05331500

C	-11.43176200	1.49463000	0.01921800
C	-10.35062400	2.35674000	0.23990200
C	-10.50255200	3.70970500	0.49375000
C	-11.79306900	4.20462200	0.52562300
H	-13.61890700	1.40941200	-0.10632100
H	-9.64844500	4.35463300	0.66083400
F	-12.02697100	5.49158000	0.76287300
F	-14.10436600	3.88882700	0.34994500
H	-9.02210900	-1.81313700	-0.48609900
H	9.20353300	-1.76466200	0.22475400
H	-3.07364800	-4.40383800	-1.96639800
H	-4.83895500	-4.38083500	-2.05235900
H	-3.90684100	-2.99538700	-2.64461900
H	-4.13025400	-3.79935400	1.60672500
H	-4.97550200	-4.85233000	0.45986700
H	-3.21066300	-4.88313600	0.54938800
H	0.99449000	2.03725200	2.06889800
H	-0.77102300	2.06560300	1.98938500
H	0.06064800	0.65218600	2.65949000
H	1.12056000	2.51705300	-0.44499500
H	0.26608300	1.46971900	-1.58988000
H	-0.64477900	2.55271000	-0.52401300
S	4.68952900	-4.35433800	0.59784000
C	6.11019200	-5.47165900	0.61455200
H	6.76663100	-5.27634000	1.46376000
H	5.68935400	-6.47184200	0.72154300
H	6.66794400	-5.42387900	-0.32162400

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Input Script of energy of cation taken from cation optimized geometry of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTR+e+

1 2

C	1.00935900	-0.11813900	0.00052200
C	0.57691700	-1.48265300	0.00029700
C	1.49329000	-2.55404000	0.00002100
C	2.83154300	-2.24886400	-0.00004200
C	3.26280800	-0.88396400	0.00017600
C	2.34970800	0.18559100	0.00046100
H	1.14399000	-3.58119300	-0.00013700
H	2.70117700	1.21182300	0.00062700
C	-0.17515700	0.84419600	0.00081400
C	-0.18616300	1.71983300	-1.26267000
C	-0.18597200	1.71927500	1.26469200
C	4.02161400	-3.20500700	-0.00033600
C	4.03633600	-4.08137300	1.26261200

C	4.03606200	-4.08095600	-1.26357300
C	-0.83810800	-1.45814600	0.00040200
C	-1.32275500	-0.13962600	0.00068100
C	-2.69942400	-0.07318400	0.00073600
C	-3.30977700	-1.34871400	0.00050000
S	-2.09666700	-2.62608100	0.00021900
H	-3.27767700	0.84233700	0.00096600
C	4.68729900	-0.90000600	0.00002500
C	5.16185400	-2.21265100	-0.00028100
C	6.54827800	-2.26262700	-0.00041200
C	7.14145400	-0.98758100	-0.00020400
S	5.92950400	0.28513500	0.00015800
H	7.15105500	-3.16294100	-0.00063300
C	-4.70206400	-1.59340700	0.00045500
C	-5.42703900	-2.81239100	0.00050300
S	-5.77990200	-0.21259400	0.00044100
C	-6.80777300	-2.58319900	0.00039200
C	-7.17703100	-1.23984300	0.00025700
H	-7.55450700	-3.36564500	0.00031500
C	-8.56536800	-0.89527700	-0.00005800
C	-10.68545700	0.49988300	-0.00062300
C	-9.22822500	0.29626600	-0.00032300
C	-8.59146200	1.63851400	-0.00014400
C	-11.66618500	-0.46186300	-0.00125200
C	-11.40079300	-1.86300500	-0.00169800
C	-13.05781500	-0.15213900	-0.00152500
O	-7.39561800	1.87456600	-0.00007000
N	-11.19836600	-3.00740000	-0.00205600

N	-14.19793900	0.06957500	-0.00175600
C	-11.98396400	4.08420800	0.00014200
C	-12.09687500	2.70452900	-0.00018100
C	-10.91711600	1.95624200	-0.00027700
C	-9.68062400	2.62102200	-0.00003600
C	-9.56604700	4.00340400	0.00027400
C	-10.73897800	4.73274500	0.00035700
H	-13.08798800	2.27279100	-0.00033000
H	-8.60129600	4.49558500	0.00044600
F	-10.72062100	6.05615300	0.00064700
F	-13.07270600	4.83618500	0.00025800
C	8.56339000	-0.87602100	-0.00027700
C	10.89401600	0.12790500	-0.00006100
C	9.42533200	0.18457300	-0.00002700
C	9.03509500	1.61641000	0.00002600
C	11.69341400	-0.99016200	0.00024400
C	11.19189900	-2.32482800	0.00067500
C	13.11765100	-0.92689000	0.00019400
O	7.90144100	2.06364400	0.00016800
N	10.80150400	-3.41956600	0.00102200
N	14.27911800	-0.90798300	0.00015000
C	12.80537800	3.42836500	-0.00074300
C	12.67388700	2.05026800	-0.00058100
C	11.38089500	1.52108200	-0.00030700
C	10.28146100	2.39266800	-0.00020800
C	10.41123200	3.77327900	-0.00035500
C	11.69423600	4.28521400	-0.00062700
H	13.57334900	1.45067200	-0.00068800

H	9.54745700	4.42673500	-0.00026600
F	11.90864300	5.59210000	-0.00079500
F	14.01036400	3.97756200	-0.00102100
H	9.01682900	-1.86022400	-0.00056500
H	-9.17819700	-1.78857800	-0.00008900
H	3.16975400	-4.74691400	1.27752700
H	4.93434000	-4.70329700	1.28021400
H	4.02111300	-3.47349600	2.16931800
H	4.02064500	-3.47278200	-2.17007600
H	4.93406000	-4.70287700	-1.28157200
H	3.16947800	-4.74649400	-1.27852200
H	-1.07661200	2.35272200	-1.27839600
H	0.68858400	2.37403900	-1.27888700
H	-0.17809300	1.11179500	-2.16930300
H	-1.07641500	2.35216100	1.28083500
H	-0.17776900	1.11083400	2.17105400
H	0.68878300	2.37346800	1.28107000
S	-4.67125300	-4.38258800	0.00064700
C	-6.08217900	-5.51276400	0.00085100
H	-6.68674600	-5.39130900	-0.89834000
H	-5.64661500	-6.51210100	0.00025900
H	-6.68590100	-5.39203300	0.90070600

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Input Script of energy of anion taken from anion optimized geometry of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTR-e-

-1 2

C	1.01964500	-0.13261000	-0.00069600
C	0.58815500	-1.49125900	0.00042800
C	1.51602400	-2.54705800	0.00152500
C	2.85742500	-2.23048600	0.00147000
C	3.28842000	-0.87433500	0.00032800
C	2.35873300	0.18262200	-0.00076500
H	1.17797200	-3.57872200	0.00239600
H	2.69780500	1.21400500	-0.00163500
C	-0.17507500	0.81994300	-0.00175000
C	-0.18874700	1.69529600	-1.26353500
C	-0.18917900	1.69761300	1.25840900
C	4.04988600	-3.18602600	0.00253700
C	4.06026300	-4.06152400	1.26414600
C	4.06068400	-4.06387300	-1.25742600
C	-0.83802200	-1.46873500	0.00019300
C	-1.32296000	-0.16668400	-0.00104300
C	-2.71063600	-0.09268700	-0.00147500
C	-3.32841000	-1.35304800	-0.00057200

S	-2.10705500	-2.63092100	0.00096400
H	-3.28422900	0.82603400	-0.00260200
C	4.71388100	-0.88755600	0.00054200
C	5.19808500	-2.19946500	0.00180300
C	6.57648300	-2.25502000	0.00202200
C	7.19404200	-0.97921200	0.00090300
S	5.96014700	0.29515700	-0.00042200
H	7.17567400	-3.15836100	0.00292800
C	-4.72521100	-1.59735000	-0.00051600
C	-5.46197500	-2.80382100	-0.00121600
S	-5.80571100	-0.21581800	0.00043200
C	-6.83421800	-2.58546300	-0.00113800
C	-7.22850000	-1.23512900	-0.00036000
H	-7.57945900	-3.36955900	-0.00168500
C	-8.58585700	-0.88967100	-0.00018400
C	-10.70171800	0.49837400	0.00061300
C	-9.27464900	0.32506700	0.00053800
C	-8.65240200	1.65335400	0.00127800
C	-11.70246100	-0.47557100	0.00012800
C	-11.45856700	-1.87515800	-0.00050700
C	-13.08852600	-0.16673300	0.00024300
O	-7.46239200	1.93693300	0.00152700
N	-11.30646700	-3.03064100	-0.00103700
N	-14.23402800	0.04689900	0.00031500
C	-12.07170400	4.07589800	0.00252600
C	-12.16473500	2.68988600	0.00176100
C	-10.97827800	1.95755900	0.00138800
C	-9.75656600	2.64151700	0.00179800

C	-9.66081400	4.01988700	0.00257000
C	-10.84636000	4.73857100	0.00292700
H	-13.14861500	2.24175400	0.00149600
H	-8.69946500	4.51948300	0.00288200
F	-10.83809500	6.07561800	0.00366000
F	-13.18707200	4.81227300	0.00290100
C	8.58850700	-0.86311800	0.00093700
C	10.91610600	0.13097900	0.00014600
C	9.47703200	0.21182500	-0.00004400
C	9.09918000	1.62926800	-0.00161300
C	11.72903400	-0.99995300	0.00146600
C	11.24419700	-2.33623400	0.00296200
C	13.14878500	-0.93838300	0.00145900
O	7.97892000	2.11900100	-0.00219500
N	10.89309900	-3.44695400	0.00421200
N	14.31348400	-0.92898900	0.00149700
C	12.89162600	3.41257400	-0.00344900
C	12.74059000	2.03251200	-0.00188300
C	11.44360900	1.51952900	-0.00137000
C	10.36059600	2.40605100	-0.00242000
C	10.50750700	3.78041300	-0.00396900
C	11.79998800	4.27962000	-0.00448600
H	13.63076000	1.41915000	-0.00113800
H	9.64850900	4.44064500	-0.00475000
F	12.02669200	5.59616800	-0.00598000
F	14.11739900	3.94346500	-0.00399500
H	9.05052700	-1.84390600	0.00193800
H	-9.20848000	-1.77669000	-0.00071000

H	3.18501300	-4.71686100	1.28584200
H	4.95468700	-4.69030900	1.28580500
H	4.05090500	-3.44662900	2.16641200
H	4.05158500	-3.45066600	-2.16084400
H	4.95513700	-4.69266600	-1.27763600
H	3.18547300	-4.71929400	-1.27818200
H	-1.08694700	2.31853700	-1.28632100
H	0.68255500	2.35581300	-1.28387700
H	-0.17499000	1.08032700	-2.16567500
H	-1.08741000	2.32086100	1.27976900
H	-0.17569000	1.08431000	2.16168700
H	0.68208700	2.35820800	1.27782600
S	-4.70036500	-4.39526800	-0.00238700
C	-6.13213300	-5.49730500	-0.00222200
H	-6.74137400	-5.36186600	-0.89715000
H	-5.72332400	-6.50837500	-0.00263600
H	-6.74077500	-5.36233900	0.89318400

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Input Script of neutral molecules' energies, that are calculated utilizing optimized cation geometries of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTR+e0

0 1

C	1.00935900	-0.11813900	0.00052200
C	0.57691700	-1.48265300	0.00029700
C	1.49329000	-2.55404000	0.00002100
C	2.83154300	-2.24886400	-0.00004200
C	3.26280800	-0.88396400	0.00017600
C	2.34970800	0.18559100	0.00046100
H	1.14399000	-3.58119300	-0.00013700
H	2.70117700	1.21182300	0.00062700
C	-0.17515700	0.84419600	0.00081400
C	-0.18616300	1.71983300	-1.26267000
C	-0.18597200	1.71927500	1.26469200
C	4.02161400	-3.20500700	-0.00033600
C	4.03633600	-4.08137300	1.26261200
C	4.03606200	-4.08095600	-1.26357300
C	-0.83810800	-1.45814600	0.00040200
C	-1.32275500	-0.13962600	0.00068100
C	-2.69942400	-0.07318400	0.00073600
C	-3.30977700	-1.34871400	0.00050000
S	-2.09666700	-2.62608100	0.00021900
H	-3.27767700	0.84233700	0.00096600
C	4.68729900	-0.90000600	0.00002500
C	5.16185400	-2.21265100	-0.00028100
C	6.54827800	-2.26262700	-0.00041200

C	7.14145400	-0.98758100	-0.00020400
S	5.92950400	0.28513500	0.00015800
H	7.15105500	-3.16294100	-0.00063300
C	-4.70206400	-1.59340700	0.00045500
C	-5.42703900	-2.81239100	0.00050300
S	-5.77990200	-0.21259400	0.00044100
C	-6.80777300	-2.58319900	0.00039200
C	-7.17703100	-1.23984300	0.00025700
H	-7.55450700	-3.36564500	0.00031500
C	-8.56536800	-0.89527700	-0.00005800
C	-10.68545700	0.49988300	-0.00062300
C	-9.22822500	0.29626600	-0.00032300
C	-8.59146200	1.63851400	-0.00014400
C	-11.66618500	-0.46186300	-0.00125200
C	-11.40079300	-1.86300500	-0.00169800
C	-13.05781500	-0.15213900	-0.00152500
O	-7.39561800	1.87456600	-0.00007000
N	-11.19836600	-3.00740000	-0.00205600
N	-14.19793900	0.06957500	-0.00175600
C	-11.98396400	4.08420800	0.00014200
C	-12.09687500	2.70452900	-0.00018100
C	-10.91711600	1.95624200	-0.00027700
C	-9.68062400	2.62102200	-0.00003600
C	-9.56604700	4.00340400	0.00027400
C	-10.73897800	4.73274500	0.00035700
H	-13.08798800	2.27279100	-0.00033000
H	-8.60129600	4.49558500	0.00044600
F	-10.72062100	6.05615300	0.00064700

F	-13.07270600	4.83618500	0.00025800
C	8.56339000	-0.87602100	-0.00027700
C	10.89401600	0.12790500	-0.00006100
C	9.42533200	0.18457300	-0.00002700
C	9.03509500	1.61641000	0.00002600
C	11.69341400	-0.99016200	0.00024400
C	11.19189900	-2.32482800	0.00067500
C	13.11765100	-0.92689000	0.00019400
O	7.90144100	2.06364400	0.00016800
N	10.80150400	-3.41956600	0.00102200
N	14.27911800	-0.90798300	0.00015000
C	12.80537800	3.42836500	-0.00074300
C	12.67388700	2.05026800	-0.00058100
C	11.38089500	1.52108200	-0.00030700
C	10.28146100	2.39266800	-0.00020800
C	10.41123200	3.77327900	-0.00035500
C	11.69423600	4.28521400	-0.00062700
H	13.57334900	1.45067200	-0.00068800
H	9.54745700	4.42673500	-0.00026600
F	11.90864300	5.59210000	-0.00079500
F	14.01036400	3.97756200	-0.00102100
H	9.01682900	-1.86022400	-0.00056500
H	-9.17819700	-1.78857800	-0.00008900
H	3.16975400	-4.74691400	1.27752700
H	4.93434000	-4.70329700	1.28021400
H	4.02111300	-3.47349600	2.16931800
H	4.02064500	-3.47278200	-2.17007600
H	4.93406000	-4.70287700	-1.28157200

H	3.16947800	-4.74649400	-1.27852200
H	-1.07661200	2.35272200	-1.27839600
H	0.68858400	2.37403900	-1.27888700
H	-0.17809300	1.11179500	-2.16930300
H	-1.07641500	2.35216100	1.28083500
H	-0.17776900	1.11083400	2.17105400
H	0.68878300	2.37346800	1.28107000
S	-4.67125300	-4.38258800	0.00064700
C	-6.08217900	-5.51276400	0.00085100
H	-6.68674600	-5.39130900	-0.89834000
H	-5.64661500	-6.51210100	0.00025900
H	-6.68590100	-5.39203300	0.90070600

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Input Script of neutral molecules' energies, that are calculated utilizing optimized anion geometries of IDSTR

%nprocshared=3

%mem=2GB

umpw1pw91/6-31g(d,p) geom=connectivity

IDSTR-e0

0 1

C	1.01964500	-0.13261000	-0.00069600
C	0.58815500	-1.49125900	0.00042800
C	1.51602400	-2.54705800	0.00152500
C	2.85742500	-2.23048600	0.00147000
C	3.28842000	-0.87433500	0.00032800
C	2.35873300	0.18262200	-0.00076500
H	1.17797200	-3.57872200	0.00239600
H	2.69780500	1.21400500	-0.00163500
C	-0.17507500	0.81994300	-0.00175000
C	-0.18874700	1.69529600	-1.26353500
C	-0.18917900	1.69761300	1.25840900
C	4.04988600	-3.18602600	0.00253700
C	4.06026300	-4.06152400	1.26414600
C	4.06068400	-4.06387300	-1.25742600
C	-0.83802200	-1.46873500	0.00019300
C	-1.32296000	-0.16668400	-0.00104300
C	-2.71063600	-0.09268700	-0.00147500
C	-3.32841000	-1.35304800	-0.00057200
S	-2.10705500	-2.63092100	0.00096400
H	-3.28422900	0.82603400	-0.00260200
C	4.71388100	-0.88755600	0.00054200
C	5.19808500	-2.19946500	0.00180300
C	6.57648300	-2.25502000	0.00202200
C	7.19404200	-0.97921200	0.00090300
S	5.96014700	0.29515700	-0.00042200
H	7.17567400	-3.15836100	0.00292800
C	-4.72521100	-1.59735000	-0.00051600
C	-5.46197500	-2.80382100	-0.00121600

S	-5.80571100	-0.21581800	0.00043200
C	-6.83421800	-2.58546300	-0.00113800
C	-7.22850000	-1.23512900	-0.00036000
H	-7.57945900	-3.36955900	-0.00168500
C	-8.58585700	-0.88967100	-0.00018400
C	-10.70171800	0.49837400	0.00061300
C	-9.27464900	0.32506700	0.00053800
C	-8.65240200	1.65335400	0.00127800
C	-11.70246100	-0.47557100	0.00012800
C	-11.45856700	-1.87515800	-0.00050700
C	-13.08852600	-0.16673300	0.00024300
O	-7.46239200	1.93693300	0.00152700
N	-11.30646700	-3.03064100	-0.00103700
N	-14.23402800	0.04689900	0.00031500
C	-12.07170400	4.07589800	0.00252600
C	-12.16473500	2.68988600	0.00176100
C	-10.97827800	1.95755900	0.00138800
C	-9.75656600	2.64151700	0.00179800
C	-9.66081400	4.01988700	0.00257000
C	-10.84636000	4.73857100	0.00292700
H	-13.14861500	2.24175400	0.00149600
H	-8.69946500	4.51948300	0.00288200
F	-10.83809500	6.07561800	0.00366000
F	-13.18707200	4.81227300	0.00290100
C	8.58850700	-0.86311800	0.00093700
C	10.91610600	0.13097900	0.00014600
C	9.47703200	0.21182500	-0.00004400
C	9.09918000	1.62926800	-0.00161300

C	11.72903400	-0.99995300	0.00146600
C	11.24419700	-2.33623400	0.00296200
C	13.14878500	-0.93838300	0.00145900
O	7.97892000	2.11900100	-0.00219500
N	10.89309900	-3.44695400	0.00421200
N	14.31348400	-0.92898900	0.00149700
C	12.89162600	3.41257400	-0.00344900
C	12.74059000	2.03251200	-0.00188300
C	11.44360900	1.51952900	-0.00137000
C	10.36059600	2.40605100	-0.00242000
C	10.50750700	3.78041300	-0.00396900
C	11.79998800	4.27962000	-0.00448600
H	13.63076000	1.41915000	-0.00113800
H	9.64850900	4.44064500	-0.00475000
F	12.02669200	5.59616800	-0.00598000
F	14.11739900	3.94346500	-0.00399500
H	9.05052700	-1.84390600	0.00193800
H	-9.20848000	-1.77669000	-0.00071000
H	3.18501300	-4.71686100	1.28584200
H	4.95468700	-4.69030900	1.28580500
H	4.05090500	-3.44662900	2.16641200
H	4.05158500	-3.45066600	-2.16084400
H	4.95513700	-4.69266600	-1.27763600
H	3.18547300	-4.71929400	-1.27818200
H	-1.08694700	2.31853700	-1.28632100
H	0.68255500	2.35581300	-1.28387700
H	-0.17499000	1.08032700	-2.16567500
H	-1.08741000	2.32086100	1.27976900

H	-0.17569000	1.08431000	2.16168700
H	0.68208700	2.35820800	1.27782600
S	-4.70036500	-4.39526800	-0.00238700
C	-6.13213300	-5.49730500	-0.00222200
H	-6.74137400	-5.36186600	-0.89715000
H	-5.72332400	-6.50837500	-0.00263600
H	-6.74077500	-5.36233900	0.89318400

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