Supplementary Information File for the article:

On the directionality of anion–π interactions

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Summary:

Cartesian Coordinates Pages 2-14

Hexafluorobenzene, Z = 3.05

o:

Energy = -1283.432129990

C	-1.2083170	0.6976220	-0.2446138
C	-1.2083170	-0.6976220	-0.2446138
C	0.0000000	-1.3952450	-0.2446138
C	1.2083170	-0.6976220	-0.2446138
C	1.2083170	0.6976220	-0.2446138
C	0.0000000	1.3952450	-0.2446138
F	2.3781050	-1.3729990	-0.2227768
F	0.0000000	-2.7459990	-0.2227768
F	-2.3781050	-1.3729990	-0.2227768
F	2.3781050	1.3729990	-0.2227768
F	0.0000000	2.7459990	-0.2227768
F	-2.3781050	1.3729990	-0.2227768
Cl	0.0000000	0.0000000	2.8043442

x_1:

Energy = -1283.432060957

C	0.6707904	-0.2446138	-1.2083170
C	-0.7244536	-0.2446138	-1.2083170
C	-1.4220766	-0.2446138	0.0000000
C	-0.7244536	-0.2446138	1.2083170
C	0.6707904	-0.2446138	1.2083170
C	1.3684134	-0.2446138	0.0000000
F	-1.3998306	-0.2227768	2.3781050
F	-2.7728306	-0.2227768	0.0000000
F	-1.3998306	-0.2227768	-2.3781050
F	1.3461674	-0.2227768	2.3781050
F	2.7191674	-0.2227768	0.0000000
F	1.3461674	-0.2227768	-2.3781050
Cl	0.3219794	2.8043442	0.0000000

x_2:

Energy = -1283.431911741

C	0.6439588	-0.2446138	-1.2083170
C	-0.7512852	-0.2446138	-1.2083170
C	-1.4489082	-0.2446138	0.0000000
C	-0.7512852	-0.2446138	1.2083170
C	0.6439588	-0.2446138	1.2083170
C	1.3415818	-0.2446138	0.0000000
F	-1.4266622	-0.2227768	2.3781050
F	-2.7996622	-0.2227768	0.0000000
F	-1.4266622	-0.2227768	-2.3781050
F	1.3193358	-0.2227768	2.3781050
F	2.6923358	-0.2227768	0.0000000
F	1.3193358	-0.2227768	-2.3781050
Cl	0.6439588	2.8043442	0.0000000

x_3:

Energy = -1283.431743898

C	0.6171272	-0.2446138	-1.2083170
C	-0.7781168	-0.2446138	-1.2083170
C	-1.4757398	-0.2446138	0.0000000
C	-0.7781168	-0.2446138	1.2083170
C	0.6171272	-0.2446138	1.2083170
C	1.3147502	-0.2446138	0.0000000
F	-1.4534938	-0.2227768	2.3781050
F	-2.8264938	-0.2227768	0.0000000
F	-1.4534938	-0.2227768	-2.3781050
F	1.2925042	-0.2227768	2.3781050
F	2.6655042	-0.2227768	0.0000000
F	1.2925042	-0.2227768	-2.3781050

```
Cl    0.9659382    2.8043442    0.0000000
```
x_4:
```
Energy = -1283.431439370
C     0.5902955   -0.2446138   -1.2083170
C    -0.8049485   -0.2446138   -1.2083170
C    -1.5025715   -0.2446138    0.0000000
C    -0.8049485   -0.2446138    1.2083170
C     0.5902955   -0.2446138    1.2083170
C     1.2879185   -0.2446138    0.0000000
F    -1.4803255   -0.2227768    2.3781050
F    -2.8533255   -0.2227768    0.0000000
F    -1.4803255   -0.2227768   -2.3781050
F     1.2656725   -0.2227768    2.3781050
F     2.6386725   -0.2227768    0.0000000
F     1.2656725   -0.2227768   -2.3781050
Cl    1.2879185    2.8043442    0.0000000
```
y_1:
```
Energy = -1283.432077076
C    -1.2315538    0.2446138    0.6976220
C    -1.2315538    0.2446138   -0.6976220
C    -0.0232368    0.2446138   -1.3952450
C     1.1850802    0.2446138   -0.6976220
C     1.1850802    0.2446138    0.6976220
C    -0.0232368    0.2446138    1.3952450
F     2.3548682    0.2227768   -1.3729990
F    -0.0232368    0.2227768   -2.7459990
F    -2.4013418    0.2227768   -1.3729990
F     2.3548682    0.2227768    1.3729990
F    -0.0232368    0.2227768    2.7459990
F    -2.4013418    0.2227768    1.3729990
Cl    0.2788422   -2.8043442    0.0000000
```
y_2:
```
Energy = -1283.431954402
C    -1.2547908    0.2446138    0.6976220
C    -1.2547908    0.2446138   -0.6976220
C    -0.0464738    0.2446138   -1.3952450
C     1.1618432    0.2446138   -0.6976220
C     1.1618432    0.2446138    0.6976220
C    -0.0464738    0.2446138    1.3952450
F     2.3316312    0.2227768   -1.3729990
F    -0.0464738    0.2227768   -2.7459990
F    -2.4245788    0.2227768   -1.3729990
F     2.3316312    0.2227768    1.3729990
F    -0.0464738    0.2227768    2.7459990
F    -2.4245788    0.2227768    1.3729990
Cl    0.5576852   -2.8043442    0.0000000
```
y_3:
```
Energy = -1283.431820937
C    -1.2780276    0.2446138    0.6976220
C    -1.2780276    0.2446138   -0.6976220
C    -0.0697106    0.2446138   -1.3952450
C     1.1386064    0.2446138   -0.6976220
C     1.1386064    0.2446138    0.6976220
C    -0.0697106    0.2446138    1.3952450
F     2.3083944    0.2227768   -1.3729990
F    -0.0697106    0.2227768   -2.7459990
F    -2.4478156    0.2227768   -1.3729990
F     2.3083944    0.2227768    1.3729990
F    -0.0697106    0.2227768    2.7459990
F    -2.4478156    0.2227768    1.3729990
Cl    0.8365274   -2.8043442    0.0000000
```

y_4:

Energy = -1283.431667446

C	-1.3012645	0.2446138	0.6976220
C	-1.3012645	0.2446138	-0.6976220
C	-0.0929475	0.2446138	-1.3952450
C	1.1153695	0.2446138	-0.6976220
C	1.1153695	0.2446138	0.6976220
C	-0.0929475	0.2446138	1.3952450
F	2.2851575	0.2227768	-1.3729990
F	-0.0929475	0.2227768	-2.7459990
F	-2.4710525	0.2227768	-1.3729990
F	2.2851575	0.2227768	1.3729990
F	-0.0929475	0.2227768	2.7459990
F	-2.4710525	0.2227768	1.3729990
Cl	1.1153695	-2.8043442	0.0000000

Y = 0

z_1:

Energy = -1283.434208836

C	-1.2083170	0.6976220	-0.2715369
C	-1.2083170	-0.6976220	-0.2715369
C	0.0000000	-1.3952450	-0.2715369
C	1.2083170	-0.6976220	-0.2715369
C	1.2083170	0.6976220	-0.2715369
C	0.0000000	1.3952450	-0.2715369
F	2.3781050	-1.3729990	-0.2496999
F	0.0000000	-2.7459990	-0.2496999
F	-2.3781050	-1.3729990	-0.2496999
F	2.3781050	1.3729990	-0.2496999
F	0.0000000	2.7459990	-0.2496999
F	-2.3781050	1.3729990	-0.2496999
Cl	0.0000000	0.0000000	3.1274211

z_2:

Energy = -1283.432622854

C	-1.2083170	0.6976220	-0.2984600
C	-1.2083170	-0.6976220	-0.2984600
C	0.0000000	-1.3952450	-0.2984600
C	1.2083170	-0.6976220	-0.2984600
C	1.2083170	0.6976220	-0.2984600
C	0.0000000	1.3952450	-0.2984600
F	2.3781050	-1.3729990	-0.2766230
F	0.0000000	-2.7459990	-0.2766230
F	-2.3781050	-1.3729990	-0.2766230
F	2.3781050	1.3729990	-0.2766230
F	0.0000000	2.7459990	-0.2766230
F	-2.3781050	1.3729990	-0.2766230
Cl	0.0000000	0.0000000	3.4504980

z_3:

Energy = -1283.430312282

C	-1.2083170	0.6976220	-0.3253831
C	-1.2083170	-0.6976220	-0.3253831
C	0.0000000	-1.3952450	-0.3253831
C	1.2083170	-0.6976220	-0.3253831
C	1.2083170	0.6976220	-0.3253831
C	0.0000000	1.3952450	-0.3253831
F	2.3781050	-1.3729990	-0.3035461
F	0.0000000	-2.7459990	-0.3035461
F	-2.3781050	-1.3729990	-0.3035461
F	2.3781050	1.3729990	-0.3035461
F	0.0000000	2.7459990	-0.3035461
F	-2.3781050	1.3729990	-0.3035461

Cl	0.0000000	0.0000000	3.7735749

z_4:

Energy = -1283.428068126

C	-1.2083170	0.6976220	-0.3523062
C	-1.2083170	-0.6976220	-0.3523062
C	0.0000000	-1.3952450	-0.3523062
C	1.2083170	-0.6976220	-0.3523062
C	1.2083170	0.6976220	-0.3523062
C	0.0000000	1.3952450	-0.3523062
F	2.3781050	-1.3729990	-0.3304692
F	0.0000000	-2.7459990	-0.3304692
F	-2.3781050	-1.3729990	-0.3304692
F	2.3781050	1.3729990	-0.3304692
F	0.0000000	2.7459990	-0.3304692
F	-2.3781050	1.3729990	-0.3304692
Cl	0.0000000	0.0000000	4.0966518

xz_1:

Energy = -1283.433797159

C	0.6439588	-0.2715369	-1.2083170
C	-0.7512852	-0.2715369	-1.2083170
C	-1.4489082	-0.2715369	0.0000000
C	-0.7512852	-0.2715369	1.2083170
C	0.6439588	-0.2715369	1.2083170
C	1.3415818	-0.2715369	0.0000000
F	-1.4266622	-0.2496999	2.3781050
F	-2.7996622	-0.2496999	0.0000000
F	-1.4266622	-0.2496999	-2.3781050
F	1.3193358	-0.2496999	2.3781050
F	2.6923358	-0.2496999	0.0000000
F	1.3193358	-0.2496999	-2.3781050
Cl	0.6439588	3.1274211	0.0000000

xz_2:

Energy = -1283.432525807

C	0.6707904	-0.2984600	-1.2083170
C	-0.7244536	-0.2984600	-1.2083170
C	-1.4220766	-0.2984600	0.0000000
C	-0.7244536	-0.2984600	1.2083170
C	0.6707904	-0.2984600	1.2083170
C	1.3684134	-0.2984600	0.0000000
F	-1.3998306	-0.2766230	2.3781050
F	-2.7728306	-0.2766230	0.0000000
F	-1.3998306	-0.2766230	-2.3781050
F	1.3461674	-0.2766230	2.3781050
F	2.7191674	-0.2766230	0.0000000
F	1.3461674	-0.2766230	-2.3781050
Cl	0.3219794	3.4504980	0.0000000

xz_3:

Energy = -1283.429513105

C	0.6171272	-0.3253831	-1.2083170
C	-0.7781168	-0.3253831	-1.2083170
C	-1.4757398	-0.3253831	0.0000000
C	-0.7781168	-0.3253831	1.2083170
C	0.6171272	-0.3253831	1.2083170
C	1.3147502	-0.3253831	0.0000000
F	-1.4534938	-0.3035461	2.3781050
F	-2.8264938	-0.3035461	0.0000000
F	-1.4534938	-0.3035461	-2.3781050
F	1.2925042	-0.3035461	2.3781050
F	2.6655042	-0.3035461	0.0000000
F	1.2925042	-0.3035461	-2.3781050
Cl	0.9659382	3.7735749	0.0000000

xz_4:
Energy = -1283.426849024

C	0.5902955	-0.3523062	-1.2083170
C	-0.8049485	-0.3523062	-1.2083170
C	-1.5025715	-0.3523062	0.0000000
C	-0.8049485	-0.3523062	1.2083170
C	0.5902955	-0.3523062	1.2083170
C	1.2879185	-0.3523062	0.0000000
F	-1.4803255	-0.3304692	2.3781050
F	-2.8533255	-0.3304692	0.0000000
F	-1.4803255	-0.3304692	-2.3781050
F	1.2656725	-0.3304692	2.3781050
F	2.6386725	-0.3304692	0.0000000
F	1.2656725	-0.3304692	-2.3781050
Cl	1.2879185	4.0966518	0.0000000

Trifluorotriazine, Z = 2.94
o:
Energy = -1034.933760665

C	-1.1666259	-0.4811915	-0.2927560
C	1.0000551	-0.7697735	-0.2742160
C	0.1664051	1.2507365	-0.2731060
N	1.2786851	0.5274295	-0.2906460
N	-1.0959479	0.8438505	-0.3114360
N	-0.1824279	-1.3709735	-0.3128460
F	2.0595951	-1.5865135	-0.2859760
F	-2.4033249	-0.9910835	-0.3240260
F	0.3435631	2.5775065	-0.2842460
Cl	0.0000231	0.0000125	2.6492540

x_1:
Energy = -1034.933471558

C	-1.1707854	-0.5124596	-0.2927560
C	0.9958956	-0.8010416	-0.2742160
C	0.1622456	1.2194684	-0.2731060
N	1.2745256	0.4961614	-0.2906460
N	-1.1001074	0.8125824	-0.3114360
N	-0.1865874	-1.4022416	-0.3128460
F	2.0554356	-1.6177816	-0.2859760
F	-2.4074844	-1.0223516	-0.3240260
F	0.3394036	2.5462384	-0.2842460
Cl	0.0374586	0.2814254	2.6492540

x_2:
Energy = -1034.932954925

C	-1.1749450	-0.5437277	-0.2927560
C	0.9917360	-0.8323097	-0.2742160
C	0.1580860	1.1882003	-0.2731060
N	1.2703660	0.4648933	-0.2906460
N	-1.1042670	0.7813143	-0.3114360
N	-0.1907470	-1.4335097	-0.3128460
F	2.0512760	-1.6490497	-0.2859760
F	-2.4116440	-1.0536197	-0.3240260
F	0.3352440	2.5149703	-0.2842460
Cl	0.0748950	0.5628383	2.6492540

x_3:
Energy = -1034.932381922

C	-1.1791046	-0.5749958	-0.2927560
C	0.9875764	-0.8635778	-0.2742160
C	0.1539264	1.1569322	-0.2731060
N	1.2662064	0.4336252	-0.2906460
N	-1.1084266	0.7500462	-0.3114360
N	-0.1949066	-1.4647778	-0.3128460

```
F     2.0471164   -1.6803178   -0.2859760
F    -2.4158036   -1.0848878   -0.3240260
F     0.3310844    2.4837022   -0.2842460
Cl    0.1123314    0.8442512    2.6492540
```

x_4:

```
Energy = -1034.931640821
C    -1.1832641   -0.6062639   -0.2927560
C     0.9834169   -0.8948459   -0.2742160
C     0.1497669    1.1256641   -0.2731060
N     1.2620469    0.4023571   -0.2906460
N    -1.1125861    0.7187781   -0.3114360
N    -0.1990661   -1.4960459   -0.3128460
F     2.0429569   -1.7115859   -0.2859760
F    -2.4199631   -1.1161559   -0.3240260
F     0.3269249    2.4524341   -0.2842460
Cl    0.1497669    1.1256641    2.6492540
```

y_1:

```
Energy = -1034.933427493
C    -1.1951094   -0.4781619   -0.2927560
C     0.9715716   -0.7667439   -0.2742160
C     0.1379216    1.2537661   -0.2731060
N     1.2502016    0.5304591   -0.2906460
N    -1.1244314    0.8468801   -0.3114360
N    -0.2109114   -1.3679439   -0.3128460
F     2.0311116   -1.5834839   -0.2859760
F    -2.4318084   -0.9880539   -0.3240260
F     0.3150796    2.5805361   -0.2842460
Cl    0.2563746   -0.0272539    2.6492540
```

y_2:

```
Energy = -1034.932662394
C    -1.2235930   -0.4751323   -0.2927560
C     0.9430880   -0.7637143   -0.2742160
C     0.1094380    1.2567957   -0.2731060
N     1.2217180    0.5334887   -0.2906460
N    -1.1529150    0.8499097   -0.3114360
N    -0.2393950   -1.3649143   -0.3128460
F     2.0026280   -1.5804543   -0.2859760
F    -2.4602920   -0.9850243   -0.3240260
F     0.2865960    2.5835657   -0.2842460
Cl    0.5127270   -0.0545203    2.6492540
```

y_3:

```
Energy = -1034.931599835
C    -1.2520761   -0.4721026   -0.2927560
C     0.9146049   -0.7606846   -0.2742160
C     0.0809549    1.2598254   -0.2731060
N     1.1932349    0.5365184   -0.2906460
N    -1.1813981    0.8529394   -0.3114360
N    -0.2678781   -1.3618846   -0.3128460
F     1.9741449   -1.5774246   -0.2859760
F    -2.4887751   -0.9819946   -0.3240260
F     0.2581129    2.5865954   -0.2842460
Cl    0.7690749   -0.0817876    2.6492540
```

y_4:

```
Energy = -1034.930389431
C    -1.2805601   -0.4690730   -0.2927560
C     0.8861209   -0.7576550   -0.2742160
C     0.0524709    1.2628550   -0.2731060
N     1.1647509    0.5395480   -0.2906460
N    -1.2098821    0.8559690   -0.3114360
N    -0.2963621   -1.3588550   -0.3128460
F     1.9456609   -1.5743950   -0.2859760
```

F -2.5172591 -0.9789650 -0.3240260
F 0.2296289 2.5896250 -0.2842460
Cl 1.0254309 -0.1090540 2.6492540

xy_1:

Energy = -1034.933213766
C -1.1985923 -0.4943770 -0.2927560
C 0.9680887 -0.7829590 -0.2742160
C 0.1344387 1.2375510 -0.2731060
N 1.2467187 0.5142440 -0.2906460
N -1.1279143 0.8306650 -0.3114360
N -0.2143943 -1.3841590 -0.3128460
F 2.0276287 -1.5996990 -0.2859760
F -2.4352913 -1.0042690 -0.3240260
F 0.3115967 2.5643210 -0.2842460
Cl 0.2877207 0.1186820 2.6492540

xy_2:

Energy = -1034.931784637
C -1.2305588 -0.5075624 -0.2927560
C 0.9361222 -0.7961444 -0.2742160
C 0.1024722 1.2243656 -0.2731060
N 1.2147522 0.5010586 -0.2906460
N -1.1598808 0.8174796 -0.3114360
N -0.2463608 -1.3973444 -0.3128460
F 1.9956622 -1.6128844 -0.2859760
F -2.4672578 -1.0174544 -0.3240260
F 0.2796302 2.5511356 -0.2842460
Cl 0.5754192 0.2373506 2.6492540

xy_3:

Energy = -1034.929750514
C -1.2625251 -0.5207478 -0.2927560
C 0.9041559 -0.8093298 -0.2742160
C 0.0705059 1.2111802 -0.2731060
N 1.1827859 0.4878732 -0.2906460
N -1.1918471 0.8042942 -0.3114360
N -0.2783271 -1.4105298 -0.3128460
F 1.9636959 -1.6260698 -0.2859760
F -2.4992241 -1.0306398 -0.3240260
F 0.2476639 2.5379502 -0.2842460
Cl 0.8631159 0.3560192 2.6492540

xy_4:

Energy = -1034.927632495
C -1.2944921 -0.5339332 -0.2927560
C 0.8721889 -0.8225152 -0.2742160
C 0.0385389 1.1979948 -0.2731060
N 1.1508189 0.4746878 -0.2906460
N -1.2238141 0.7911088 -0.3114360
N -0.3102941 -1.4237152 -0.3128460
F 1.9317289 -1.6392552 -0.2859760
F -2.5311911 -1.0438252 -0.3240260
F 0.2156969 2.5247648 -0.2842460
Cl 1.1508189 0.4746878 2.6492540

Y = 0

z_1:

Energy = -1034.936013320
C -1.1637365 -0.4798534 -0.3277560
C 1.0029445 -0.7684354 -0.3092160
C 0.1692945 1.2520746 -0.3081060
N 1.2815745 0.5287676 -0.3256460
N -1.0930585 0.8451886 -0.3464360
N -0.1795385 -1.3696354 -0.3478460
F 2.0624845 -1.5851754 -0.3209760

F -2.4004355 -0.9897454 -0.3590260
F 0.3464525 2.5788446 -0.3192460
Cl -0.0259815 -0.0120304 2.9642540

z_2:

Energy = -1034.934003808
C -1.1637365 -0.4798534 -0.3627560
C 1.0029445 -0.7684354 -0.3442160
C 0.1692945 1.2520746 -0.3431060
N 1.2815745 0.5287676 -0.3606460
N -1.0930585 0.8451886 -0.3814360
N -0.1795385 -1.3696354 -0.3828460
F 2.0624845 -1.5851754 -0.3559760
F -2.4004355 -0.9897454 -0.3940260
F 0.3464525 2.5788446 -0.3542460
Cl -0.0259815 -0.0120304 3.2792540

z_3:

Energy = -1034.931051946
C -1.1637365 -0.4798534 -0.3977560
C 1.0029445 -0.7684354 -0.3792160
C 0.1692945 1.2520746 -0.3781060
N 1.2815745 0.5287676 -0.3956460
N -1.0930585 0.8451886 -0.4164360
N -0.1795385 -1.3696354 -0.4178460
F 2.0624845 -1.5851754 -0.3909760
F -2.4004355 -0.9897454 -0.4290260
F 0.3464525 2.5788446 -0.3892460
Cl -0.0259815 -0.0120304 3.5942540

z_4:

Energy = -1034.928254998
C -1.1637365 -0.4798534 -0.4327560
C 1.0029445 -0.7684354 -0.4142160
C 0.1692945 1.2520746 -0.4131060
N 1.2815745 0.5287676 -0.4306460
N -1.0930585 0.8451886 -0.4514360
N -0.1795385 -1.3696354 -0.4528460
F 2.0624845 -1.5851754 -0.4259760
F -2.4004355 -0.9897454 -0.4640260
F 0.3464525 2.5788446 -0.4242460
Cl -0.0259815 -0.0120304 3.9092540

xz_1:

Energy = -1034.935143136
C -1.1749450 -0.5437277 -0.3277560
C 0.9917360 -0.8323097 -0.3092160
C 0.1580860 1.1882003 -0.3081060
N 1.2703660 0.4648933 -0.3256460
N -1.1042670 0.7813143 -0.3464360
N -0.1907470 -1.4335097 -0.3478460
F 2.0512760 -1.6490497 -0.3209760
F -2.4116440 -1.0536197 -0.3590260
F 0.3352440 2.5149703 -0.3192460
Cl 0.0748950 0.5628383 2.9642540

xz_2:

Energy = -1034.933803234
C -1.1707854 -0.5124596 -0.3627560
C 0.9958956 -0.8010416 -0.3442160
C 0.1622456 1.2194684 -0.3431060
N 1.2745256 0.4961614 -0.3606460
N -1.1001074 0.8125824 -0.3814360
N -0.1865874 -1.4022416 -0.3828460
F 2.0554356 -1.6177816 -0.3559760
F -2.4074844 -1.0223516 -0.3940260

```
F     0.3394036    2.5462384   -0.3542460
Cl    0.0374586    0.2814254    3.2792540
```
xz_3:
```
Energy = -1034.929822258
C    -1.1791046   -0.5749958   -0.3977560
C     0.9875764   -0.8635778   -0.3792160
C     0.1539264    1.1569322   -0.3781060
N     1.2662064    0.4336252   -0.3956460
N    -1.1084266    0.7500462   -0.4164360
N    -0.1949066   -1.4647778   -0.4178460
F     2.0471164   -1.6803178   -0.3909760
F    -2.4158036   -1.0848878   -0.4290260
F     0.3310844    2.4837022   -0.3892460
Cl    0.1123314    0.8442512    3.5942540
```
xz_4:
```
Energy = -1034.926637105
C    -1.1832641   -0.6062639   -0.4327560
C     0.9834169   -0.8948459   -0.4142160
C     0.1497669    1.1256641   -0.4131060
N     1.2620469    0.4023571   -0.4306460
N    -1.1125861    0.7187781   -0.4514360
N    -0.1990661   -1.4960459   -0.4528460
F     2.0429569   -1.7115859   -0.4259760
F    -2.4199631   -1.1161559   -0.4640260
F     0.3269249    2.4524341   -0.4242460
Cl    0.1497669    1.1256641    3.9092540
```

Benzene, Z = 2.42

o:
```
Energy = -392.4357566834
C    -1.2228780    0.7060290   -0.1727589
C    -1.2228780   -0.7060290   -0.1727589
C     0.0000000   -1.4120570   -0.1727589
C     1.2228780   -0.7060290   -0.1727589
C     1.2228780    0.7060290   -0.1727589
C     0.0000000    1.4120570   -0.1727589
H    -2.1690950    1.2523270   -0.2021049
H    -2.1690950   -1.2523270   -0.2021049
H     0.0000000   -2.5046550   -0.2021049
H     2.1690950   -1.2523270   -0.2021049
H     2.1690950    1.2523270   -0.2021049
H     0.0000000    2.5046550   -0.2021049
Na    0.0000000    0.0000000    2.2491831
```
x_1:
```
Energy = -392.4346312112
C     0.6788741   -0.1727589   -1.2228780
C    -0.7331839   -0.1727589   -1.2228780
C    -1.4392119   -0.1727589    0.0000000
C    -0.7331839   -0.1727589    1.2228780
C     0.6788741   -0.1727589    1.2228780
C     1.3849021   -0.1727589    0.0000000
H     1.2251721   -0.2021049   -2.1690950
H    -1.2794819   -0.2021049   -2.1690950
H    -2.5318099   -0.2021049    0.0000000
H    -1.2794819   -0.2021049    2.1690950
H     1.2251721   -0.2021049    2.1690950
H     2.4775001   -0.2021049    0.0000000
Na    0.3258591    2.2491831    0.0000000
```
x_2:
```
Energy = -392.4317902012
C     0.6517191   -0.1727589   -1.2228780
```

C	-0.7603389	-0.1727589	-1.2228780
C	-1.4663669	-0.1727589	0.0000000
C	-0.7603389	-0.1727589	1.2228780
C	0.6517191	-0.1727589	1.2228780
C	1.3577471	-0.1727589	0.0000000
H	1.1980171	-0.2021049	-2.1690950
H	-1.3066369	-0.2021049	-2.1690950
H	-2.5589649	-0.2021049	0.0000000
H	-1.3066369	-0.2021049	2.1690950
H	1.1980171	-0.2021049	2.1690950
H	2.4503451	-0.2021049	0.0000000
Na	0.6517191	2.2491831	0.0000000

x_3:

Energy = -392.4284803862

C	0.6245642	-0.1727589	-1.2228780
C	-0.7874938	-0.1727589	-1.2228780
C	-1.4935218	-0.1727589	0.0000000
C	-0.7874938	-0.1727589	1.2228780
C	0.6245642	-0.1727589	1.2228780
C	1.3305922	-0.1727589	0.0000000
H	1.1708622	-0.2021049	-2.1690950
H	-1.3337918	-0.2021049	-2.1690950
H	-2.5861198	-0.2021049	0.0000000
H	-1.3337918	-0.2021049	2.1690950
H	1.1708622	-0.2021049	2.1690950
H	2.4231902	-0.2021049	0.0000000
Na	0.9775782	2.2491831	0.0000000

x_4:

Energy = -392.4257786396

C	0.5974092	-0.1727589	-1.2228780
C	-0.8146488	-0.1727589	-1.2228780
C	-1.5206768	-0.1727589	0.0000000
C	-0.8146488	-0.1727589	1.2228780
C	0.5974092	-0.1727589	1.2228780
C	1.3034372	-0.1727589	0.0000000
H	1.1437072	-0.2021049	-2.1690950
H	-1.3609468	-0.2021049	-2.1690950
H	-2.6132748	-0.2021049	0.0000000
H	-1.3609468	-0.2021049	2.1690950
H	1.1437072	-0.2021049	2.1690950
H	2.3960352	-0.2021049	0.0000000
Na	1.3034372	2.2491831	0.0000000

y_1:

Energy = -392.4349036792

C	-1.2463948	0.1727589	0.7060290
C	-1.2463948	0.1727589	-0.7060290
C	-0.0235168	0.1727589	-1.4120570
C	1.1993612	0.1727589	-0.7060290
C	1.1993612	0.1727589	0.7060290
C	-0.0235168	0.1727589	1.4120570
H	-2.1926118	0.2021049	1.2523270
H	-2.1926118	0.2021049	-1.2523270
H	-0.0235168	0.2021049	-2.5046550
H	2.1455782	0.2021049	-1.2523270
H	2.1455782	0.2021049	1.2523270
H	-0.0235168	0.2021049	2.5046550
Na	0.2822022	-2.2491831	0.0000000

y_2:

Energy = -392.4326602048

C	-1.2699118	0.1727589	0.7060290
C	-1.2699118	0.1727589	-0.7060290

```
C    -0.0470338    0.1727589   -1.4120570
C     1.1758442    0.1727589   -0.7060290
C     1.1758442    0.1727589    0.7060290
C    -0.0470338    0.1727589    1.4120570
H    -2.2161288    0.2021049    1.2523270
H    -2.2161288    0.2021049   -1.2523270
H    -0.0470338    0.2021049   -2.5046550
H     2.1220612    0.2021049   -1.2523270
H     2.1220612    0.2021049    1.2523270
H    -0.0470338    0.2021049    2.5046550
Na    0.5644052   -2.2491831    0.0000000
```

y_3:

```
Energy = -392.4298297739
C    -1.2934286    0.1727589    0.7060290
C    -1.2934286    0.1727589   -0.7060290
C    -0.0705506    0.1727589   -1.4120570
C     1.1523274    0.1727589   -0.7060290
C     1.1523274    0.1727589    0.7060290
C    -0.0705506    0.1727589    1.4120570
H    -2.2396456    0.2021049    1.2523270
H    -2.2396456    0.2021049   -1.2523270
H    -0.0705506    0.2021049   -2.5046550
H     2.0985444    0.2021049   -1.2523270
H     2.0985444    0.2021049    1.2523270
H    -0.0705506    0.2021049    2.5046550
Na    0.8466074   -2.2491831    0.0000000
```

y_4:

```
Energy = -392.4272815038
C    -1.3169455    0.1727589    0.7060290
C    -1.3169455    0.1727589   -0.7060290
C    -0.0940675    0.1727589   -1.4120570
C     1.1288105    0.1727589   -0.7060290
C     1.1288105    0.1727589    0.7060290
C    -0.0940675    0.1727589    1.4120570
H    -2.2631625    0.2021049    1.2523270
H    -2.2631625    0.2021049   -1.2523270
H    -0.0940675    0.2021049   -2.5046550
H     2.0750275    0.2021049   -1.2523270
H     2.0750275    0.2021049    1.2523270
H    -0.0940675    0.2021049    2.5046550
Na    1.1288105   -2.2491831    0.0000000
```

Y = 0

z_1:

```
Energy = -392.4330240076
C    -1.2228780    0.7060290   -0.1996820
C    -1.2228780   -0.7060290   -0.1996820
C     0.0000000   -1.4120570   -0.1996820
C     1.2228780   -0.7060290   -0.1996820
C     1.2228780    0.7060290   -0.1996820
C     0.0000000    1.4120570   -0.1996820
H    -2.1690950    1.2523270   -0.2290280
H    -2.1690950   -1.2523270   -0.2290280
H     0.0000000   -2.5046550   -0.2290280
H     2.1690950   -1.2523270   -0.2290280
H     2.1690950    1.2523270   -0.2290280
H     0.0000000    2.5046550   -0.2290280
Na    0.0000000    0.0000000    2.5722600
```

z_2:

```
Energy = -392.4267148630
C    -1.2228780    0.7060290   -0.2266051
```

```
C    -1.2228780   -0.7060290   -0.2266051
C     0.0000000   -1.4120570   -0.2266051
C     1.2228780   -0.7060290   -0.2266051
C     1.2228780    0.7060290   -0.2266051
C     0.0000000    1.4120570   -0.2266051
H    -2.1690950    1.2523270   -0.2559511
H    -2.1690950   -1.2523270   -0.2559511
H     0.0000000   -2.5046550   -0.2559511
H     2.1690950   -1.2523270   -0.2559511
H     2.1690950    1.2523270   -0.2559511
H     0.0000000    2.5046550   -0.2559511
Na    0.0000000    0.0000000    2.8953369
```

z_3:

```
Energy = -392.4204868488
C    -1.2228780    0.7060290   -0.2535282
C    -1.2228780   -0.7060290   -0.2535282
C     0.0000000   -1.4120570   -0.2535282
C     1.2228780   -0.7060290   -0.2535282
C     1.2228780    0.7060290   -0.2535282
C     0.0000000    1.4120570   -0.2535282
H    -2.1690950    1.2523270   -0.2828742
H    -2.1690950   -1.2523270   -0.2828742
H     0.0000000   -2.5046550   -0.2828742
H     2.1690950   -1.2523270   -0.2828742
H     2.1690950    1.2523270   -0.2828742
H     0.0000000    2.5046550   -0.2828742
Na    0.0000000    0.0000000    3.2184138
```

z_4:

```
Energy = -392.4153467729
C    -1.2228780    0.7060290   -0.2804512
C    -1.2228780   -0.7060290   -0.2804512
C     0.0000000   -1.4120570   -0.2804512
C     1.2228780   -0.7060290   -0.2804512
C     1.2228780    0.7060290   -0.2804512
C     0.0000000    1.4120570   -0.2804512
H    -2.1690950    1.2523270   -0.3097972
H    -2.1690950   -1.2523270   -0.3097972
H     0.0000000   -2.5046550   -0.3097972
H     2.1690950   -1.2523270   -0.3097972
H     2.1690950    1.2523270   -0.3097972
H     0.0000000    2.5046550   -0.3097972
Na    0.0000000    0.0000000    3.5414908
```

xz_1:

```
Energy = -392.4312213789
C     0.6517191   -0.1996820   -1.2228780
C    -0.7603389   -0.1996820   -1.2228780
C    -1.4663669   -0.1996820    0.0000000
C    -0.7603389   -0.1996820    1.2228780
C     0.6517191   -0.1996820    1.2228780
C     1.3577471   -0.1996820    0.0000000
H     1.1980171   -0.2290280   -2.1690950
H    -1.3066369   -0.2290280   -2.1690950
H    -2.5589649   -0.2290280    0.0000000
H    -1.3066369   -0.2290280    2.1690950
H     1.1980171   -0.2290280    2.1690950
H     2.4503451   -0.2290280    0.0000000
Na    0.6517191    2.5722600    0.0000000
```

xz_2:

```
Energy = -392.4243821505
C     0.6245642   -0.2266051   -1.2228780
C    -0.7874938   -0.2266051   -1.2228780
```

C	-1.4935218	-0.2266051	0.0000000
C	-0.7874938	-0.2266051	1.2228780
C	0.6245642	-0.2266051	1.2228780
C	1.3305922	-0.2266051	0.0000000
H	1.1708622	-0.2559511	-2.1690950
H	-1.3337918	-0.2559511	-2.1690950
H	-2.5861198	-0.2559511	0.0000000
H	-1.3337918	-0.2559511	2.1690950
H	1.1708622	-0.2559511	2.1690950
H	2.4231902	-0.2559511	0.0000000
Na	0.9775782	2.8953369	0.0000000

xz_3:

Energy = -392.4203087092

C	0.6788741	-0.2535282	-1.2228780
C	-0.7331839	-0.2535282	-1.2228780
C	-1.4392119	-0.2535282	0.0000000
C	-0.7331839	-0.2535282	1.2228780
C	0.6788741	-0.2535282	1.2228780
C	1.3849021	-0.2535282	0.0000000
H	1.2251721	-0.2828742	-2.1690950
H	-1.2794819	-0.2828742	-2.1690950
H	-2.5318099	-0.2828742	0.0000000
H	-1.2794819	-0.2828742	2.1690950
H	1.2251721	-0.2828742	2.1690950
H	2.4775001	-0.2828742	0.0000000
Na	0.3258591	3.2184138	0.0000000

xz_4:

Energy = -392.4130362902

C	0.5974092	-0.2804512	-1.2228780
C	-0.8146488	-0.2804512	-1.2228780
C	-1.5206768	-0.2804512	0.0000000
C	-0.8146488	-0.2804512	1.2228780
C	0.5974092	-0.2804512	1.2228780
C	1.3034372	-0.2804512	0.0000000
H	1.1437072	-0.3097972	-2.1690950
H	-1.3609468	-0.3097972	-2.1690950
H	-2.6132748	-0.3097972	0.0000000
H	-1.3609468	-0.3097972	2.1690950
H	1.1437072	-0.3097972	2.1690950
H	2.3960352	-0.3097972	0.0000000
Na	1.3034372	3.5414908	0.0000000