Coordinates of B3PW91/6-31G(d,p) optimizations and DEDS4 from reference 19:

p-fluorophenol

```
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 0.455756 -0.088640 -0.000261
2 6 0 1.842377 -0.114798 0.000730
3 6 0 2.542474 1.090175 0.000810
4 6 0 1.852656 2.305438 -0.000004
5 6 0 0.454994 2.310084 -0.000959
6 6 0 -0.247084 1.109628 -0.001121
7 1 0 2.362135 -1.066955 0.001378
8 1 0 3.630393 1.079572 0.001444
9 1 0 -0.067280 3.261008 -0.001518
10 1 0 -1.331853 1.094269 -0.001849
11 8 0 2.482999 3.513521 -0.000102
12 1 0 3.436220 3.371841 0.002421
13 9 0 -0.224710 -1.251494 -0.000369
```

```
1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C6H5F1O1|JANE|05-Feb-
2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||p-fluorophenol B3PW
91/6-31G(d,p) opt||0,1|C,0.4557563742,-0.0886398461,-0.0002607753|C,1.
8423767701,-0.1147978163,0.0007301889|C,2.5424742377,1.090175184,0.000
8096595|C,1.852656004,2.3054380438,-0.0000041645|C,0.4549936435,2.3100
837662,-0.0009589588|C,-0.2470837405,1.1096283677,-0.0011209959|H,2.36
2134821,-1.0669550177,0.0013783239|H,3.630392795,1.0795717634,0.001444
1637|H,-0.0672799291,3.2610084908,-0.0015184099|H,-1.3318525175,1.0942
68942,-0.0018487256|O,2.4829985972,3.5135211064,-0.0001021576|H,3.4362
202563,3.3718409666,0.0024211265|F,-0.2247099017,-1.2514936509,-0.0003
689649||Version=EM64W-G16RevC.01|State=1-A|HF=-406.5555822|RMSD=4.131e
-009|RMSF=1.619e-004|Dipole=0.7447894,0.2235331,0.0016539|Quadrupole=6
.0837892,-3.1934395,-2.8903496,-0.7064857,0.0122214,0.0053416|PG=C01 [
X(C6H5F1O1)]||@
```

p-nitrophenol

```
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 -1.387889 -0.006673 -0.000017
2 6 0 -0.698521 -1.215856 0.000042
3 6 0 0.688348 -1.202901 0.000155
4 6 0 1.377070 0.017544 0.000210
5 6 0 0.668844 1.227162 0.000146
6 6 0 -0.715350 1.215295 0.000028
7 1 0 -1.256937 -2.144230 -0.000002
8 1 0 1.239367 -2.140524 0.000201
9 1 0 1.223785 2.159000 0.000192
10 1 0 -1.289185 2.134235 -0.000024
11 8 0 2.726269 0.093409 0.000317
12 1 0 3.101488 -0.795260 0.000432
13 7 0 -2.845489 -0.019573 -0.000148
14 8 0 -3.425422 1.061471 -0.000062
15 8 0 -3.406745 -1.110851 -0.000039
```

```
1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C6H5N1O3|JANE|05-Feb-
2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||p-nitrophenol B3PW9
1/6-31G(d,p) opt||0,1|C,-1.3878891535,-0.0066725387,-0.0000166014|C,-0
.6985214461,-1.2158559047,0.0000415617|C,0.6883481009,-1.2029007982,0.
0001553522|C,1.3770703314,0.0175441836,0.0002100989|C,0.668843542,1.22
71623589,0.0001459803|C,-0.7153498886,1.2152951522,0.0000283081|H,-1.2
569369157,-2.1442296324,-0.0000023276|H,1.2393665471,-2.1405241059,0.0
002007737|H,1.2237846069,2.159000214,0.0001916722|H,-1.2891850786,2.13
42348943,-0.0000236652|O,2.7262686444,0.0934093311,0.0003169665|H,3.10
14877914,-0.795260209,0.0004319611|N,-2.8454893708,-0.0195728477,-0.00
01477575|O,-3.4254220314,1.0614705119,-0.0000620122|O,-3.4067445295,-1
.1108510993,-0.0000386408||Version=EM64W-G16RevC.01|State=1-A|HF=-511.
7874798|RMSD=8.666e-009|RMSF=4.296e-005|Dipole=2.0399048,-0.5223219,0.
0000824|Quadrupole=-3.8759701,4.306167,-0.4301969,-4.5198163,0.000881,
-0.0004339|PG=C01 [X(C6H5N1O3)]||@
```

anthracene

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-6.199447	-0.542799	-0.014381
2	6	0	-4.831229	-0.542476	-0.009470
3	6	0	-4.097771	0.681959	-0.010199
4	6	0	-4.828481	1.924957	-0.016164
5	6	0	-6.255056	1.879574	-0.021145
6	6	0	-6.920761	0.684216	-0.020302
7	6	0	-2.699644	0.714392	-0.005325
8	6	0	-4.120173	3.130832	-0.016906
9	6	0	-2.722046	3.163266	-0.012030
10	6	0	-1.991335	1.920267	-0.006083
11	6	0	-0.564760	1.965648	-0.001155
12	1	0	-0.015569	1.027321	0.003304
13	6	0	0.100945	3.161005	-0.002053
14	6	0	-0.620369	4.388022	-0.007897
15	6	0	-1.988586	4.387700	-0.012733
16	1	0	-2.148209	-0.223636	-0.000810
17	1	0	-6.744540	-1.482484	-0.013797
18	1	0	-4.278449	-1.478693	-0.004934
19	1	0	-6.804246	2.817902	-0.025640
20	1	0	-8.006923	0.664945	-0.024153
21	1	0	-4.671599	4.068865	-0.021392
22	1	0	1.187108	3.180279	0.001725
23	1	0	-0.075280	5.327709	-0.008517
24	1	0	-2.541363	5.323919	-0.017201

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C14H10|JANE|05-Feb-20
24|0||# opt b3pw91/6-31g(d,p) geom=connectivity||anthracene||0,1|C,-6.
199446531,-0.5427992137,-0.0143812788|C,-4.8312291268,-0.5424756053,-0
.0094696552|C,-4.0977709615,0.6819587442,-0.010199227|C,-4.8284809597,
1.9249571677,-0.0161642158|C,-6.2550560772,1.8795744191,-0.021144678|C
,-6.9207606972,0.6842163365,-0.0203018913|C,-2.6996438482,0.7143922826
,-0.0053254921|C,-4.1201726003,3.1308321676,-0.0169058695|C,-2.7220455
734,3.1632661886,-0.0120303791|C,-1.9913354119,1.920267227,-0.00608271
23|C,-0.5647602495,1.9656482587,-0.0011553047|H,-0.0155689471,1.027321
3743,0.0033044968|C,0.1009451938,3.1610053205,-0.0020534872|C,-0.62036
86332,4.3880216804,-0.0078965497|C,-1.9885860618,4.3877000097,-0.01273
32614|H,-2.1482093173,-0.2236356202,-0.0008102433|H,-6.7445397917,-1.4
824840271,-0.013797235|H,-4.2784493466,-1.4786927727,-0.0049341081|H,-
6.8042460005,2.817901811,-0.0256397918|H,-8.0069230957,0.6649452765,-0
.0241532004|H,-4.6715988133,4.0688650596,-0.0213916057|H,1.1871076552,
3.1802794025,0.0017249532|H,-0.0752796531,5.3277090271,-0.0085166669|H
,-2.5413626718,5.3239193252,-0.0172005968||Version=EM64W-G16RevC.01|St
ate=1-A|HF=-539.3392264|RMSD=6.611e-009|RMSF=1.717e-005|Dipole=-0.0000
015,0.0000056,-0.0000104|Quadrupole=4.3525847,4.0518984,-8.4044831,0.2
702468,0.0446099,-0.0327321|PG=C01 [X(C14H10)]||@

o-bromophenol

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-1.413424	-0.007730	-0.000078
2	6	0	-0.707715	-1.207321	-0.000033
3	6	0	0.681881	-1.182896	0.000095
4	6	0	1.396888	0.022050	0.000186
5	6	0	0.672954	1.219075	0.000158
6	6	0	-0.716039	1.201124	0.000019
7	1	0	-1.225077	-2.160810	-0.000099
8	1	0	1.230028	2.150376	0.000247
9	1	0	-1.259254	2.141558	-0.000002
10	8	0	2.744605	0.086182	0.000275
11	1	0	3.091850	-0.820021	0.000476
12	35	0	1.672435	-2.809443	0.000194
13	1	0	-2.498604	-0.020986	-0.000188

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C6H5Br1O1|JANE|05-Feb
-2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||o-bromophenol B3PW
91/6-31G(d,p) opt||0,1|C,-1.4134244663,-0.0077295835,-0.0000780611|C,-
0.7077149011,-1.2073214611,-0.0000332438|C,0.6818807477,-1.182896174,0

.0000950241|C,1.396888405,0.0220503377,0.0001862825|C,0.672953717,1.21
9074813,0.0001584871|C,-0.7160394897,1.2011239219,0.0000193962|H,-1.22
50765189,-2.1608097843,-0.0000988961|H,1.2300281814,2.1503759132,0.000
246767|H,-1.2592540233,2.1415577831,-0.0000017462|O,2.744605077,0.0861
815033,0.0002747149|H,3.091849695,-0.8200213354,0.0004762324|Br,1.6724
354148,-2.8094431489,0.0001944538|H,-2.4986040887,-0.0209856749,-0.000
1876708||Version=EM64W-G16RevC.01|State=1-A|HF=-2878.45404|RMSD=9.481e
-009|RMSF=8.124e-005|Dipole=-0.3557113,0.0047397,0.0000806|Quadrupole=
2.654957,1.1505717,-3.8055287,-2.4158586,0.0011369,0.0000098|PG=C01 [X
(C6H5Br1O1)]||@

o-nitrophenol

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.167977	-1.441288	-0.000257
2	6	0	-0.787780	-1.439764	-0.000124
3	6	0	-0.090180	-0.224326	0.000116
4	6	0	-0.772028	1.016830	0.000155
5	6	0	-2.176847	0.986374	0.000075
6	6	0	-2.856854	-0.217673	-0.000133
7	1	0	-0.211998	-2.357787	-0.000139
8	1	0	-2.698943	1.937124	0.000115
9	1	0	-3.943156	-0.211810	-0.000227
10	8	0	-0.164960	2.199883	0.000159
11	1	0	0.804499	2.005811	-0.000206
12	1	0	-2.711978	-2.379542	-0.000418
13	7	0	1.349460	-0.268244	0.000435
14	8	0	1.969936	0.815523	0.000735
15	8	0	1.915753	-1.348484	-0.000711

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C6H5N1O3|JANE|05-Feb-
2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||o-nitrophenol B3PW9
1/6-31G(d,p) opt||0,1|C,-2.1679769855,-1.4412879182,-0.0002566224|C,-0
.7877800797,-1.4397638567,-0.0001236507|C,-0.0901804955,-0.2243258337,
0.0001156568|C,-0.7720279888,1.0168297153,0.0001545475|C,-2.1768466463
,0.9863736249,0.0000752941|C,-2.8568543876,-0.2176727448,-0.0001329243
|H,-0.211997943,-2.3577866852,-0.0001394694|H,-2.698942916,1.937124125
2,0.0001150321|H,-3.9431564457,-0.211810424,-0.000227215|O,-0.16495950
53,2.1998827194,0.0001594244|H,0.8044989076,2.0058110278,-0.0002063983
|H,-2.7119780012,-2.3795423687,-0.0004180912|N,1.3494598961,-0.2682441
792,0.0004353463|O,1.9699362257,0.8155227558,0.000734937|O,1.915753035
1,-1.3484840278,-0.0007107668||Version=EM64W-G16RevC.01|State=1-A|HF=-
511.7947711|RMSD=6.094e-009|RMSF=8.017e-005|Dipole=-1.377976,-0.265321
5,-0.0000553|Quadrupole=-0.0874749,0.6774722,-0.5899973,2.2335103,0.00
07199,-0.0026285|PG=C01 [X(C6H5N1O3)]||@

biphenyl

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	-2.805345	0.545158	0.402145
2	6	0	-1.413367	0.545746	0.403286
3	6	0	-0.692781	1.679749	0.000302
4	6	0	-1.413077	2.813749	-0.403510
5	6	0	-2.804979	2.814262	-0.403599
6	6	0	-3.507584	1.679689	-0.000984
7	1	0	-3.343062	-0.341676	0.726366
8	1	0	-0.874729	-0.333614	0.745643
9	1	0	-0.874067	3.692997	-0.745564
10	1	0	-3.342473	3.701022	-0.728395
11	1	0	-4.593899	1.679686	-0.001417
12	6	0	0.789128	1.679820	0.000839
13	6	0	1.509315	2.814428	0.403134
14	6	0	1.509822	0.545348	-0.400625
15	6	0	2.901217	2.815075	0.403222
16	1	0	0.970221	3.694081	0.744015
17	6	0	2.901801	0.544894	-0.399485
18	1	0	0.971269	-0.334522	-0.741804
19	6	0	3.603931	1.680032	0.002124
20	1	0	3.438626	3.702319	0.726834

```
21 1 0 3.439602 -0.342322 -0.722518
22 1 0 4.690246 1.680134 0.002559
```

```
1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C12H10|JANE|05-Feb-20
24|0||# opt b3pw91/6-31g(d,p) geom=connectivity||biphenyl B3PW91/6-31G
(d,p)||0,1|C,-2.8053452139,0.5451576232,0.4021448482|C,-1.4133668983,0
.545746499,0.4032863674|C,-0.6927810189,1.6797487883,0.0003017028|C,-1
.413076743,2.813748659,-0.4035098019|C,-2.8049790796,2.8142623882,-0.4
035991866|C,-3.5075844716,1.6796893622,-0.0009844864|H,-3.3430622926,-
0.3416763461,0.7263656098|H,-0.8747287713,-0.3336141759,0.7456428075|H
,-0.8740672551,3.6929973804,-0.7455642994|H,-3.3424734031,3.7010218465
,-0.7283949831|H,-4.5938990477,1.6796862191,-0.0014173666|C,0.78912750
85,1.6798204089,0.0008389655|C,1.5093146806,2.8144280742,0.4031342026|
C,1.5098220914,0.545347879,-0.4006247125|C,2.9012167507,2.8150750795,0
.4032220716|H,0.970221495,3.6940812267,0.7440147142|C,2.9018005871,0.5
448940921,-0.3994845066|H,0.9712686282,-0.3345218286,-0.7418043066|C,3
.6039310723,1.6800320468,0.0021243301|H,3.4386261931,3.7023188685,0.72
68336345|H,3.4396017348,-0.3423223336,-0.7225175275|H,4.6902456837,1.6
801339625,0.0025585729||Version=EM64W-G16RevC.01|State=1-A|HF=-463.143
1495|RMSD=5.310e-009|RMSF=1.656e-005|Dipole=0.0000001,-0.0000489,0.000
0016|Quadrupole=3.7493705,2.3244123,-6.0737828,0.0000683,0.0043225,-0.
0056138|PG=C01 [X(C12H10)]||@
```

planar biphenyl (single-point)

```
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 -2.853461 -1.134284 -0.403067
2 6 0 -1.461483 -1.134281 -0.402361
3 6 0 -0.740954 -0.000043 0.000062
4 6 0 -1.461308 1.134440 0.402413
5 6 0 -2.853210 1.134628 0.403219
6 6 0 -3.555758 0.000184 0.000141
7 1 0 -3.391130 -2.027020 -0.710750
8 1 0 -0.922787 -2.032453 -0.691684
9 1 0 -0.922356 2.032541 0.691472
10 1 0 -3.390754 2.027463 0.710834
11 1 0 -4.642073 0.000246 0.000234
12 6 0 0.740954 -0.000042 -0.000063
13 6 0 1.461376 1.134262 0.402669
14 6 0 1.461415 -1.134280 -0.402608
15 6 0 2.853278 1.134842 0.402136
16 1 0 0.922477 2.013712 0.744379
17 6 0 2.853394 -1.134801 -0.402090
18 1 0 0.922667 -2.013896 -0.744135
19 6 0 3.555758 0.000034 -0.000035
20 1 0 3.390875 2.021844 0.726101
21 1 0 3.391008 -2.021827 -0.725957
22 1 0 4.642073 0.000084 -0.000087
```

```
1|1|UNPC-LAPTOP-15J01059|SP|RB3PW91|6-31G(d,p)|C12H10|JANE|06-Feb-2024
|0||# b3pw91/6-31g(d,p) geom=connectivity||bplanar iphenyl B3PW91/6-31
G(d,p) sp||0,1|C,0,-2.85346142,-1.13428431,-0.40306725|C,0,-1.46148259
,-1.13428098,-0.40236139|C,0,-0.7409544,-0.00004256,0.00006184|C,0,-1.
46130812,1.13443968,0.40241269|C,0,-2.85321041,1.13462814,0.40321873|C
,0,-3.55575833,0.00018372,0.00014127|H,0,-3.39112951,-2.02702048,-0.71
074985|H,0,-0.92278698,-2.03245338,-0.69168422|H,0,-0.92235603,2.03254
11,0.69147234|H,0,-3.39075395,2.02746337,0.71083401|H,0,-4.64207307,0.
00024635,0.00023368|C,0,0.74095433,-0.00004215,-0.00006307|C,0,1.46137
583,1.13426171,0.40266943|C,0,1.46141492,-1.13428033,-0.4026078|C,0,2.
85327793,1.13484211,0.40213574|H,0,0.9224773,2.01371241,0.74437936|C,0
,2.85339387,-1.13480143,-0.40208993|H,0,0.92266669,-2.01389585,-0.7441
3539|C,0,3.5557584,0.00003405,-0.00003541|H,0,3.39087464,2.02184352,0.
72610075|H,0,3.39100797,-2.02182728,-0.72595686|H,0,4.64207318,0.00008
373,-0.00008654||Version=EM64W-G16RevC.01|State=1-A|HF=-463.1384623|RM
SD=4.928e-009|Dipole=0.,-0.0000212,-0.0000058|Quadrupole=3.8075263,2.3
751879,-6.1827141,-0.0000149,0.0000264,3.4742652|PG=C01 [X(C12H10)]||@
```

phenanthrene

```
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 -5.069292 -3.151111 -0.004037
2 6 0 -3.690562 -3.141427 -0.005116
3 6 0 -2.969927 -1.926926 -0.003697
4 6 0 -3.674884 -0.689696 -0.001052
5 6 0 -5.086413 -0.733474 -0.000059
6 6 0 -5.770317 -1.933311 -0.001509
7 6 0 -1.537333 -1.928829 -0.004943
8 6 0 -2.921126 0.554074 0.000473
9 6 0 -1.498116 0.501707 -0.000925
10 6 0 -0.833460 -0.767369 -0.003668
11 6 0 -0.754979 1.702574 0.000469
12 1 0 0.330666 1.641912 -0.000653
13 6 0 -1.384436 2.929261 0.003209
14 6 0 -2.788408 2.987135 0.004672
15 6 0 -3.535540 1.825618 0.003333
16 1 0 -1.023063 -2.886648 -0.006963
17 1 0 -5.611580 -4.092255 -0.005148
18 1 0 -3.134379 -4.075752 -0.007112
19 1 0 -5.656341 0.189513 0.001824
20 1 0 -6.856680 -1.933713 -0.000708
21 1 0 0.253616 -0.780001 -0.004691
22 1 0 -0.801096 3.845527 0.004259
23 1 0 -3.290787 3.950356 0.006889
24 1 0 -4.617497 1.903700 0.004578
```


```
1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C14H10|JANE|06-Feb-20
24|0||# opt b3pw91/6-31g(d,p) geom=connectivity||phenanthrene B3PW91/6
-31G(d,p) opt||0,1|C,-5.0692920503,-3.15111136,-0.0040369081|C,-3.6905
62155,-3.141427245,-0.0051155585|C,-2.9699270594,-1.9269261021,-0.0036
968004|C,-3.6748842624,-0.689695941,-0.0010519459|C,-5.0864125784,-0.7
334743986,-0.0000589792|C,-5.7703172944,-1.9333113055,-0.0015090404|C,
-1.5373333514,-1.92882944,-0.0049432235|C,-2.9211263333,0.5540743912,0
.0004727255|C,-1.498116398,0.5017070446,-0.0009249086|C,-0.8334599475,
-0.7673687914,-0.003668379|C,-0.754979343,1.7025743422,0.0004689794|H,
0.3306656416,1.6419123936,-0.0006531491|C,-1.3844362022,2.9292614337,0
.0032085739|C,-2.7884076857,2.987134842,0.0046716902|C,-3.5355403125,1
.8256181134,0.003333331|H,-1.0230634821,-2.8866480351,-0.0069632232|H,
-5.6115804249,-4.0922550502,-0.0051476749|H,-3.1343786886,-4.075751729
6,-0.0071121243|H,-5.6563409582,0.1895132552,0.0018242257|H,-6.8566800
266,-1.9337130385,-0.0007082202|H,0.2536156754,-0.7800014414,-0.004690
5139|H,-0.8010955746,3.8455268355,0.0042589061|H,-3.2907866959,3.95035
58487,0.0068891923|H,-4.6174967727,1.9036995784,0.0045780025||Version=E
M64W-G16RevC.01|State=1-A|HF=-539.3476309|RMSD=6.323e-009|RMSF=6.793e-
005|Dipole=-0.0101269,0.0061367,0.0000207|Quadrupole=4.1223142,4.30340
03,-8.4257145,0.1734838,-0.0104866,0.0216841|PG=C01 [X(C14H10)]||@
```


trinitromethane

```
---------------------------------------------------------------------
Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
---------------------------------------------------------------------
1 6 0 0.000098 -0.000077 0.139599
2 7 0 -0.714428 1.232954 -0.362881
3 8 0 -1.740746 1.476935 0.240610
4 8 0 -0.223765 1.826132 -1.298766
5 7 0 1.425026 0.002479 -0.363347
6 8 0 2.149569 0.769110 0.240317
7 8 0 1.693183 -0.718421 -1.299769
8 7 0 -0.710399 -1.235232 -0.363525
9 8 0 -1.468735 -1.106782 -1.299988
10 8 0 -0.409394 -2.246108 0.240319
11 1 0 0.000146 -0.000369 1.226164
```


```
1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C1H1N3O6|JANE|06-Feb-
2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||trinitromethane B3P
W91/6-31G(d,p) opt||0,1|C,0.0000975319,-0.0000769686,0.1395992869|N,-0
.7144276768,1.2329537249,-0.3628806942|O,-1.7407464801,1.4769346572,0.
2406096706|O,-0.2237646703,1.826131736,-1.2987662737|N,1.4250264692,0.
0024788842,-0.363346521|O,2.1495686875,0.7691097465,0.2403172214|O,1.6
```

931832945,-0.7184207108,-1.2997689158|N,-0.7103993527,-1.2352317121,-0
.3635254488|O,-1.4687351936,-1.1067819873,-1.2999875465|O,-0.409393674
3,-2.2461080038,0.2403188646|H,0.0001456845,-0.0003687461,1.2261643064
||Version=EM64W-G16RevC.01|State=1-A|HF=-653.7143575|RMSD=6.593e-009|R
MSF=2.224e-005|Dipole=0.0001552,-0.0002174,0.8825976|Quadrupole=-1.788
414,-1.789364,3.577778,-0.0021606,0.0010204,-0.0005231|PG=C01 [X(C1H1N
3O6)]||@

chlorotrinitromethane

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

---

1 6 0 0.000105 -0.000105 0.228310
2 7 0 -0.739272 1.231455 -0.355942
3 8 0 -1.775939 1.520404 0.193171
4 8 0 -0.208265 1.751636 -1.312265
5 7 0 1.436130 0.024532 -0.356491
6 8 0 2.205192 0.776982 0.193109
7 8 0 1.620244 -0.693906 -1.314121
8 7 0 -0.696849 -1.255972 -0.356306
9 8 0 -1.411466 -1.056008 -1.313618
10 8 0 -0.429830 -2.298289 0.193243
11 17 0 0.000374 -0.000248 1.941608

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C1Cl1N3O6|JANE|06-Feb
-2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||chlorotrinitrometh
ane B3PW91/6-31G(d,p) opt||0,1|C,0.0001051744,-0.0001046143,0.22831023
69|N,-0.7392724235,1.2314554932,-0.355941951|O,-1.7759391957,1.5204040
202,0.1931713365|O,-0.2082652063,1.751636358,-1.3122648907|N,1.4361296
83,0.0245322129,-0.3564908927|O,2.2051921219,0.7769824891,0.1931089644
|O,1.6202435271,-0.693905845,-1.3141210762|N,-0.6968490758,-1.25597191
3,-0.3563059723|O,-1.4114657381,-1.056008193,-1.3136183271|O,-0.429829
7488,-2.2982890919,0.1932430003|Cl,0.0003738817,-0.0002479162,1.941607
572||Version=EM64W-G16RevC.01|State=1-A|HF=-1113.2379193|RMSD=9.940e-0
09|RMSF=7.934e-005|Dipole=0.0001629,-0.0002837,0.8492347|Quadrupole=-1
.3685207,-1.368263,2.7367838,-0.002239,0.0011554,0.0006077|PG=C01 [X(C
1Cl1N3O6)]||@

$ClH_2SiCH_2NH_2$

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

---

1 6 0 -0.367594 -0.262864 0.048070
2 1 0 -2.713433 -0.811012 -1.338906
3 1 0 -2.808093 -1.068822 1.080480
4 1 0 0.009393 0.139627 -0.898496
5 1 0 0.033575 0.379622 0.847169
6 1 0 0.935631 -1.855934 -0.150690
7 1 0 -0.119400 -2.021439 1.084453
8 17 0 -3.021381 1.663623 0.140683
9 14 0 -2.251889 -0.267654 -0.040103
10 7 0 -0.024084 -1.686858 0.131822

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C1H6Cl1N1Si1|JANE|23-
Nov-2023|0||# opt b3pw91/6-31g(d,p) geom=connectivity||ClH2Si-CH2-NH2
B3PW91/6-31G(d,p) opt||0,1|C,-0.3675935064,-0.2628639185,0.0480695573|
H,-2.7134333663,-0.8110122013,-1.3389058512|H,-2.8080927974,-1.0688218
866,1.0804799449|H,0.0093930413,0.1396267738,-0.8984961471|H,0.0335745
852,0.3796224702,0.8471688078|H,0.9356310949,-1.8559338274,-0.15068973
02|H,-0.1194002995,-2.0214392126,1.0844525939|Cl,-3.0213805457,1.66362
29256,0.1406828933|Si,-2.2518891968,-0.2676539743,-0.0401028926|N,-0.0
240844593,-1.686858419,0.131821824||Version=EM64W-G16RevC.01|State=1-A
|HF=-846.0699657|RMSD=2.821e-009|RMSF=3.793e-005|Dipole=1.0782183,-0.5
731653,0.2476687|Quadrupole=2.6561649,-2.9200987,0.2639338,-0.2566501,
0.7008497,-1.8428722|PG=C01 [X(C1H6Cl1N1Si1)]||@

$ClH_2SiCH_2CH_2NH_2$

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

---

1 6 0 -0.784317 1.024483 -0.124762
2 1 0 -0.014083 -1.171145 1.457102
3 1 0 0.239422 -1.504920 -0.974713
4 6 0 -2.198505 0.646438 0.310988
5 1 0 -0.384135 1.878416 0.430347
6 1 0 -0.752681 1.293453 -1.188179
7 1 0 -2.252901 0.656510 1.405088
8 1 0 -2.956018 1.357409 -0.054891
9 1 0 -3.200734 -1.171405 0.356828
10 1 0 -2.609632 -0.782643 -1.117100
11 17 0 2.265358 0.088015 0.241836
12 7 0 -2.416931 -0.738863 -0.120684
13 14 0 0.253150 -0.535836 0.144837

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C2H8Cl1N1Si1|JANE|24-Nov-2023|0||# opt b3pw91/6-31g(d,p) geom=connectivity||ClH2SiCH2CH2NH2||0,1|C,-0.7843165117,1.0244830315,-0.124762224|H,-0.0140826971,-1.1711446435,1.4571017531|H,0.2394221331,-1.5049202173,-0.9747132135|C,-2.1985046859,0.6464378381,0.3109876143|H,-0.384134535,1.8784164242,0.4303468707|H,-0.7526806585,1.2934530788,-1.1881793412|H,-2.2529011414,0.6565098792,1.4050883495|H,-2.9560179975,1.3574092754,-0.0548909852|H,-3.2007339771,-1.1714054824,0.3568276233|H,-2.6096320585,-0.7826431445,-1.1170995407|Cl,2.2653580848,0.0880152413,0.2418360017|N,-2.4169308358,-0.7388626282,-0.1206837854|Si,0.2531498707,-0.5358359825,0.1448374475||Version=EM64W-G16RevC.01|State=1-A|HF=-885.3813576|RMSD=8.481e-009|RMSF=2.754e-005|Dipole=-1.9705907,0.1345676,-0.2308832|Quadrupole=0.3106985,-0.736282,0.4255835,0.632333,0.4658478,0.2383929|PG=C01 [X(C2H8Cl1N1Si1)]||@

$ClH_2SiCH_2CH_2CH_2NH_2$

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

---

1 6 0 2.088581 0.675607 -0.001864
2 6 0 0.580376 0.768799 0.240922
3 1 0 2.650282 1.319818 0.684932
4 1 0 2.326609 1.024625 -1.016064
5 1 0 0.361730 0.756233 1.316869
6 1 0 0.175840 1.716083 -0.129723
7 1 0 -0.428737 -0.784819 -2.004824
8 1 0 -0.635150 -1.875626 0.250571
9 17 0 -2.427090 0.204929 -0.286571
10 14 0 -0.455342 -0.627321 -0.529716
11 6 0 2.555395 -0.768286 0.140978
12 1 0 3.630490 -0.873458 -0.058084
13 1 0 2.373862 -1.117933 1.163685
14 7 0 1.724736 -1.580153 -0.757922
15 1 0 2.035250 -1.484352 -1.720992
16 1 0 1.757631 -2.568219 -0.526785

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C3H10Cl1N1Si1|JANE|06-Feb-2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||ClH2SiCH2CH2CH2NH2 B3PW91/6-31G(d,p) opt||0,1|C,2.088580978,0.6756067581,-0.0018637194|C,0.5803756652,0.7687992357,0.2409221055|H,2.6502818066,1.3198177172,0.6849316444|H,2.3266094114,1.0246252985,-1.0160644635|H,0.3617296113,0.7562330372,1.3168693067|H,0.1758400528,1.7160830641,-0.1297233076|H,-0.4287368073,-0.7848188173,-2.0048242834|H,-0.635149674,-1.8756257192,0.2505709576|Cl,-2.4270898967,0.2049291665,-0.2865705895|Si,-0.4553418892,-0.627321316,-0.5297156389|C,2.5553950788,-0.7682858541,0.1409780356|H,3.6304901177,-0.8734584907,-0.0580841361|H,2.3738623453,-1.1179325933,1.1636848689|N,1.7247358455,-1.5801530737,-0.7579217931|H,2.0352498823,-1.4843515456,-1.7209916509|H,1.7576314221,-2.5682187775,-0.5267848261||Version=EM64W-G16RevC.01|State=1-A|HF=-924.6905238|RMSD=5.752e-009|RMSF=4.774e-005|Dipole=2.6088096,-0.728307,-0.1129473|Quadrupole=-3.9258898,2.7900539,1.1358359,-1.3768561,-1.0538063,0.9052705|PG=C01 [X(C3H10Cl1N1Si1)]||@

$ClH_2SiCH_2CH_2CH_2CH_2NH_2$

Center Number	Atomic Number	Atomic Type	X	Y	Z
1	6	0	1.700310	1.160119	-0.401225
2	6	0	0.408315	0.987051	0.414739
3	1	0	2.062884	2.188428	-0.275415
4	1	0	1.482108	1.050587	-1.472105
5	1	0	0.640375	1.023018	1.488984
6	1	0	-0.256835	1.834835	0.223397
7	1	0	-0.329637	-1.292835	-1.205827
8	1	0	-1.015138	-1.419592	1.230751
9	17	0	-2.537639	0.230695	-0.416737
10	14	0	-0.596691	-0.587711	0.074206
11	6	0	2.842507	0.212211	-0.026063
12	1	0	3.736655	0.470372	-0.606049
13	1	0	3.113726	0.362255	1.029813
14	6	0	2.541206	-1.262666	-0.257589
15	1	0	2.255049	-1.424286	-1.303676
16	1	0	3.438863	-1.868350	-0.067078
17	7	0	1.405190	-1.693861	0.572368
18	1	0	1.212718	-2.682643	0.432082
19	1	0	1.628703	-1.580430	1.559228

1|1|UNPC-LAPTOP-15J01059|FOpt|RB3PW91|6-31G(d,p)|C4H12Cl1N1Si1|JANE|07-Feb-2024|0||# opt b3pw91/6-31g(d,p) geom=connectivity||ClH2SiCH2CH2CH2CH2NH2 B3PW91/6-31G(d,p) opt||0,1|C,1.7003102906,1.160119071,-0.4012254505|C,0.4083152346,0.9870511055,0.4147385238|H,2.062884218,2.1884282245,-0.2754150343|H,1.4821075895,1.0505874224,-1.4721051342|H,0.6403753767,1.0230184877,1.4889839859|H,-0.2568350159,1.8348353155,0.2233972412|H,-0.3296370984,-1.2928354868,-1.2058272146|H,-1.0151384534,-1.4195915921,1.2307509729|Cl,-2.5376387248,0.230694535,-0.4167366538|Si,-0.5966908217,-0.5877114965,0.074205555|C,2.8425068238,0.2122111371,-0.0260630838|H,3.7366547639,0.4703721113,-0.6060488739|H,3.1137258741,0.3622551071,1.029812697|C,2.5412057577,-1.2626664728,-0.2575892077|H,2.2550494992,-1.4242856996,-1.3036763021|H,3.4388625392,-1.8683504025,-0.067078202|N,1.4051899422,-1.6938606665,0.5723682157|H,1.2127175608,-2.6826430666,0.4320823302|H,1.6287031139,-1.5804300737,1.5592277252||Version=EM64W-G16RevC.01|State=1-A|HF=-963.9896863|RMSD=7.681e-009|RMSF=1.253e-005|Dipole=2.6077466,-0.8477025,0.6046378|Quadrupole=-6.2429803,4.621625,1.6213553,-1.0133507,-0.471858,-1.0371057|PG=C01 [X(C4H12Cl1N1Si1)]||@

DEDS4 coordinates from reference 19

DEDS Conf. 4: staple 2: opt with fixed dihedrals (-25,90,-60)

mp2/6-31++g(d,p)

S	0.86207700	-1.05342000	-0.55228700
S	-0.79357200	-0.97370300	0.66355000
C	2.03306800	0.30355800	-0.11440400
H	2.50203900	0.54387900	-1.06967500
H	2.79281300	-0.14664700	0.52498500
C	-2.01395500	0.10066300	-0.16941200
H	-2.85616700	0.06053000	0.52641500
H	-2.32779400	-0.39798500	-1.08804400
C	1.50808000	1.56071700	0.55335600
H	2.35975300	2.15022500	0.89544000
H	0.92758000	2.17411800	-0.12755800
H	0.89380800	1.32198900	1.42024800
C	-1.64309700	1.53874900	-0.46876000
H	-2.50799900	2.04083400	-0.90560600
H	-1.35271200	2.07686400	0.43113500
H	-0.83197400	1.58804200	-1.19221800