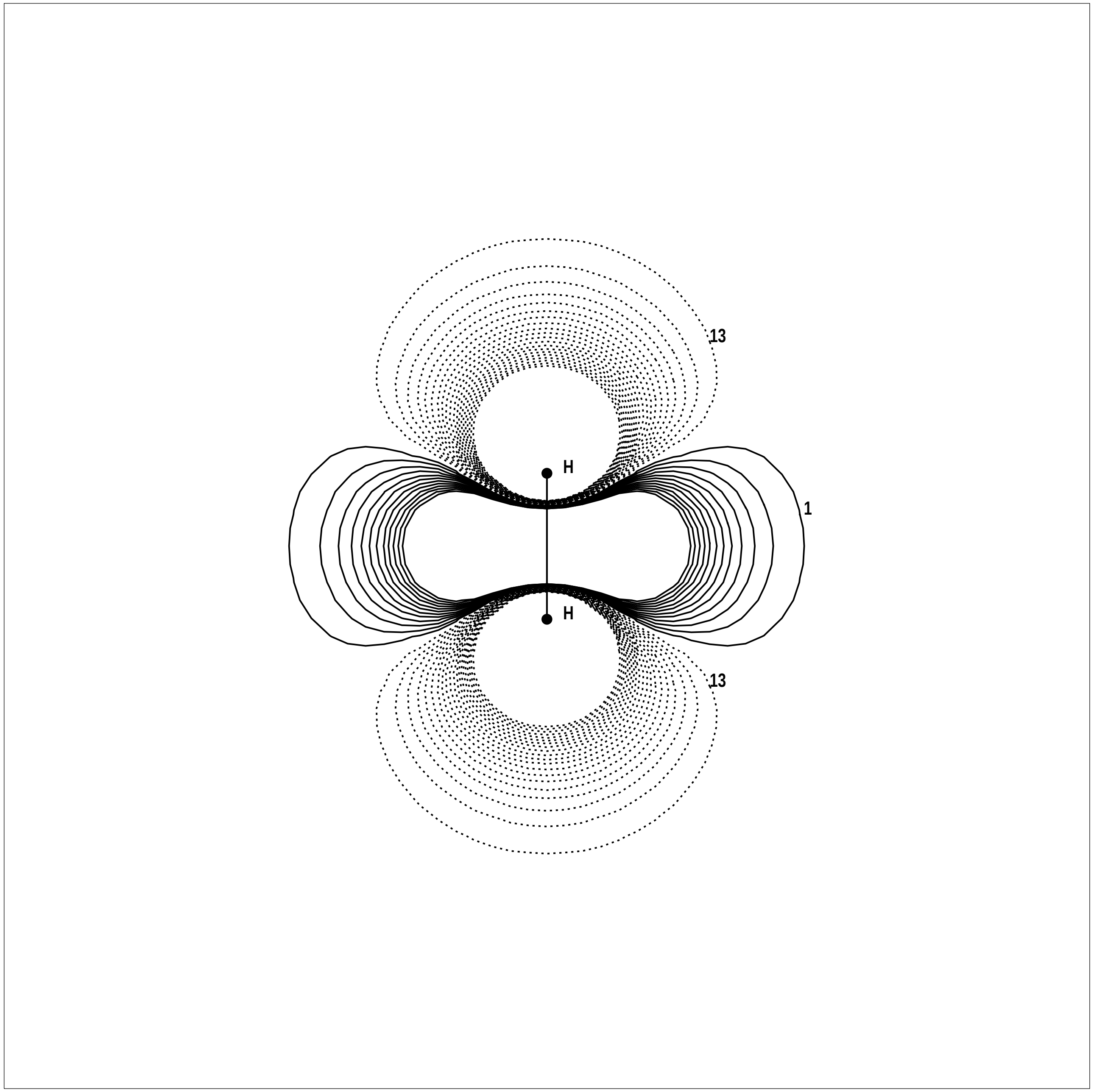


MOLDEN

H2 sto3g Molecular Density minus atoms

CENTER=(0.0 0.0 0.0) LINE=(1.0 0.0 0.
0) CUT=0.1 EDGE=10.0
BONDS FILE = H2STO_OUT POSTSCRIPT DEBUG

CONTOUR	VALUE
1	0.00050
2	0.00100
3	0.00150
4	0.00200
5	0.00250
6	0.00300
7	0.00350
8	0.00400
9	0.00450
10	0.00500
11	0.00550
12	0.00600
13	-0.00050
14	-0.00100
15	-0.00150
16	-0.00200
17	-0.00250
18	-0.00300
19	-0.00350
20	-0.00400
21	-0.00450
22	-0.00500
23	-0.00550
24	-0.00600
25	-0.00650
....	

Figure 1: H2 sto3g Molecular density minus Atomic density

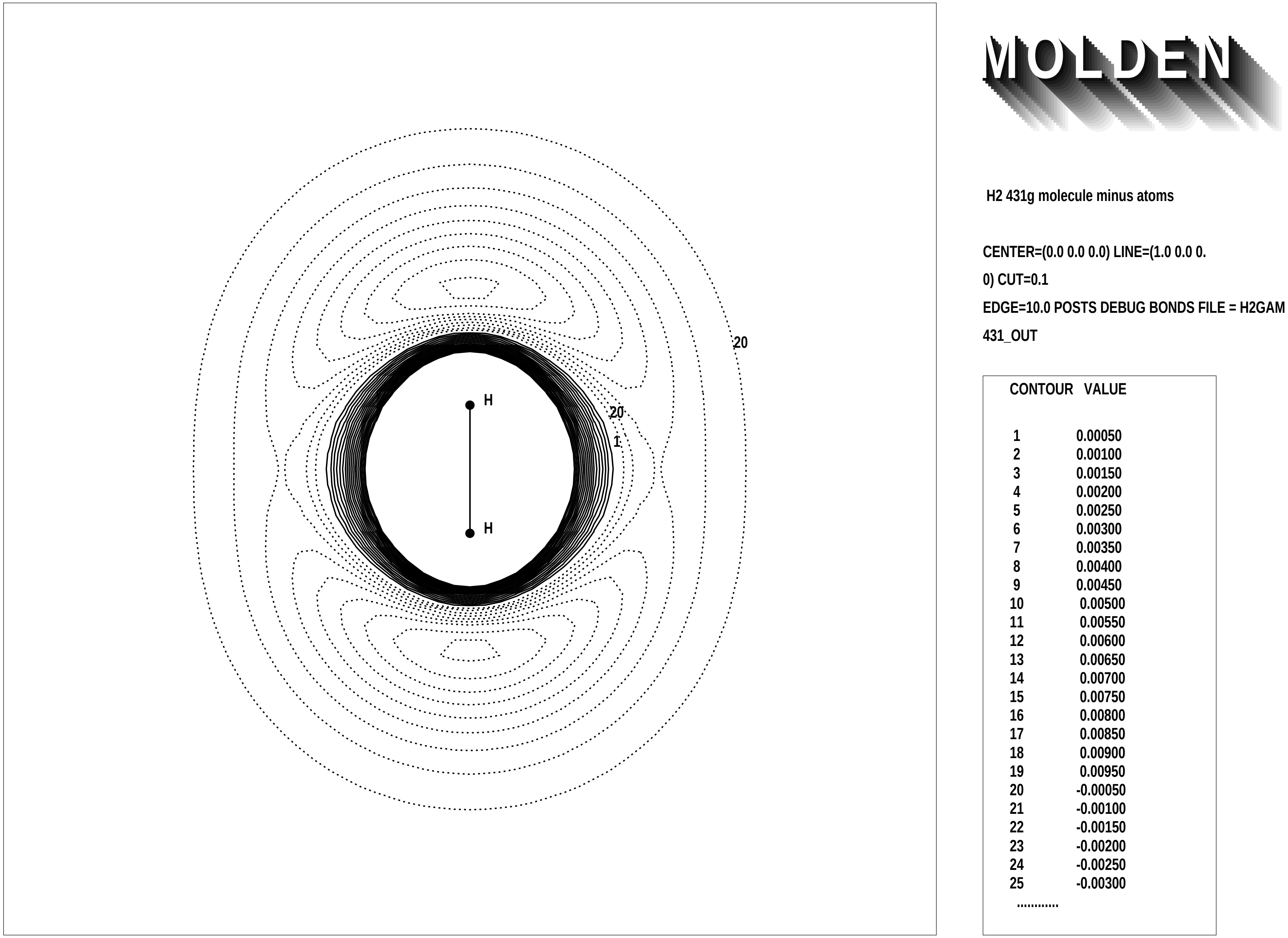
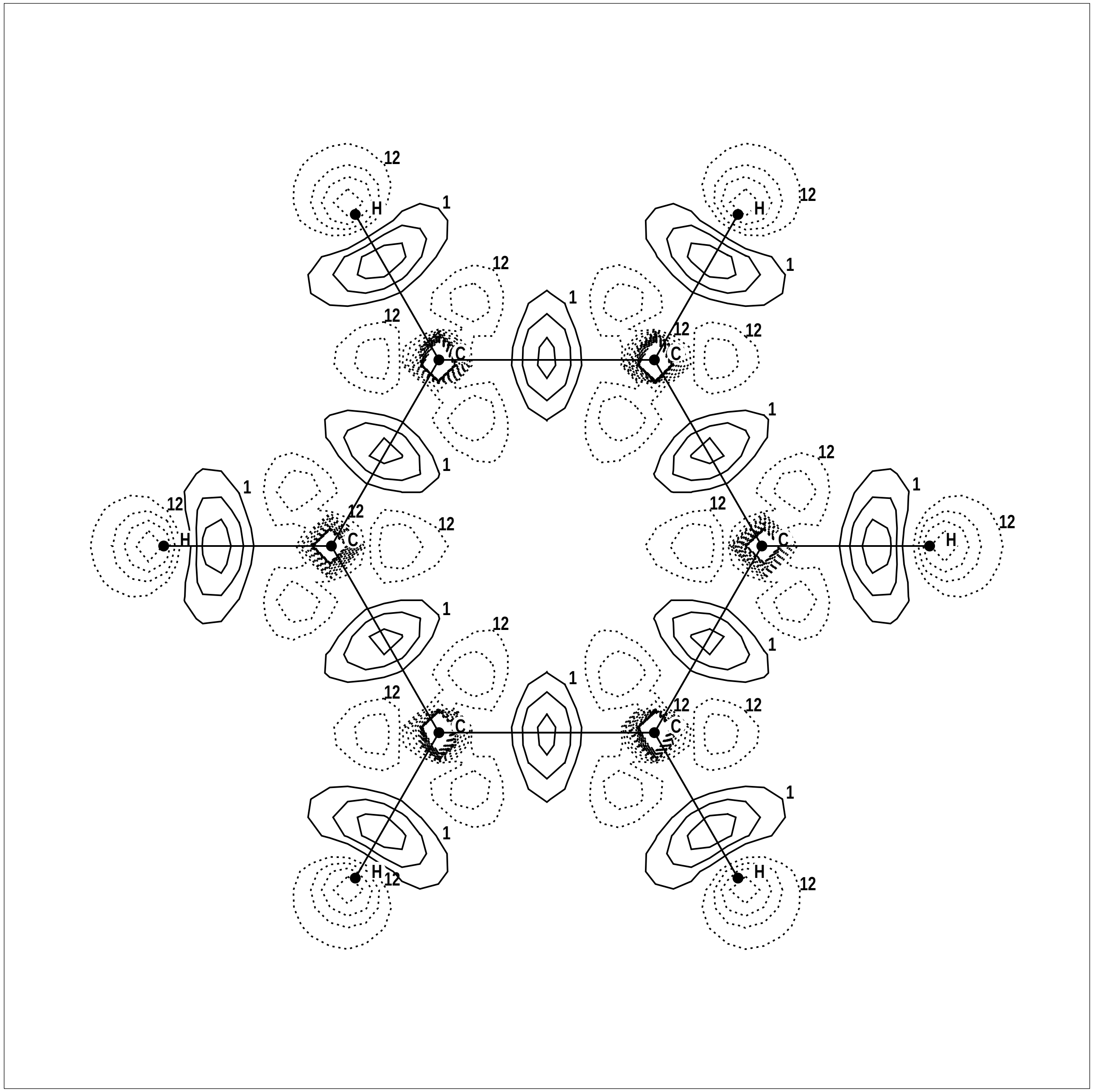


Figure 2: H2 4-31g Molecular density minus Atomic density



MOLDEN

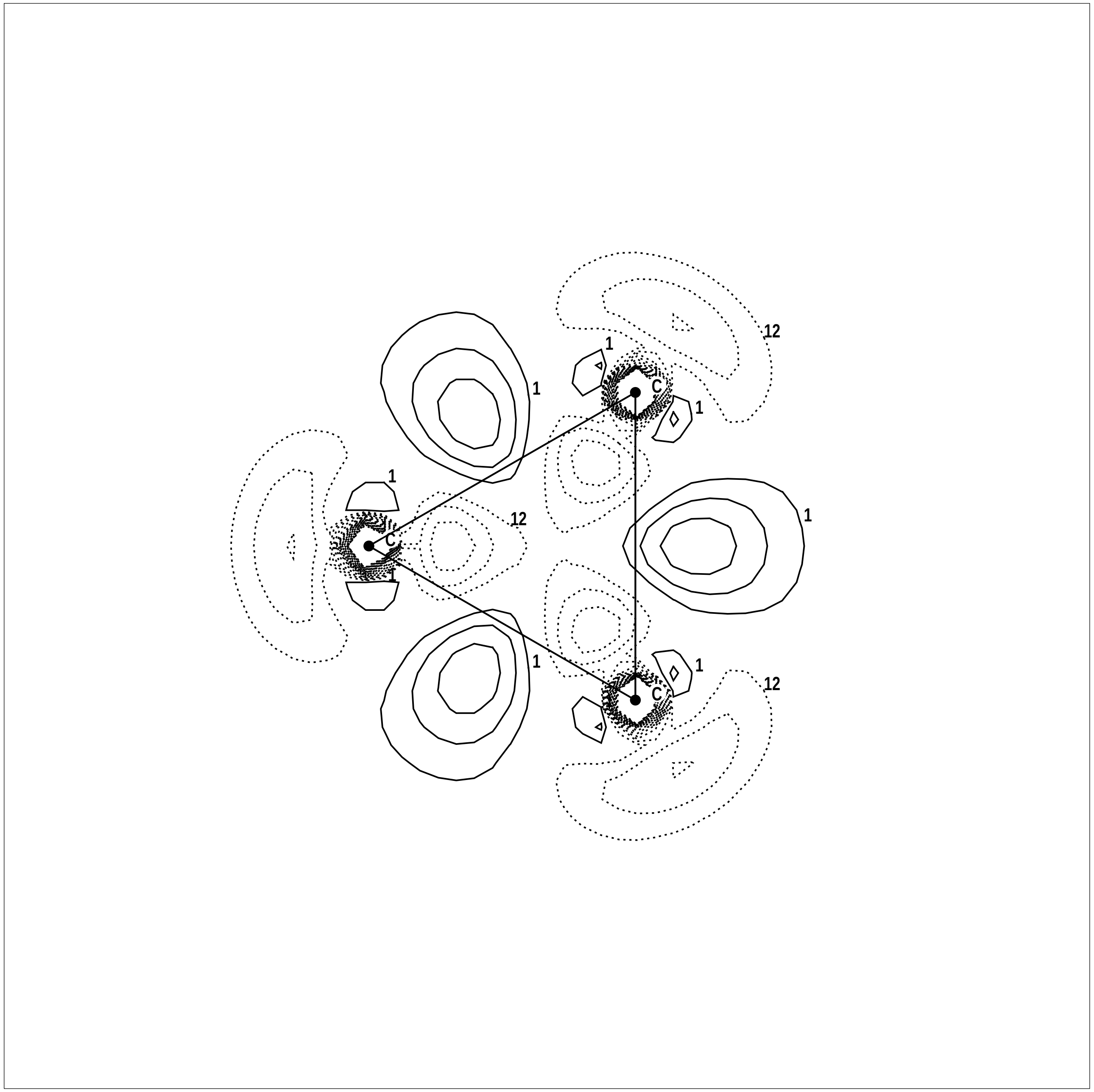
benzene sto3g molecular minus atomic den
sity

PLANE=(1 3 5) EDGE=13.22 BONDS CUT=0.0
8

FILE=BENZENE.OUT POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	-0.01250
13	-0.02500
14	-0.03750
15	-0.05000
16	-0.06250
17	-0.07500
18	-0.08750
19	-0.10000
20	-0.11250
21	-0.12500
22	-0.13750
23	-0.15000
24	-0.16250
25	-0.17500
....	

Figure 3: Benzene sto3g Molecular density minus Atomic density

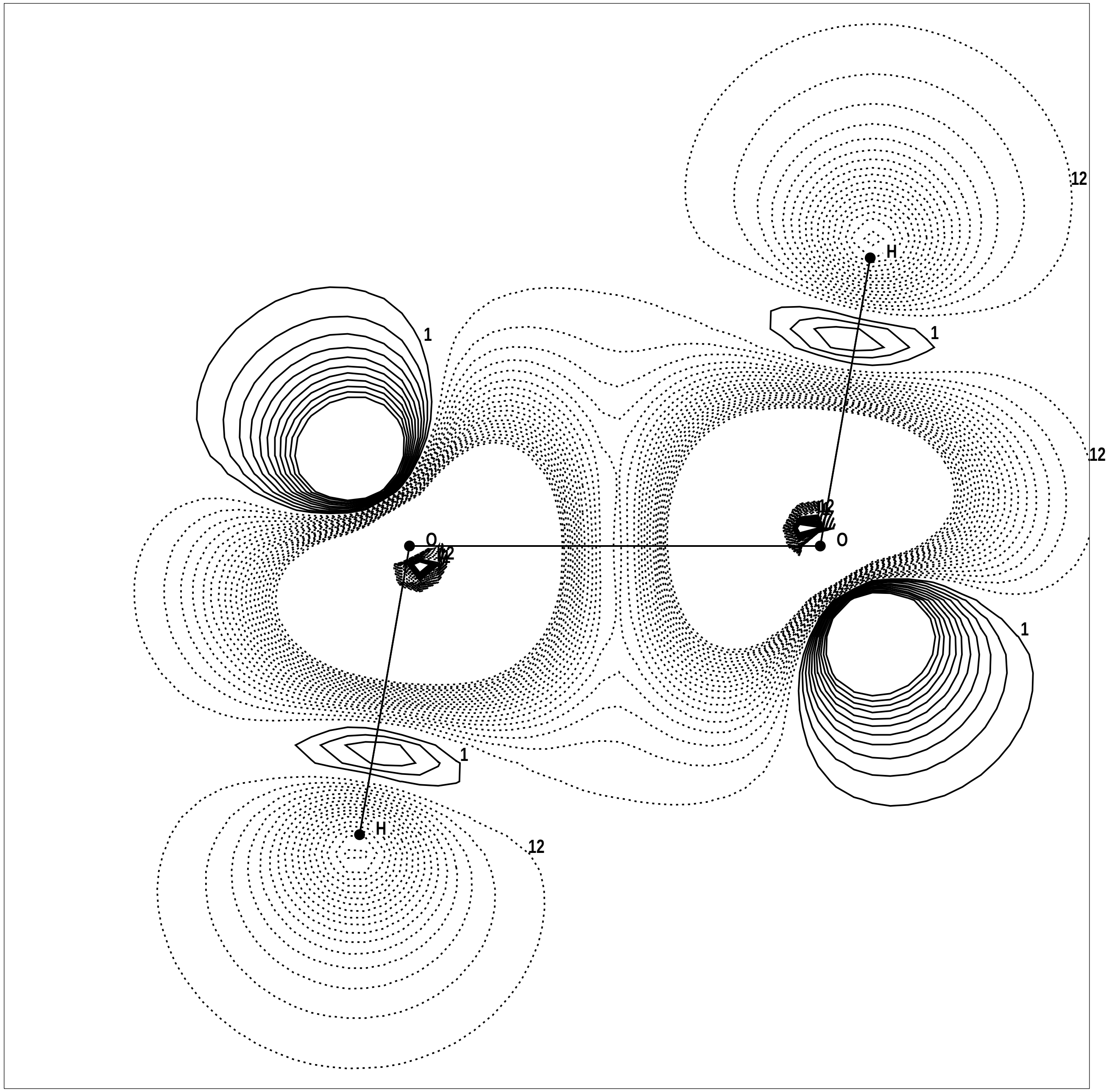


MOLDEN

cyclopropaan sto3g molecular density min
us atomic
PLANE=(1 2 3) EDGE=10.0 BONDS ORIENT C
UT=0.08
FILE=CYCLOPROPAAN.OUT POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	-0.01250
13	-0.02500
14	-0.03750
15	-0.05000
16	-0.06250
17	-0.07500
18	-0.08750
19	-0.10000
20	-0.11250
21	-0.12500
22	-0.13750
23	-0.15000
24	-0.16250
25	-0.17500
....	

Figure 4: Cyclopropane sto3g Molecular density minus Atomic density



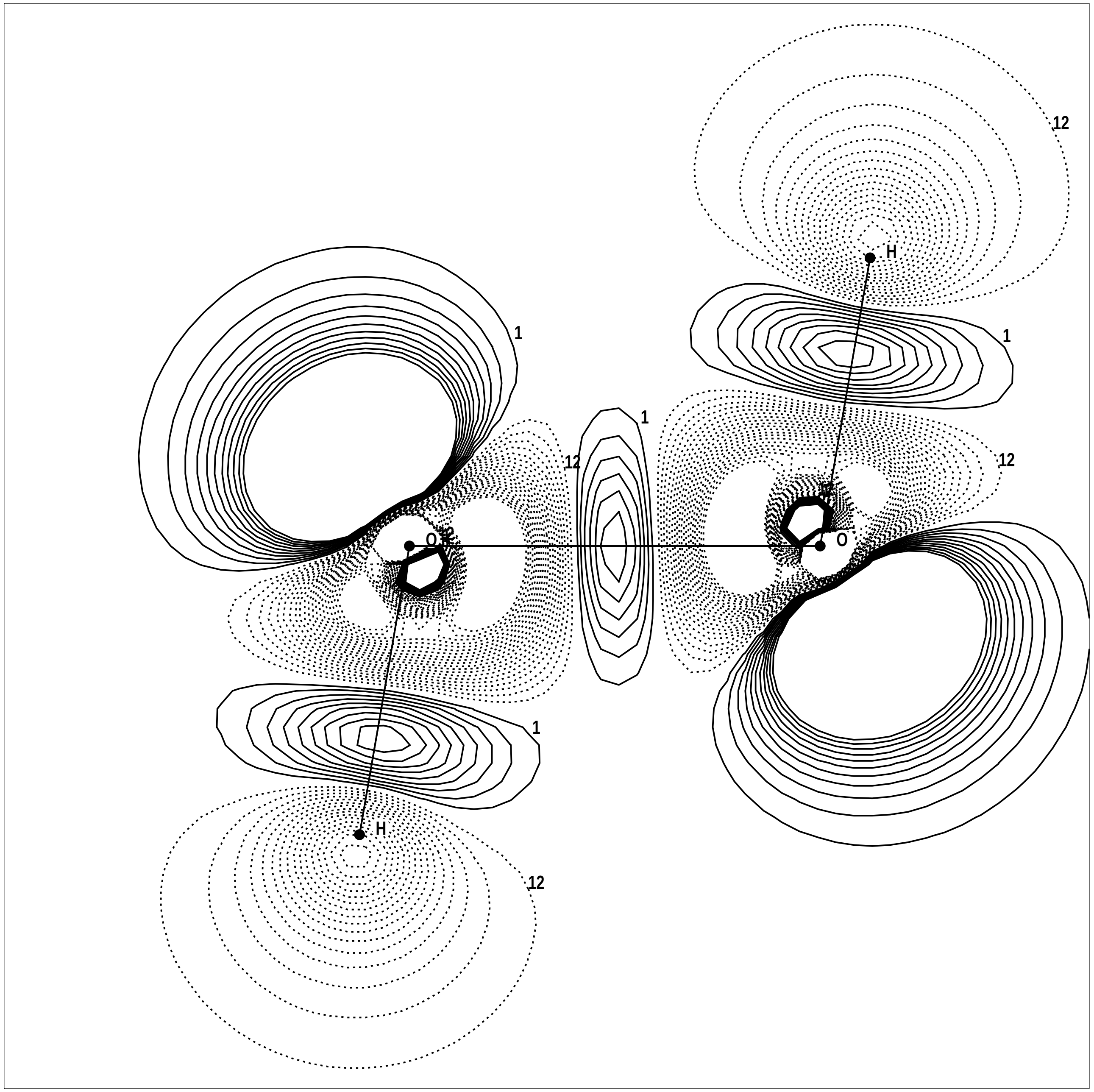
MOLDEN

H2O2 sto3g molecular density minus Spher
ical atoms
PLANE=(2 3 4) EDGE=7.0 BONDS CUT=0.1

FILE=H2O2_OUT POSTSCRIPT DEBUG

CONTOUR	VALUE
1	0.00500
2	0.01000
3	0.01500
4	0.02000
5	0.02500
6	0.03000
7	0.03500
8	0.04000
9	0.04500
10	0.05000
11	0.05500
12	-0.00500
13	-0.01000
14	-0.01500
15	-0.02000
16	-0.02500
17	-0.03000
18	-0.03500
19	-0.04000
20	-0.04500
21	-0.05000
22	-0.05500
23	-0.06000
24	-0.06500
25	-0.07000
....	

Figure 5: H2O2 sto3g Molecular density minus Spherical Atomic density



MOLDEN

H2O2 sto3g molecular density minus Orien

ted Oxygens

PLANE=(2 3 4) EDGE=7.0 BONDS ORIENT CU

T=0.1

FILE=H2O2_OUT POSTSCRIPT DEBUG

CONTOUR	VALUE
1	0.00500
2	0.01000
3	0.01500
4	0.02000
5	0.02500
6	0.03000
7	0.03500
8	0.04000
9	0.04500
10	0.05000
11	0.05500
12	-0.00500
13	-0.01000
14	-0.01500
15	-0.02000
16	-0.02500
17	-0.03000
18	-0.03500
19	-0.04000
20	-0.04500
21	-0.05000
22	-0.05500
23	-0.06000
24	-0.06500
25	-0.07000
....	

Figure 6: H2O2 sto3g Molecular density minus Oriented Oxygens

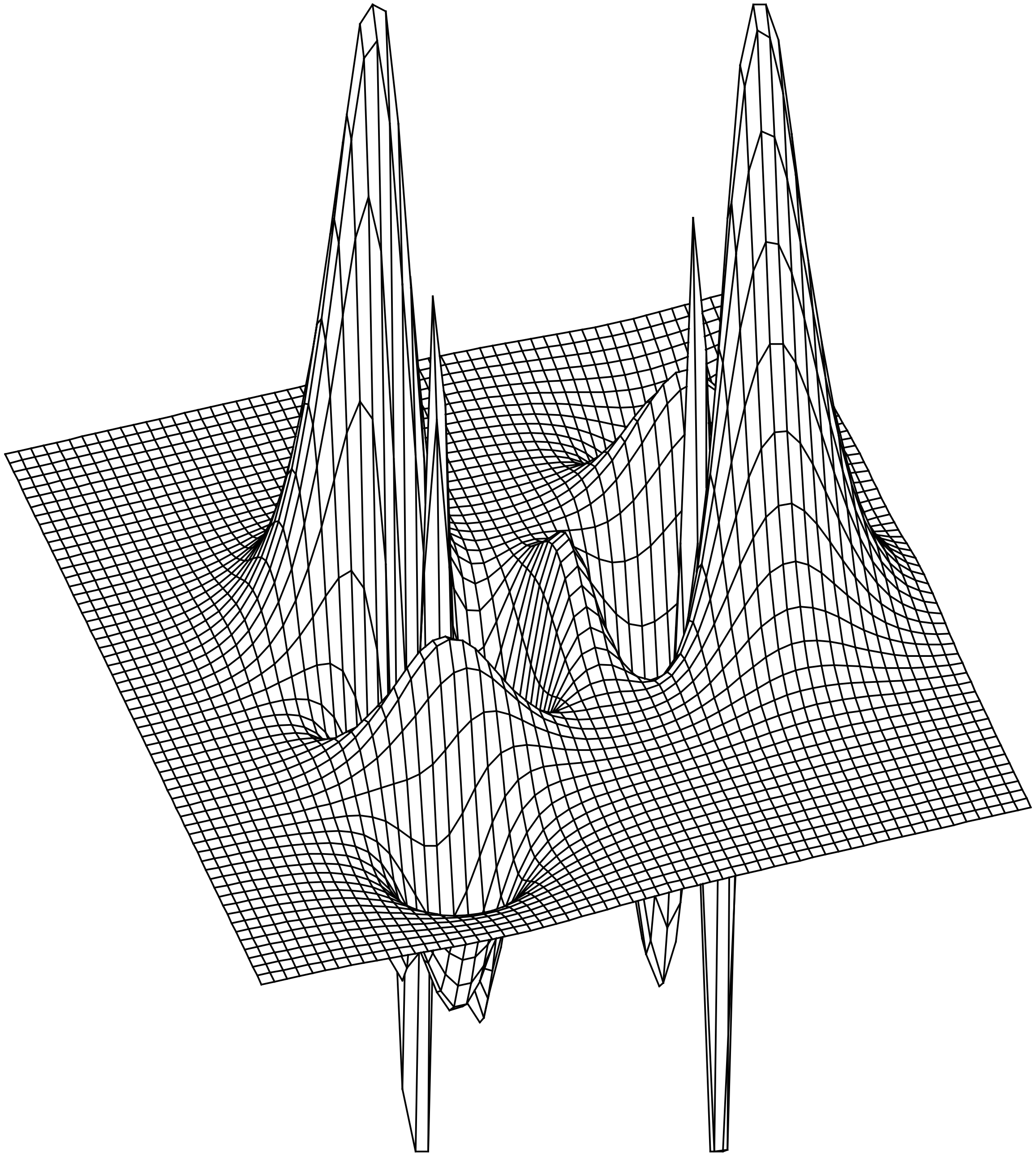
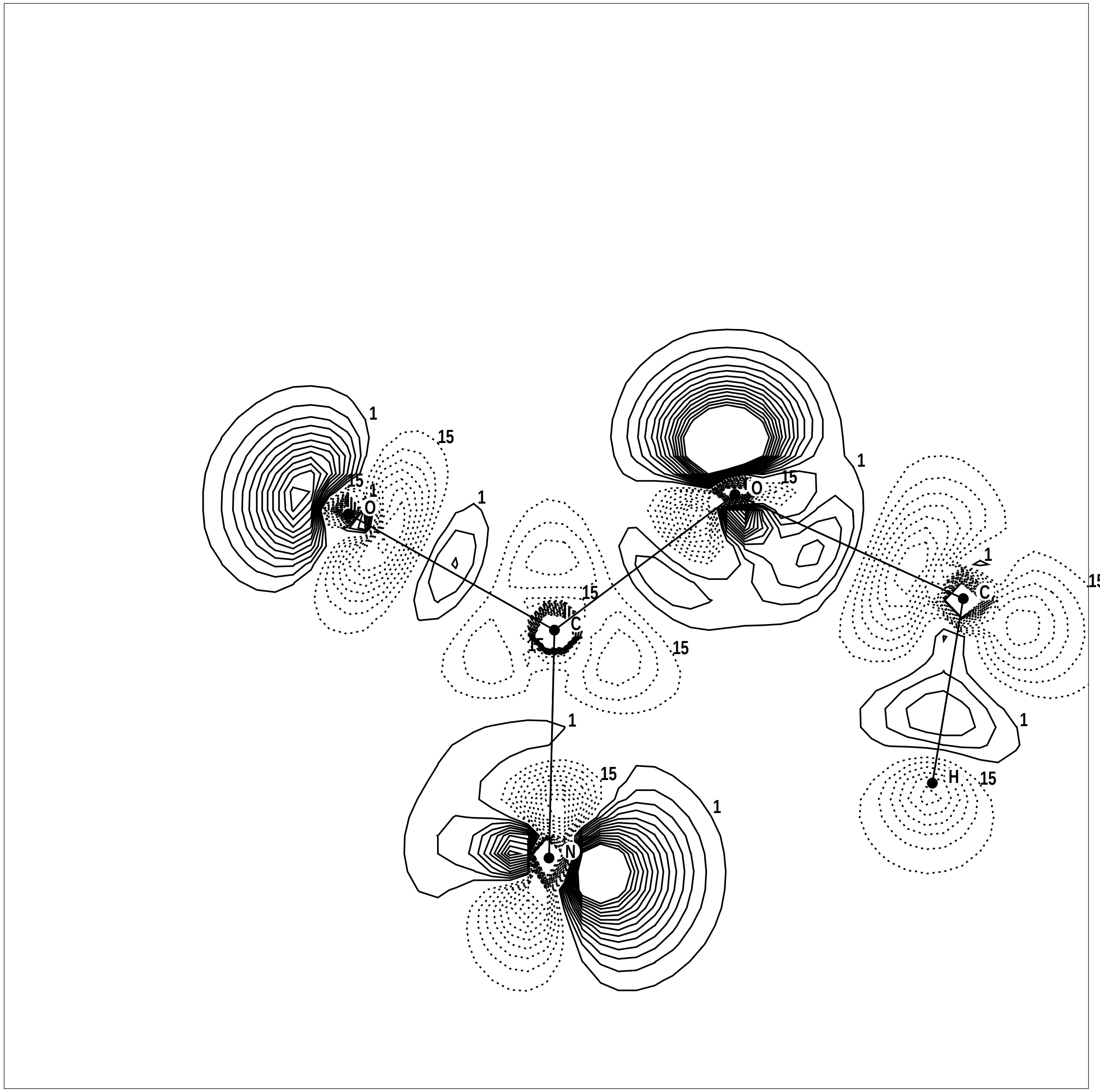


Figure 7: H2 sto3g Molecular density minus Atomic density; 3-d plot

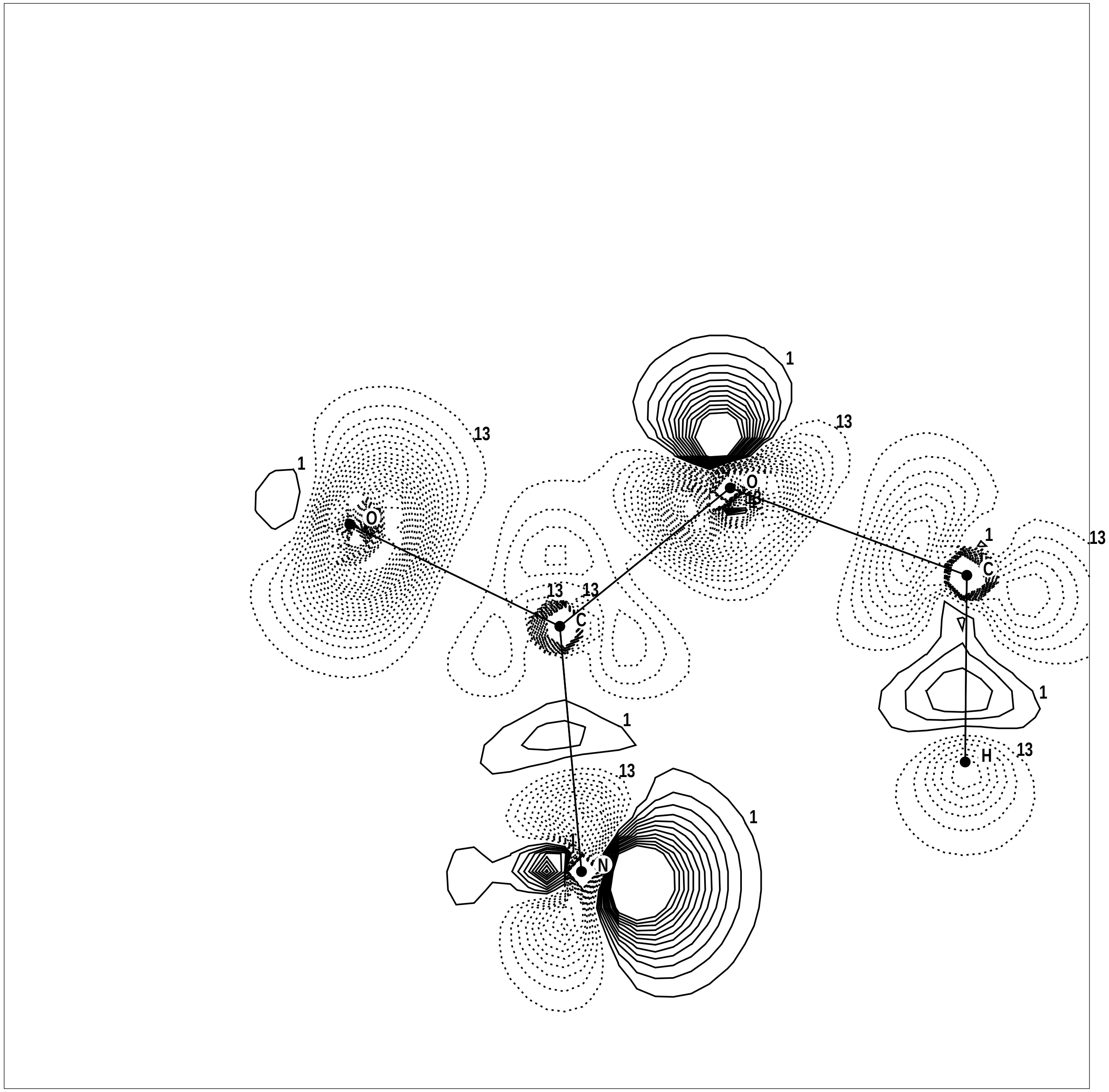


MOLDEN

NH2COOCH3+. sto3g Mol. Density - Oriente
d Atoms before Optimisation
PLANE=(1 2 3) EDGE=12.0 BONDS ORIENT C
UT=0.1
BEFORE FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	0.16250
14	0.17500
15	-0.01250
16	-0.02500
17	-0.03750
18	-0.05000
19	-0.06250
20	-0.07500
21	-0.08750
22	-0.10000
23	-0.11250
24	-0.12500
25	-0.13750
....	

Figure 8: NH2COOCH3+. sto3g Molecular density minus Oriented atoms, before optimisation



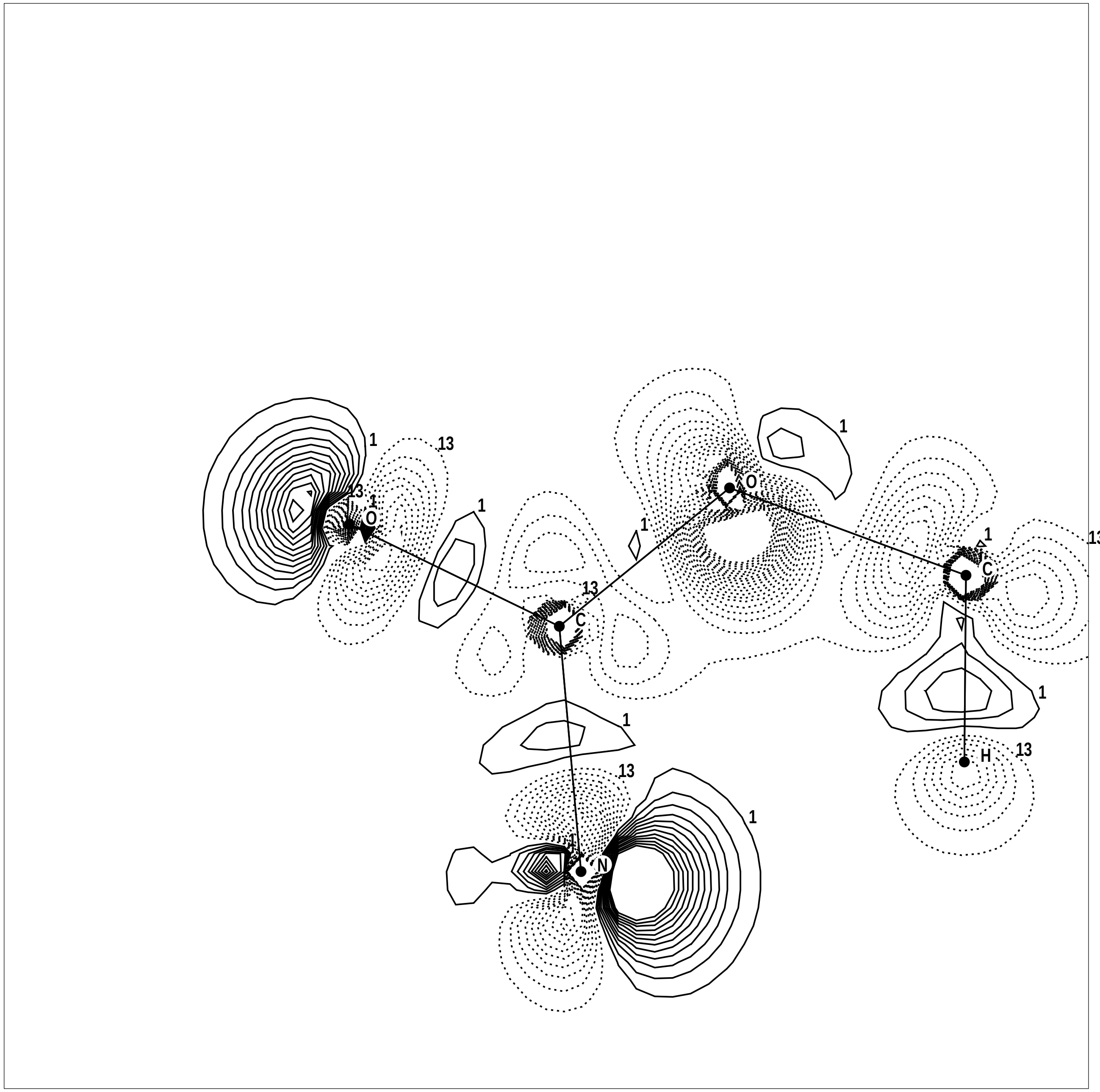
MOLDEN

NH2COOCH3+. sto3g Mol. Density - Spheric
al Atoms after Optimisation
PLANE=(1 2 3) EDGE=12.0 BONDS CUT=0.1

FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	-0.01250
14	-0.02500
15	-0.03750
16	-0.05000
17	-0.06250
18	-0.07500
19	-0.08750
20	-0.10000
21	-0.11250
22	-0.12500
23	-0.13750
24	-0.15000
25	-0.16250
....	

Figure 9: NH2COOCH3+. sto3g Molecular density minus spherical atoms, after optimisation

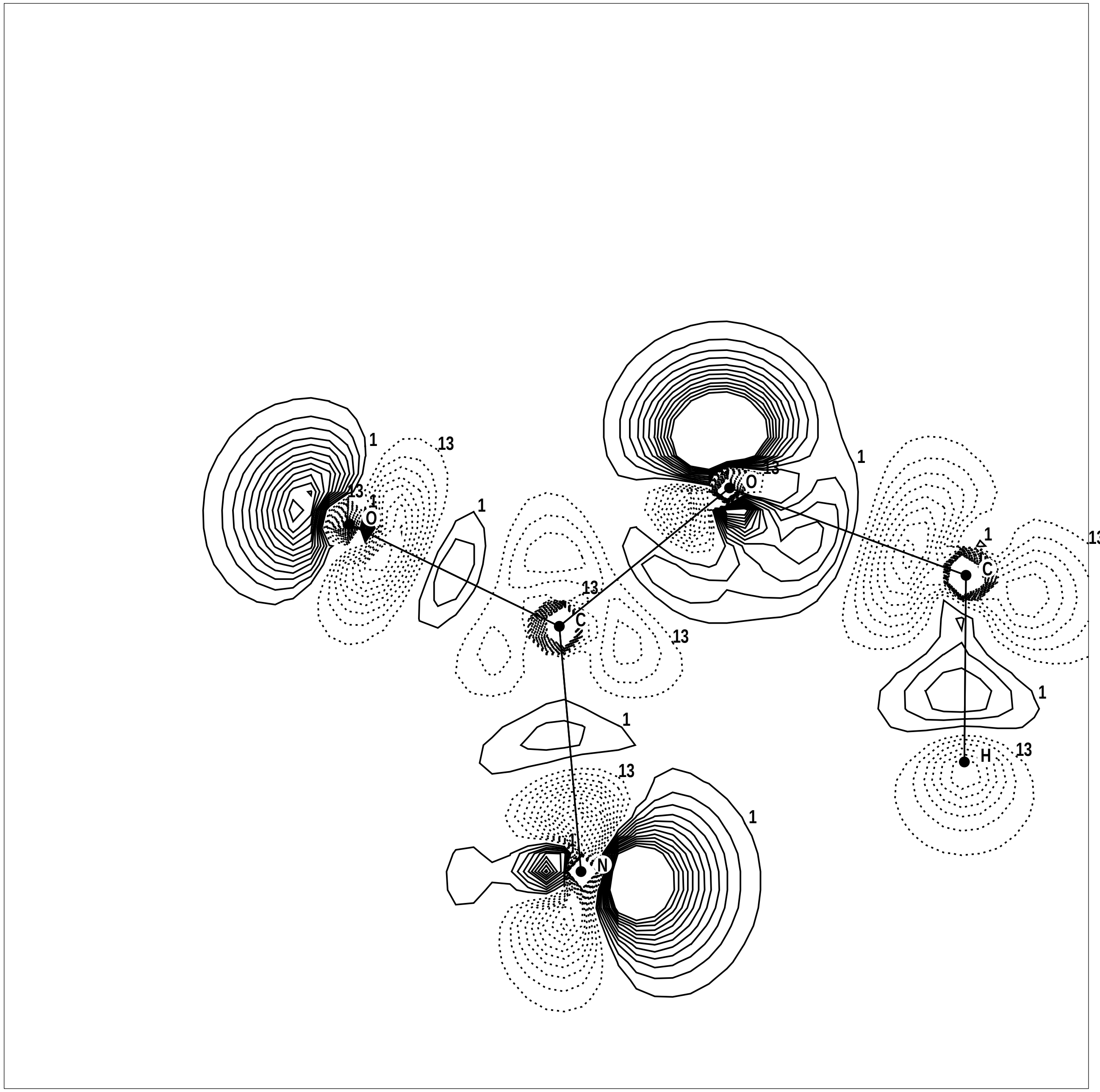


MOLDEN

NH2COOCH3+. sto3g Mol. Density - Oriente
d Atoms after Optimisation
PLANE=(1 2 3) EDGE=12.0 BONDS ORIENT C
UT=0.1
FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	-0.01250
14	-0.02500
15	-0.03750
16	-0.05000
17	-0.06250
18	-0.07500
19	-0.08750
20	-0.10000
21	-0.11250
22	-0.12500
23	-0.13750
24	-0.15000
25	-0.16250
....	

Figure 10: NH2COOCH3+. sto3g Molecular density minus Oriented atoms, after optimisation

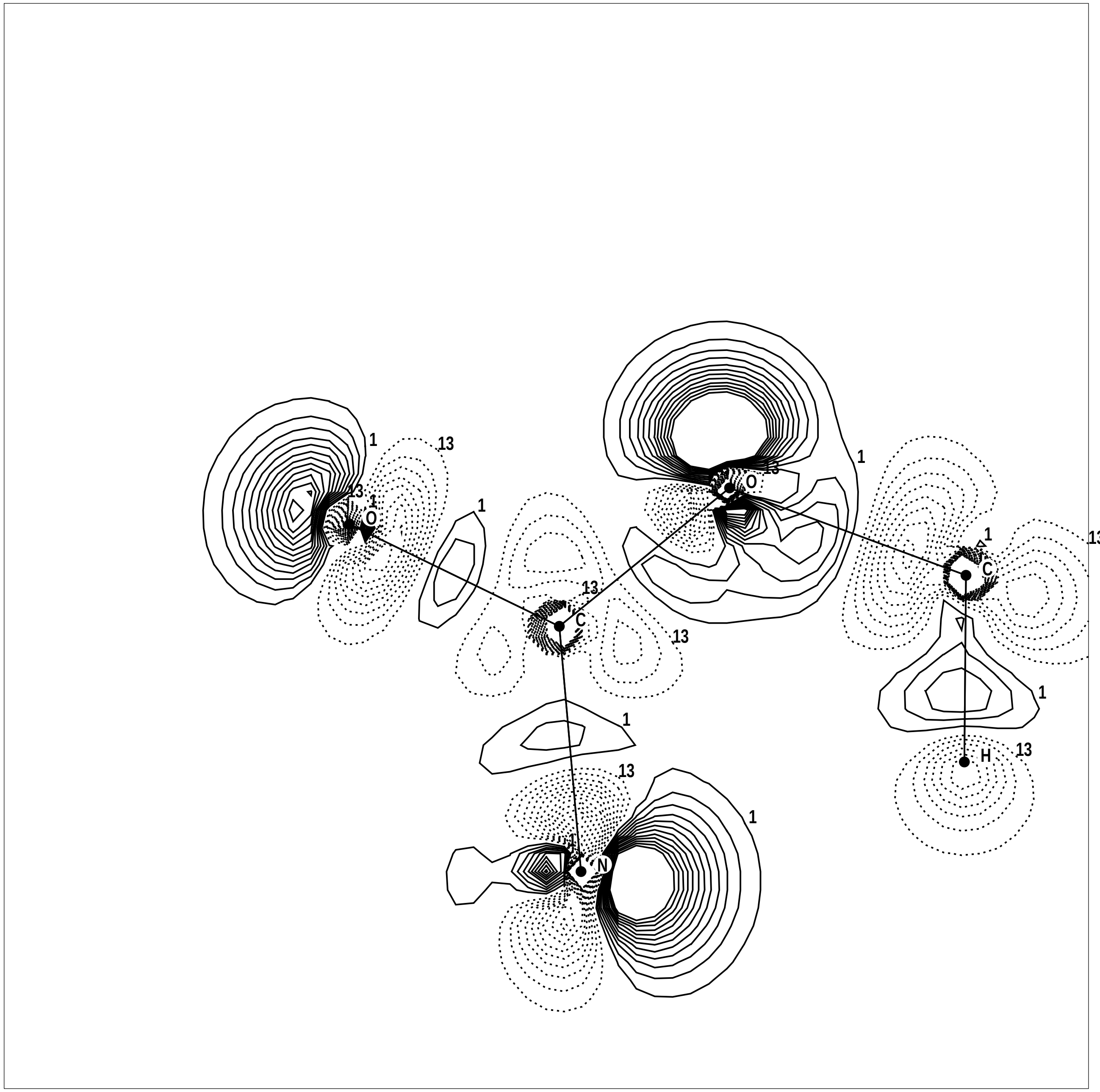


MOLDEN

NH2COOCH3+. sto3g Mol.- Atoms forced ori
entation C-O-C oxygen
PLANE=(1 2 3) EDGE=12.0 ORIENT=(2,3/0
/90) BONDS CUT=0.1
FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	-0.01250
14	-0.02500
15	-0.03750
16	-0.05000
17	-0.06250
18	-0.07500
19	-0.08750
20	-0.10000
21	-0.11250
22	-0.12500
23	-0.13750
24	-0.15000
25	-0.16250
....	

Figure 11: NH2COOCH3+. sto3g Mol. density minus Oriented Oxygens, with forced orientation of the C-O-C oxygen

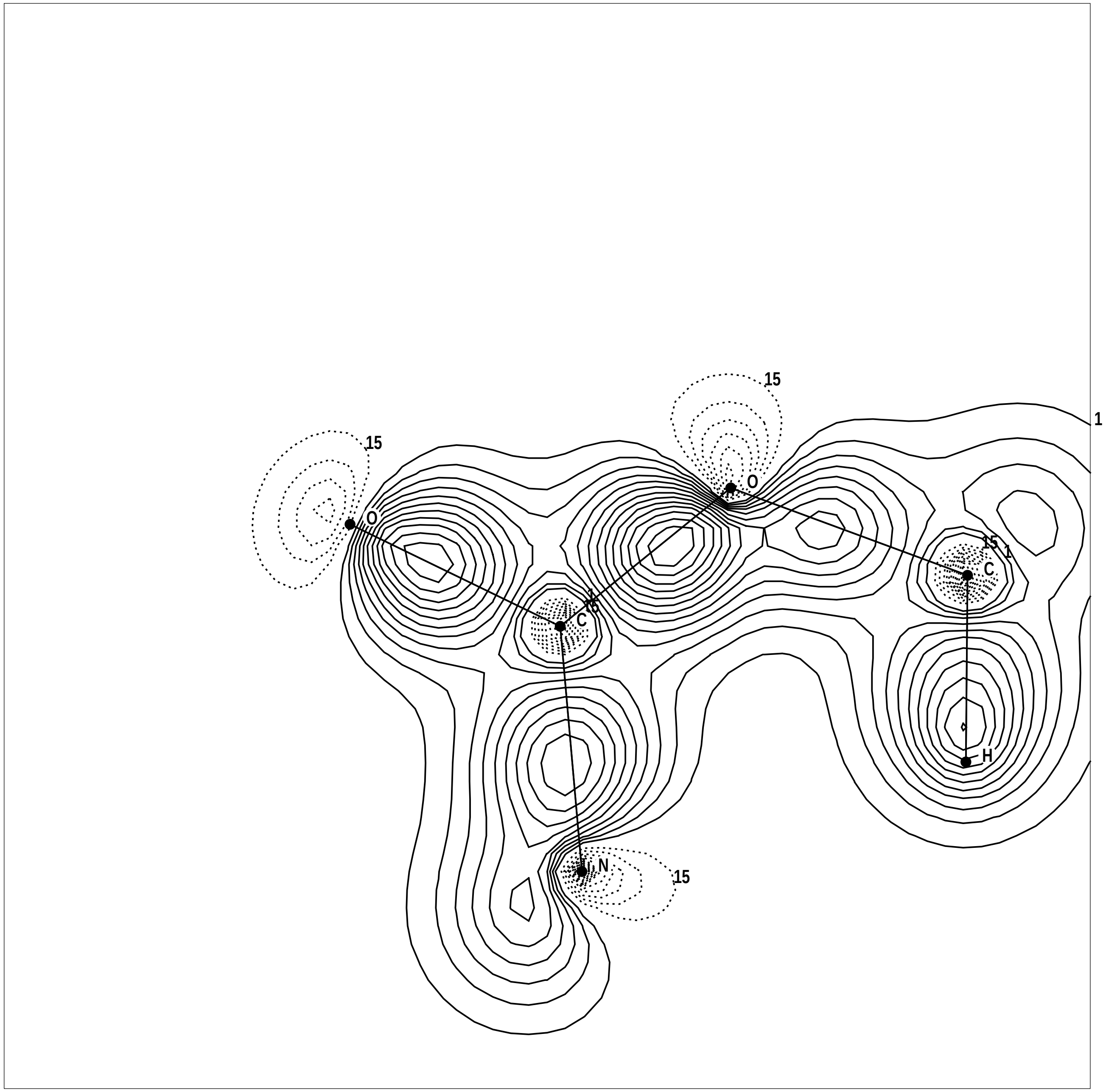


MOLDEN

NH2COOCH3+. sto3g Mol.- Atoms forced ori
entation C-O-C oxygen
PLANE=(1 2 3) EDGE=12.0 ORIENT=(2,3/0
/90) BONDS CUT=0.1
FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	-0.01250
14	-0.02500
15	-0.03750
16	-0.05000
17	-0.06250
18	-0.07500
19	-0.08750
20	-0.10000
21	-0.11250
22	-0.12500
23	-0.13750
24	-0.15000
25	-0.16250
....	

Figure 11: NH2COOCH3+. sto3g Mol. density minus Oriented Oxygens, with forced orientation of the C-O-C oxygen



NH2COOCH3+. sto3g Interatomic Overlap De
nsity

PLANE=(1 2 3) EDGE=12.0 OVERLAP

FILE=CARBS_O POSTSCRIPT DEBUG

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	0.13750
12	0.15000
13	0.16250
14	0.17500
15	-0.01250
16	-0.02500
17	-0.03750
18	-0.05000
19	-0.06250
20	-0.07500
21	-0.08750
22	-0.10000
23	-0.11250
24	-0.12500
25	-0.13750
....	

Figure 12: NH2COOCH3+. sto3g Interatomic overlap density, contour plot

MOLDEN

NH2COOCH3+. sto3g Interatomic Overlap De
nsity
PLANE=(1 2 3) EDGE=12.0 3D OVERLAP

FILE=CARBS_O POSTSCRIPT DEBUG

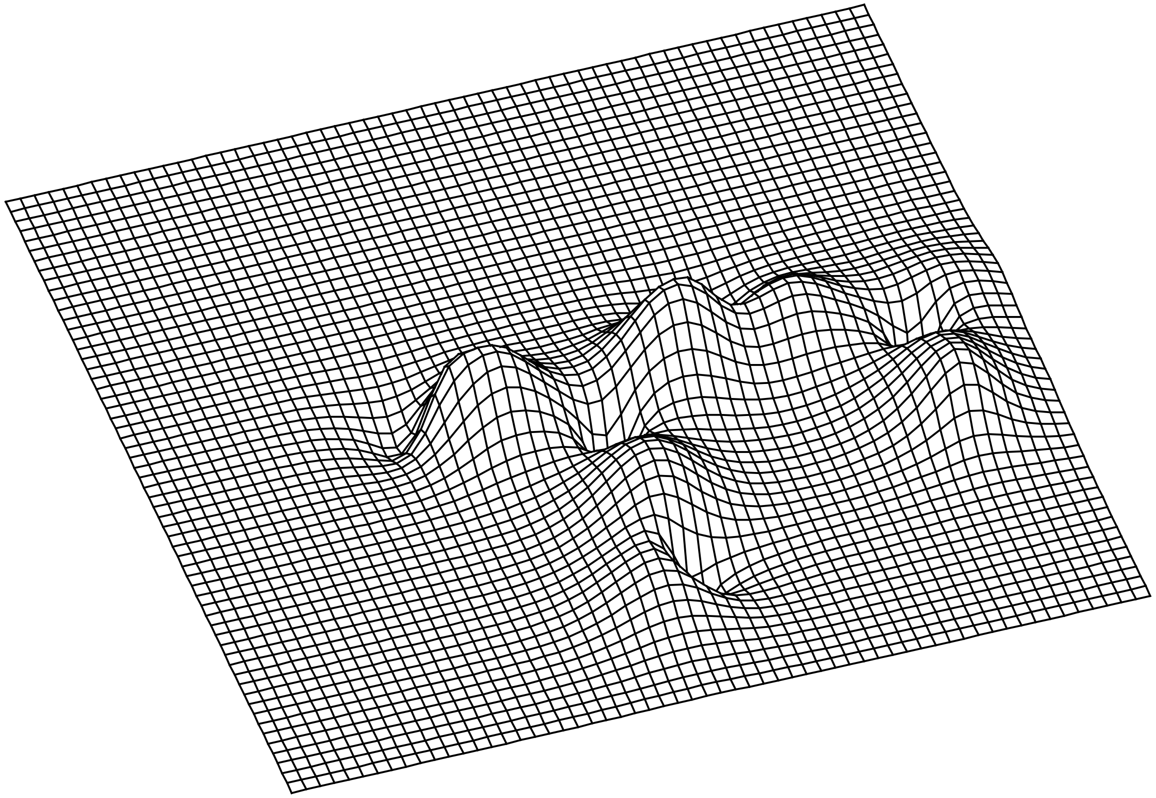
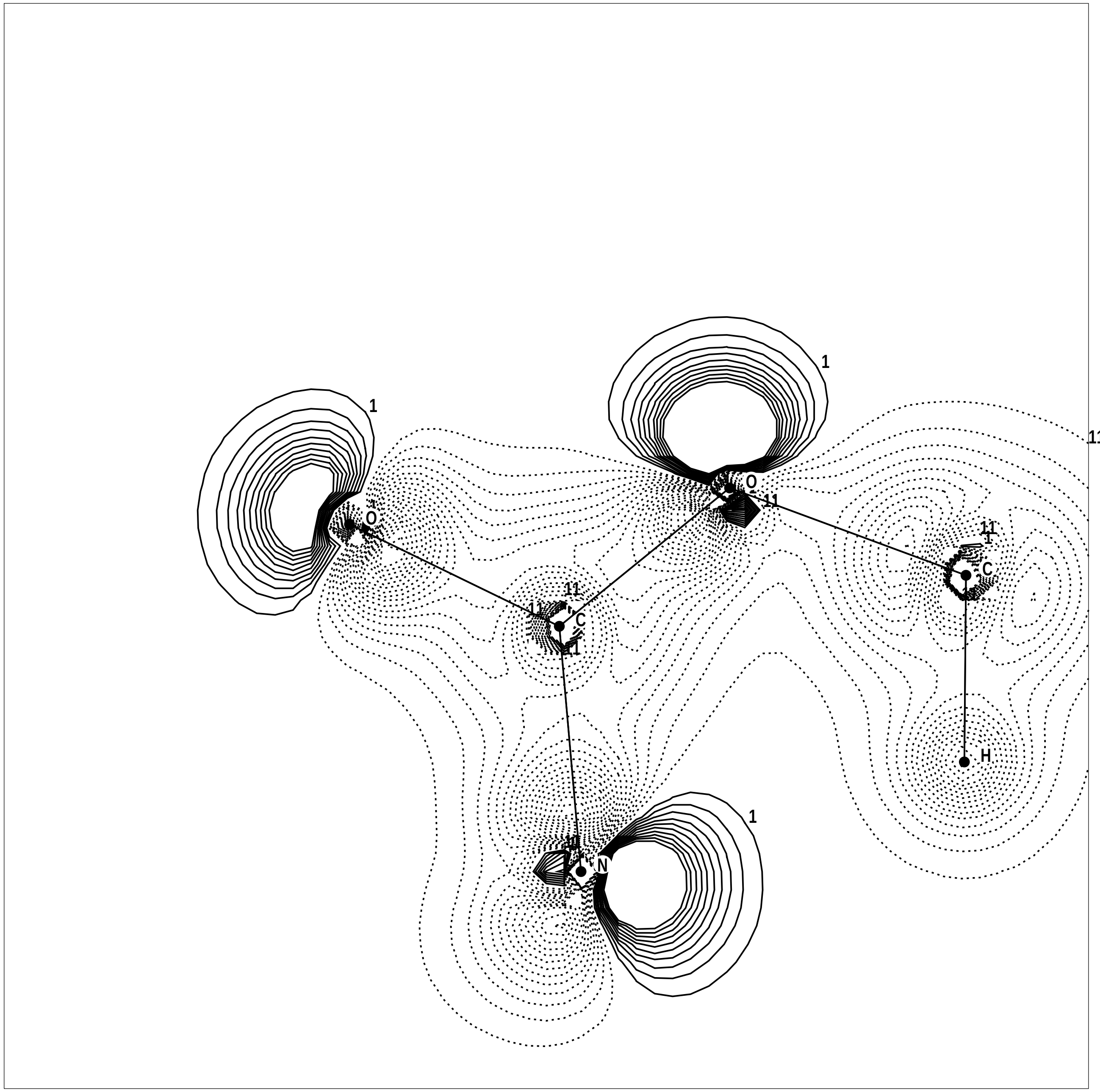


Figure 13: NH2COOCH3+. sto3g Interatomic overlap density, 3d plot



MOLDEN

NH2COOCH3+. sto3g Mol.-Atoms forced orie
ntation C-O-C Oxygen ATOMIC
PLANE=(1 2 3) EDGE=12.0 ORIENT=(2,3/0
/90) ATOMIC CUT=0.1
FILE=CARBS_O POSTSCRIPT

CONTOUR	VALUE
1	0.01250
2	0.02500
3	0.03750
4	0.05000
5	0.06250
6	0.07500
7	0.08750
8	0.10000
9	0.11250
10	0.12500
11	-0.01250
12	-0.02500
13	-0.03750
14	-0.05000
15	-0.06250
16	-0.07500
17	-0.08750
18	-0.10000
19	-0.11250
20	-0.12500
21	-0.13750
22	-0.15000
23	-0.16250
24	-0.17500
25	-0.18750
....	

Figure 14: NH2COOCH3+. sto3g Molecular density minus Oriented atoms; Atomic part of the density