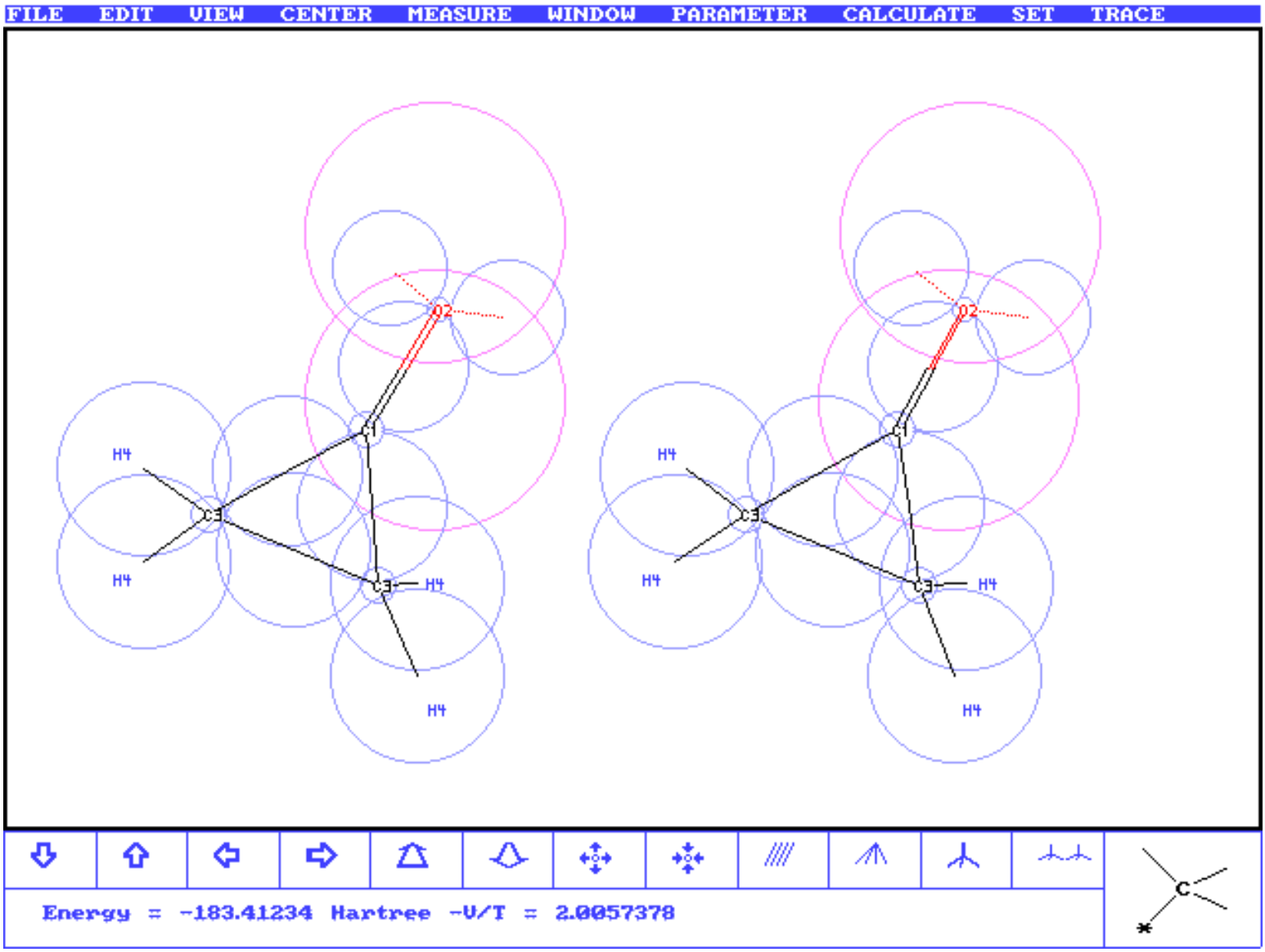


This Kimball run of **cyclo-Propanone** (set G21205.prf) shows a fairly reasonable structure and total energy. In the C-triangle one observes multiple overlaps of the crowded C-C bonds. Since the present version of Kimball.exe does not allow bonding clouds to yield towards the outside of the straight C-C connection the figure conveys the impression of a particularly high electron density in the center. However, the program correctly deals with Pauli's exclusion principle and computes an approximate exchange energy whenever two (doubly occupied) clouds overlap. The result of this is, that the density in the center of the triangle is much lower, not higher, than in the rest of the C-C clouds.

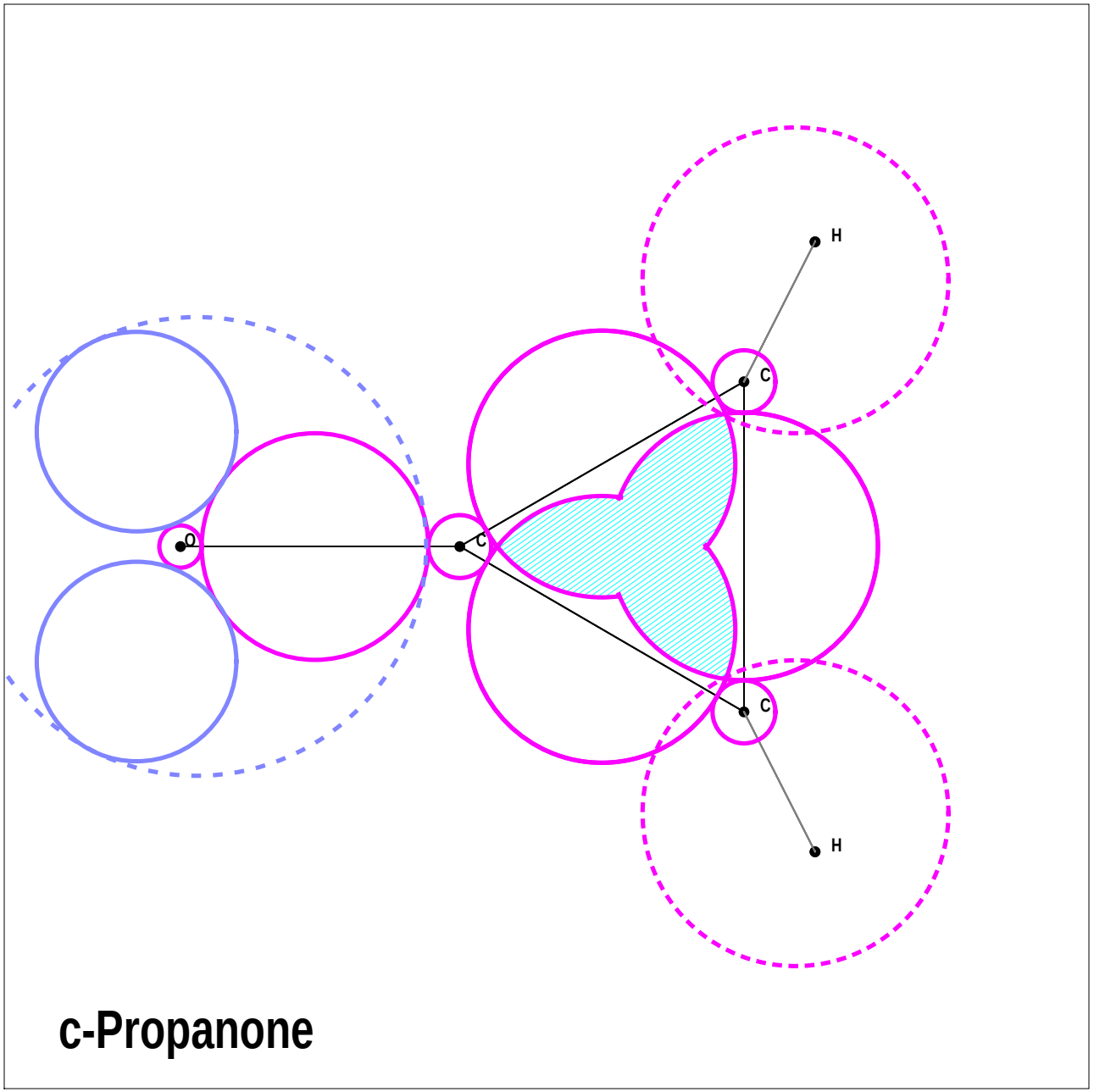
This is demonstrated by a different coloring in the next figure, where the Kimball electron distribution is overlayed onto the overlap density computed from an optimized RHF/6-31G run with Gaussian98 and plotted with Molden.3.6.

The density in the center is lower than contour 1, going around the "outside" of the molecule. The three local maxima outside the triangle depict the "banana bonds" which are also well represented by the exchange corrected rest of the Kimball clouds. Just subtract the density within the cyan exchange region to visualize this.

Incidentally, this description points out the importance of Pauli's exclusion principle in connection with strain in small ring systems. For the rest of the molecule the Kimball clouds fairly well wrap around the local maxima of overlap density, see figure.

For another example of a precise representation of the overlap density by Kimball, see Isobutene or 2-Methyl-propene-1.

Mar. 10, 2000 by ES



c-Propanone

KIMBALL

cyclo-Propanone, optimized Kimball run

Parameter set: G21205.prf

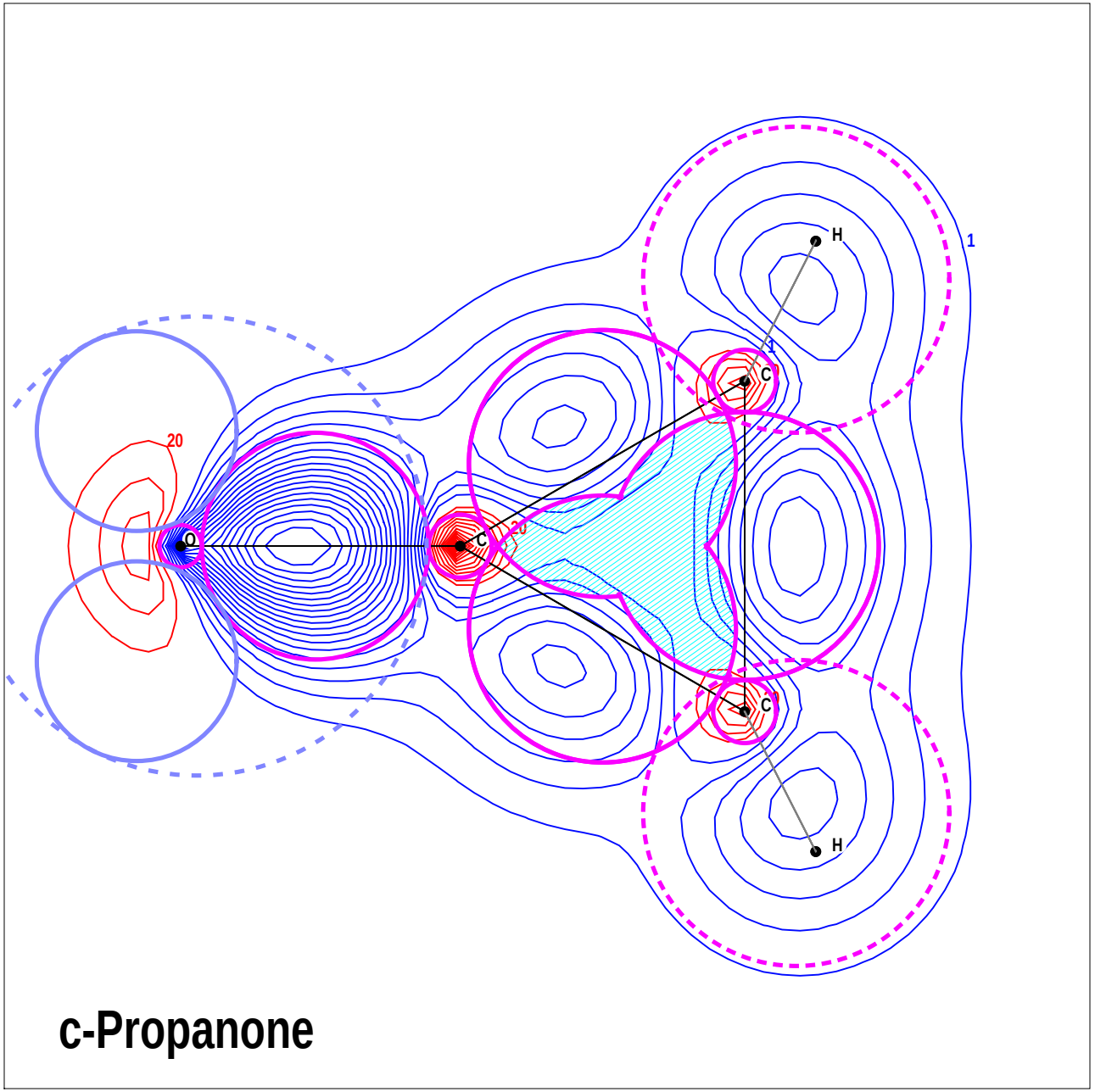
E = -183.41234 hartree (-V/T 2.0057)

Edge = 9.38 bohr

solid line: in plane; dashed: out of plane

magenta: sigma; blue: pi; cyan: Pauli excl.

CONTOUR	VALUE
1	0.00800
2	0.01600
3	0.02400
4	0.03200
5	0.04000
6	0.04800
7	0.05600
8	0.06400
9	0.07200
10	0.08000
11	0.08800
12	0.09600
13	0.10400
14	0.11200
15	0.12000
16	0.12800
17	0.13600
18	0.14400
19	0.15200
20	-0.00800
21	-0.01600
22	-0.02400
23	-0.03200
24	-0.04000
25	-0.04800
.....	



c-Propanone

MOLDEN

KIMBALL

Edge = 9.38 Overlap Contour Euclid

Contour for Gaussian98 RHF/6-31G

E = -190.6343062 hartree, optimized

Overlay Kimball set G21205.prf

E = -183.41234 hartree, optimized

CONTOUR	VALUE
1	0.00800
2	0.01600
3	0.02400
4	0.03200
5	0.04000
6	0.04800
7	0.05600
8	0.06400
9	0.07200
10	0.08000
11	0.08800
12	0.09600
13	0.10400
14	0.11200
15	0.12000
16	0.12800
17	0.13600
18	0.14400
19	0.15200
20	-0.00800
21	-0.01600
22	-0.02400
23	-0.03200
24	-0.04000
25	-0.04800
.....	