

This Kimball run of **Isobutene** (2-methylpropene-1, set G21205.prf) shows a fairly reasonable structure and a very good total energy. Since there is very little overlap of the clouds (only the diffuse  $\pi$ -clouds need to be exchange corrected in their overlap with  $\sigma$ -clouds), the virial ratio is very good, too.

That the [density distribution](#) is a fair approximation to that computed from an optimized RHF/6-31G with [Gaussian98](#) is demonstrated in the next figure, where the Kimball electron distribution is overlayed onto the Gaussian overlap density and plotted with [Molden.3.6](#).

The Kimball clouds cunningly well wrap around the local maxima of overlap density, [see figure](#).

For another example of a more problematical molding of the overlap density, see [cyclo-propanone](#).

Mar. 08, 2000 by ES

# KIMBALL

Isobutylene, optimized Kimball run

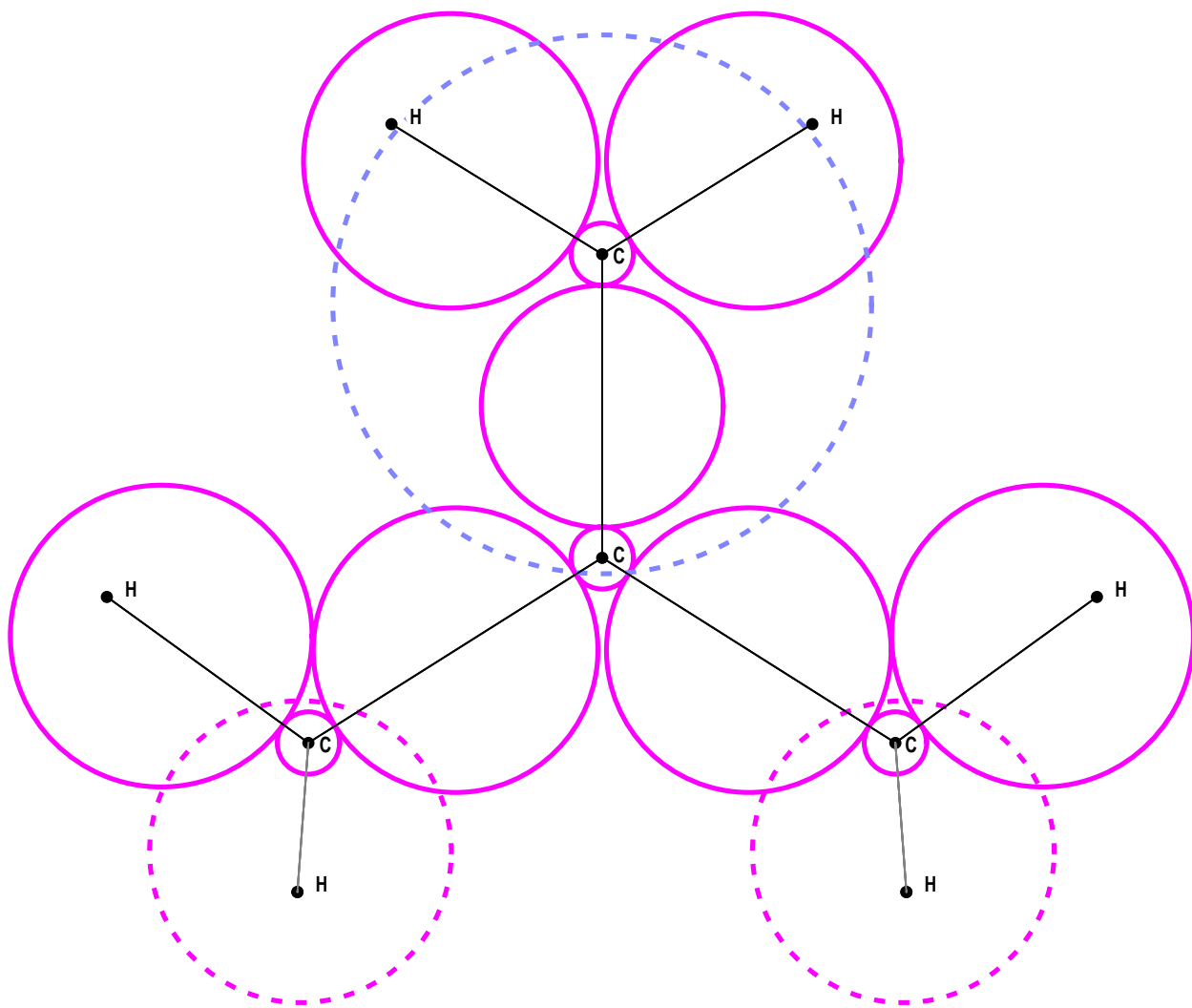
Parameter set: G21205.prf

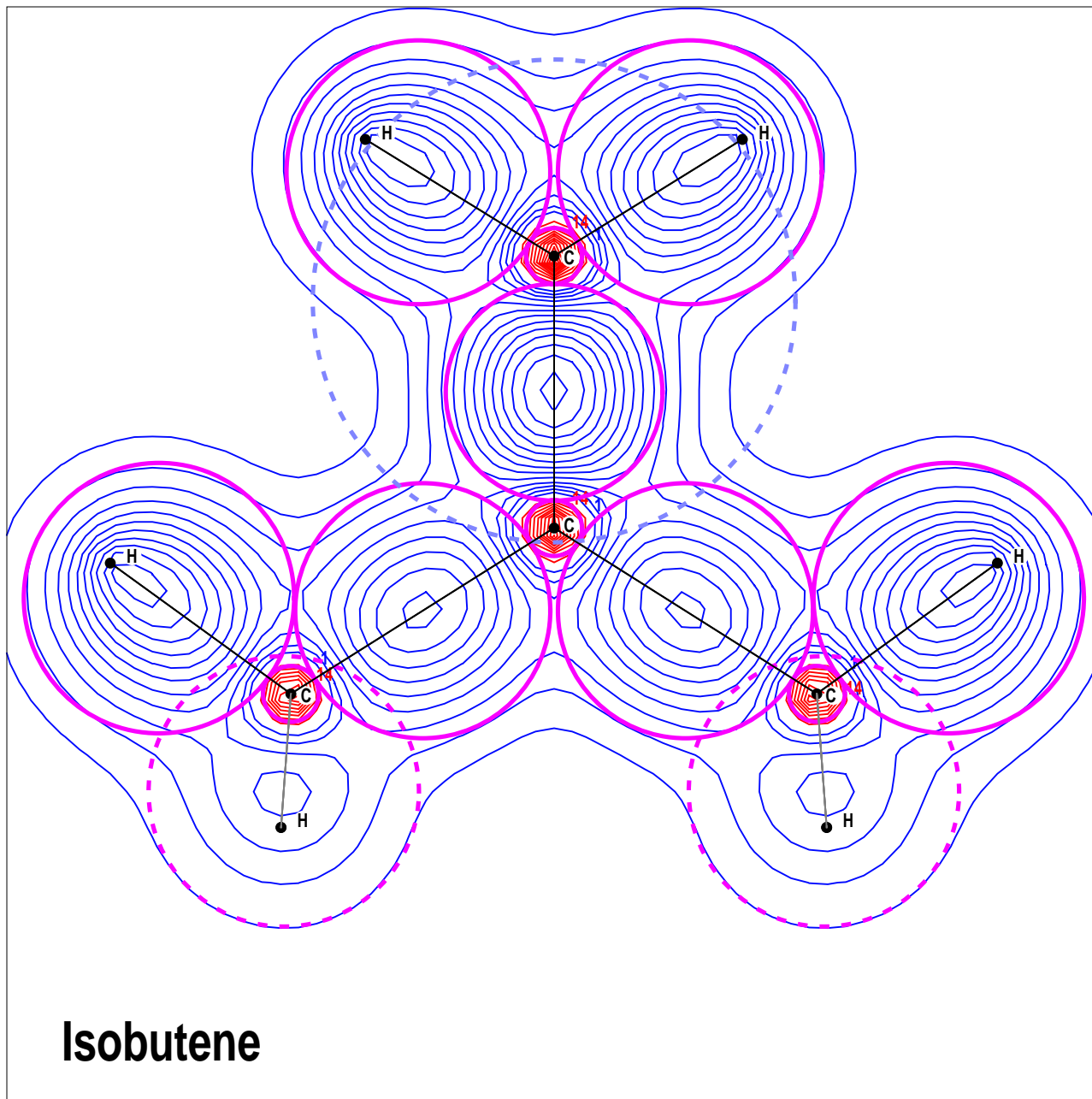
E = -156.12220 hartree (-V/T 2.000036)

Edge = 10.04 bohr

solid line: in plane; dashed: out of plane

magenta: sigma; blue: pi





# MOLDEN

## KIMBALL

Edge = 10.04 Overlay Contour Euclid

Contour for Gaussian98 RHF/6-31G\*\*(d,p)

E = -156.1238464 hartree, optimized

Overlay Kimball set G21205.prf

E = -156.12220 hartree, optimized

### 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	-0.01250
15	-0.02500
16	-0.03750
17	-0.05000
18	-0.06250
19	-0.07500
20	-0.08750
21	-0.10000
22	-0.11250
23	-0.12500
24	-0.13750
25	-0.15000