

KIMBALL

cyclo-Propanone, optimized Kimball run

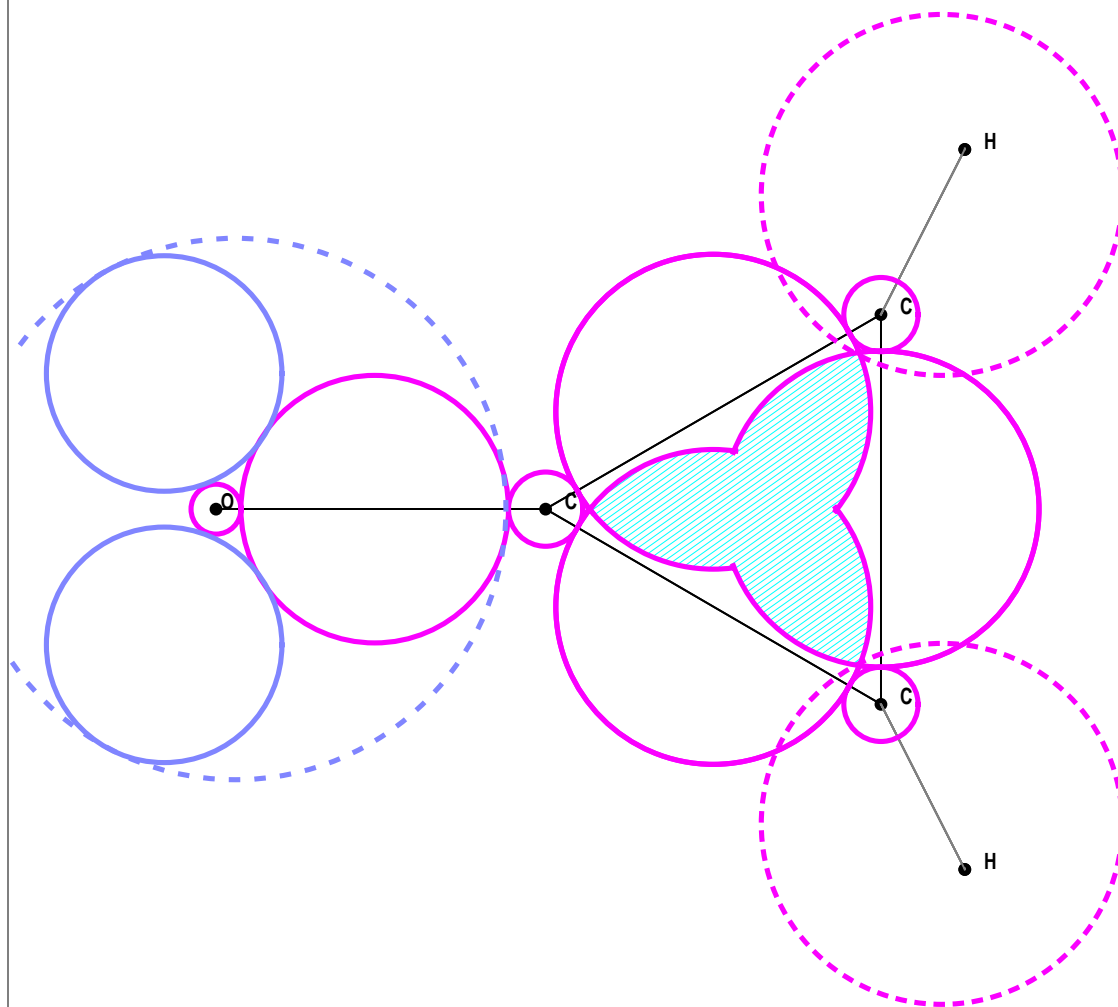
Parameter set: G21205.prf

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.



c-Propanone

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

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