BENZENO

File benzene.fchk Density MP2

Angstrom

Multipoles

Limit 2

Switch 4.0

Radius H 0.35

Punch file.punch

Add TOP1 0.0 0.0 2.00

Add TOP2 0.0 0.0 -2.00

Start

Finish

G D M A

by Anthony Stone

Distributed Multipoles from Gaussian wavefunctions

version 2.3.3 (e2d289a)

Compiled with gfortran on 05 October 2021 at 19:26:39

Starting at 19:48:52 on 03 Dec 2021

Using MP2 density matrix from file benzene.fchk

Distributed Multipole Analysis

Standard DMA for products of primitives with exponent greater than 4.00000

Using 80-point Euler-MacLaurin radial quadrature

Using 590-point Lebedev quadrature

Becke smoothing parameter = 3

Positions and radii in angstrom

Multipole moments in atomic units, ea\_0^k for rank k

C x = -0.000000 y = 1.394663 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050325

|Q1| = 0.152398 Q11s = -0.152398

|Q2| = 0.711237 Q20 = -0.689378 Q22c = -0.174975

C x = -1.207814 y = 0.697332 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050323

|Q1| = 0.152398 Q11c = 0.131981 Q11s = -0.076200

|Q2| = 0.711233 Q20 = -0.689375 Q22c = 0.087482 Q22s = -0.151530

C x = -1.207814 y = -0.697332 z = 0.000000 angstrom

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H x = -0.000000 y = 2.479089 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041400

|Q1| = 0.118058 Q11s = -0.118058

|Q2| = 0.192926 Q20 = -0.144046 Q22c = -0.128340

H x = -2.146954 y = 1.239545 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = 0.102245 Q11s = -0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = -0.111138

H x = -2.146954 y = -1.239545 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = 0.102245 Q11s = 0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = 0.111138

H x = -0.000000 y = -2.479089 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041400

|Q1| = 0.118058 Q11s = 0.118058

|Q2| = 0.192926 Q20 = -0.144046 Q22c = -0.128340

H x = 2.146954 y = -1.239545 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = -0.102245 Q11s = 0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = -0.111138

H x = 2.146954 y = 1.239545 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = -0.102245 Q11s = -0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = 0.111138

TOP1 x = 0.000000 y = 0.000000 z = 2.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = -0.275170

|Q1| = 0.289518 Q10 = 0.289518

|Q2| = 0.192943 Q20 = 0.192943 Q22c = 0.000002

TOP2 x = 0.000000 y = 0.000000 z = -2.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = -0.275170

|Q1| = 0.289518 Q10 = -0.289518

|Q2| = 0.192943 Q20 = 0.192943 Q22c = 0.000002

Total multipoles referred to origin at

x = 0.000000, y = 0.000000, z = 0.000000 angstrom

Q00 = -0.000000

|Q1| = 0.000000

|Q2| = 6.145000 Q20 = -6.145000 Q22c = -0.000285

CPU time used: 1m17.217s Total: 1m17.217s

Finished at 19:50:09 on 03 Dec 2021