

INPUT Benzene

```
#hf/6-31G(d,p) aim scf=tight
```

```
benzene - aim analysis
```

```
0 1
C    0.695 -1.204  0.000000
C    1.391  0.000  0.000000
C    0.695  1.204  0.000000
C   -0.695  1.204  0.000000
C   -1.391  0.000  0.000000
C   -0.695 -1.204  0.000000
H    1.242 -2.152  0.000000
H    2.485  0.000  0.000000
H    1.242  2.152  0.000000
H   -1.242  2.152  0.000000
H   -2.485  0.000  0.000000
H   -1.242 -2.152  0.000000
```

Or if the wavefunction is needed for further visualization use the output=wfn option

```
#hf/6-31G(d,p) aim output=wfn
```

```
benzene
```

```
0 1
C    0.695 -1.204  0.000000
C    1.391  0.000  0.000000
C    0.695  1.204  0.000000
C   -0.695  1.204  0.000000
C   -1.391  0.000  0.000000
C   -0.695 -1.204  0.000000
H    1.242 -2.152  0.000000
H    2.485  0.000  0.000000
H    1.242  2.152  0.000000
H   -1.242  2.152  0.000000
H   -2.485  0.000  0.000000
H   -1.242 -2.152  0.000000
```

c6h6.wfn

file which will be generated

OUTPUT Benzene

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.204000	0.695000
2	6	0	0.000000	0.000000	1.391000
3	6	0	0.000000	-1.204000	0.695000
4	6	0	0.000000	-1.204000	-0.695000
5	6	0	0.000000	0.000000	-1.391000
6	6	0	0.000000	1.204000	-0.695000
7	1	0	0.000000	2.152000	1.242000
8	1	0	0.000000	0.000000	2.485000
9	1	0	0.000000	-2.152000	1.242000
10	1	0	0.000000	-2.152000	-1.242000
11	1	0	0.000000	0.000000	-2.485000
12	1	0	0.000000	2.152000	-1.242000

....

This link is based on concepts and algorithms described in:

JCP 106 (1997) 3607, JCP 105 (1996) 8741,
MolPhys 88 (1996) 621, CPL 255 (1996) 315, CPL 256 (1996) 449,
MolPhys 84 (1995) 707, JCompChem 16 (1995) 1394,
CPL 219 (1994) 151, CPL 203 (1993) 137, CPL 194 (1992) 73,
JACS 114 (1992) 4392, THEOCHEM 255 (1992) 9, JACS 113 (1991) 4142,
IJQC S24 (1990) 15.

Accuracy reduced in fast calculations of atomic charges.

(Spin)orbitals with zero occupancies ignored.

Primitives contributing lt. 0.1E-04 neglected in density calculations.

PrimPairs contributing lt. 0.1E-04 neglected in atomic integrations.

MxBpIt=10, SBpMax= 2.0, NGrd=20, LookUp=100, NTrig=20, GueDis=0.1E-05,
HowFar= 5.0, PraInf=20.0, RScale= 2.0, NInCho= 7, RtFSec=20.0,
TolerR=0.1E-09, NInGrd=20, EpsInt=0.10E-01, EpsSfF= 6.0, NStRK=20,
IPrSma=0, MIILoc=10, ITILoc= 7, IDcInt=10, IPrLoc=0.

Properties of atoms in molecules using the SCF density.

I. ATTRACTORS

Attr.	Cartesian Coordinates			Nucleus (Distance)	Density	
	X	Y	Z		Total	Spin
1	0.000000	2.275231	1.313360	C (0.000001)	0.11816E+03	0.00000E+00
2	0.000000	0.000000	2.628610	C (0.000001)	0.11816E+03	0.00000E+00
3	0.000000	-2.275231	1.313360	C (0.000001)	0.11816E+03	0.00000E+00
4	0.000000	-2.275231	-1.313360	C (0.000001)	0.11816E+03	0.00000E+00
5	0.000000	0.000000	-2.628610	C (0.000001)	0.11816E+03	0.00000E+00
6	0.000000	2.275231	-1.313360	C (0.000001)	0.11816E+03	0.00000E+00
7	0.000000	4.029358	2.325497	H (0.043102)	0.42690E+00	0.00000E+00
8	0.000000	0.000000	4.652828	H (0.043141)	0.42710E+00	0.00000E+00
9	0.000000	-4.029358	2.325497	H (0.043102)	0.42690E+00	0.00000E+00
10	0.000000	-4.029358	-2.325497	H (0.043102)	0.42690E+00	0.00000E+00
11	0.000000	0.000000	-4.652828	H (0.043141)	0.42710E+00	0.00000E+00
12	0.000000	4.029358	-2.325497	H (0.043102)	0.42690E+00	0.00000E+00

12 (3, -3) critical points were found (see standard orientation, however here the coordinates are given in $a_0 = 0.529189 \text{ \AA}$) according to 6 C and 6 H atoms.

II. CRITICAL POINTS ON ATTRACTOR INTERACTION LINES

Line	Attractors		Cartesian Coordinates			Density	
	A	B	X	Y	Z	Total	Spin
1	2	1	0.000000	1.140024	1.975179	0.32446E+00	0.00000E+00
2	3	2	0.000000	-1.140024	1.975179	0.32446E+00	0.00000E+00
3	4	3	0.000000	-2.279833	0.000000	0.32488E+00	0.00000E+00
4	5	4	0.000000	-1.140024	-1.975179	0.32446E+00	0.00000E+00
5	6	1	0.000000	2.279833	0.000000	0.32488E+00	0.00000E+00
6	6	5	0.000000	1.140024	-1.975179	0.32446E+00	0.00000E+00
7	7	1	0.000000	3.381063	1.951413	0.28521E+00	0.00000E+00
8	8	2	0.000000	0.000000	3.904735	0.28550E+00	0.00000E+00
9	9	3	0.000000	-3.381063	1.951413	0.28521E+00	0.00000E+00
10	10	4	0.000000	-3.381063	-1.951413	0.28521E+00	0.00000E+00
11	11	5	0.000000	0.000000	-3.904735	0.28550E+00	0.00000E+00
12	12	6	0.000000	3.381063	-1.951413	0.28521E+00	0.00000E+00

The existence of a (3, -1) critical point between C1 and C2 (attractor A = 1 and B = 2) indicates a bond between these two centers.

Finally 12 "bonds" are found corresponding to 6 C-C and 6 C-H bonds.

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II-1. RING POINTS

Ring	Cartesian Coordinates			Attractors					
	X	Y	Z	1	2	3	4	5	6
1 (6-membered)	0.000000	0.000000	0.000000	1	2	3	4	5	6

One ring: (3, +1) critical point was found involving all 6 C atoms (attractors belonging to the C atoms)

12 attractors - 12 bond point(s) + 1 ring point(s) - 0 cage point(s) = 1

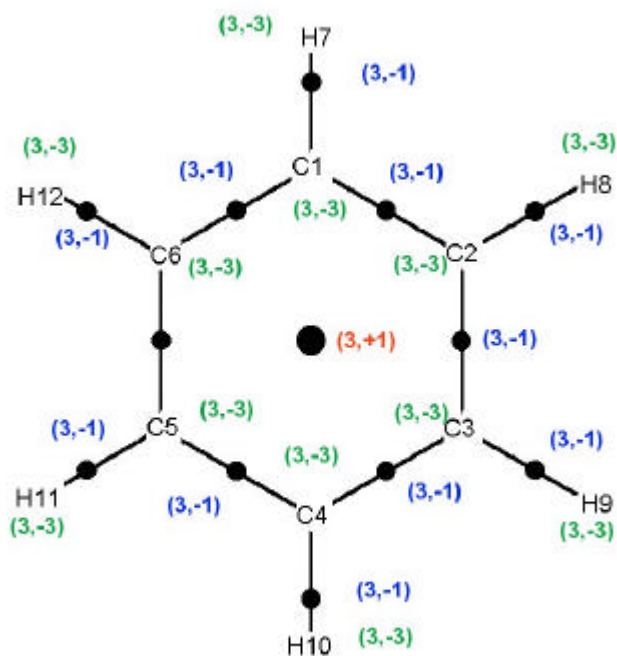


Abb.2: Benzol, Molekularer Graph

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III. PROPERTIES OF ATTRACTORS

Attr.	Number of electrons		Charge
	total	spin	
1	5.970620	0.000000	0.029380
2	5.970471	0.000000	0.029529
3	5.970620	0.000000	0.029380
4	5.970620	0.000000	0.029380
5	5.970471	0.000000	0.029529
6	5.970620	0.000000	0.029380
7	1.031643	0.000000	-0.031643
8	1.031557	0.000000	-0.031557
9	1.031643	0.000000	-0.031643
10	1.031643	0.000000	-0.031643
11	1.031557	0.000000	-0.031557
12	1.031643	0.000000	-0.031643
Total	42.013108	0.000000	-0.013108

Attr.	Kinetic energy			Dipole moment		
	G	K	L	X	Y	Z
1	0.377464E+02	0.377459E+02	-0.515E-03	0.000000	-0.023926	-0.014330
2	0.377459E+02	0.377453E+02	-0.518E-03	0.000000	0.000000	-0.027366
3	0.377464E+02	0.377459E+02	-0.515E-03	0.000000	0.023926	-0.014330
4	0.377464E+02	0.377459E+02	-0.515E-03	0.000000	0.023926	0.014330
5	0.377459E+02	0.377453E+02	-0.518E-03	0.000000	0.000000	0.027366
6	0.377464E+02	0.377459E+02	-0.515E-03	0.000000	-0.023926	0.014330
7	0.634395E+00	0.634282E+00	-0.113E-03	0.000000	-0.085607	-0.049390
8	0.634614E+00	0.634502E+00	-0.112E-03	0.000000	0.000000	-0.098809
9	0.634395E+00	0.634282E+00	-0.113E-03	0.000000	0.085607	-0.049390
10	0.634395E+00	0.634282E+00	-0.113E-03	0.000000	0.085607	0.049390
11	0.634614E+00	0.634502E+00	-0.112E-03	0.000000	0.000000	0.098809
12	0.634395E+00	0.634282E+00	-0.113E-03	0.000000	-0.085607	0.049390
Total	0.230284E+03	0.230280E+03	-0.377E-02	0.000000	0.000000	0.000000

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1|1|UNPC-UNK|SP|RHF|6-31G(d,p)|C6H6|PCUSER|04-Jul-2001|0|#HF/6-31G(D,
P) AIM||benzene||0,1|C,0,0.695,-1.204,0.|C,0,1.391,0.,0.|C,0,0.695,1.2
04,0.|C,0,-0.695,1.204,0.|C,0,-1.391,0.,0.|C,0,-0.695,-1.204,0.|H,0,1.
242,-2.152,0.|H,0,2.485,0.,0.|H,0,1.242,2.152,0.|H,0,-1.242,2.152,0.|H
,0,-2.485,0.,0.|H,0,-1.242,-2.152,0.||Version=x86-Win32-G98RevA.9|Stat
e=1-AG|HF=-230.7123161|RMSD=3.063e-006|Dipole=0.,0.,0.|PG=D02H [C2"(H1
C1.C1H1),SG(C4H4)]||@

Benzene.wfn file

Output

The „output file“ is the same as without the output option, but a new file will be generated:

Writing a WFN file to c6h6.wfn.

Wfn file

```
benzene
GAUSSIAN          21 MOL ORBITALS   210 PRIMITIVES   12 NUCLEI
C  1 (CENTRE 1)  0.00000000  2.27523009  1.31335956  CHARGE = 6.0
C  2 (CENTRE 2)  0.00000000  0.00000000  2.62860885  CHARGE = 6.0
C  3 (CENTRE 3)  0.00000000 -2.27523009  1.31335956  CHARGE = 6.0
C  4 (CENTRE 4)  0.00000000 -2.27523009 -1.31335956  CHARGE = 6.0
C  5 (CENTRE 5)  0.00000000  0.00000000 -2.62860885  CHARGE = 6.0
C  6 (CENTRE 6)  0.00000000  2.27523009 -1.31335956  CHARGE = 6.0
H  7 (CENTRE 7)  0.00000000  4.06669033  2.34703968  CHARGE = 1.0
H  8 (CENTRE 8)  0.00000000  0.00000000  4.69596908  CHARGE = 1.0
H  9 (CENTRE 9)  0.00000000 -4.06669033  2.34703968  CHARGE = 1.0
H 10 (CENTRE 10) 0.00000000 -4.06669033 -2.34703968  CHARGE = 1.0
H 11 (CENTRE 11) 0.00000000  0.00000000 -4.69596908  CHARGE = 1.0
H 12 (CENTRE 12) 0.00000000  4.06669033 -2.34703968  CHARGE = 1.0
CENTRE ASSIGNMENTS 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CENTRE ASSIGNMENTS 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2
CENTRE ASSIGNMENTS 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3
CENTRE ASSIGNMENTS 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
CENTRE ASSIGNMENTS 3 3 3 3 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
CENTRE ASSIGNMENTS 4 4 4 4 4 4 4 4 4 4 4 4 4 4 5 5 5 5 5 5 5 5
CENTRE ASSIGNMENTS 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
CENTRE ASSIGNMENTS 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
CENTRE ASSIGNMENTS 6 6 6 6 6 6 6 6 7 7 7 7 7 7 7 7 8 8 8 8 8 8
CENTRE ASSIGNMENTS 8 8 9 9 9 9 9 9 9 10 10 10 10 10 10 10 11 11 11 11 11
CENTRE ASSIGNMENTS 11 11 11 12 12 12 12 12 12 12 12
TYPE ASSIGNMENTS   1 1 1 1 1 1 1 1 1 2 2 2 3 3 3 4 4 4 1 2
TYPE ASSIGNMENTS   3 4 5 6 7 8 9 10 1 1 1 1 1 1 1 1 1 2 2 2
TYPE ASSIGNMENTS   3 3 3 4 4 4 1 2 3 4 5 6 7 8 9 10 1 1 1 1
TYPE ASSIGNMENTS   4 4 1 2 3 4 5 6 7 8 9 10 1 1 1 1 1 1 1
TYPE ASSIGNMENTS   3 4 1 1 1 1 2 3 4 1 1 1 1 2 3 4 1 1 1 1
TYPE ASSIGNMENTS   2 3 4 1 1 1 1 2 3 4
EXPONENTS
...
MOs
...

END DATA
THE HF ENERGY = -230.712316121408 THE VIRIAL(-V/T)= 2.00189699
```

Li-F example

INPUT

#hf/6-31G(d) aim scf=tight

LiF

0 1

Li

F 1 1.3

OUTPUT

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	3	0	0.000000	0.000000	-0.975000
2	9	0	0.000000	0.000000	0.325000

Properties of atoms in molecules using the SCF density.

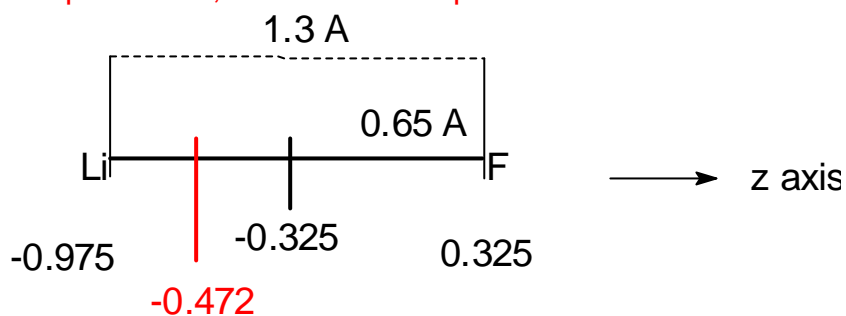
I. ATTRACTORS

Attr.	Cartesian Coordinates			Nucleus	Density	
	X	Y	Z	(Distance)	Total	Spin
1	0.000000	0.000000	-1.842550	Li (0.000067)	0.13164E+02	0.00000E+00
2	0.000000	0.000000	0.614159	F (0.000002)	0.41862E+03	0.00000E+00

II. CRITICAL POINTS ON ATTRACTOR INTERACTION LINES

Line	Attractors		Cartesian Coordinates			Density	
	A	B	X	Y	Z	Total	Spin
1	2	1	0.000000	0.000000	-0.891268	0.16435E+00	0.00000E+00

In a polar bond, the bond critical point is found closer to the electropositive atom.



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2 attractors - 1 bond point(s) + 0 ring point(s) - 0 cage point(s) = 1

III. PROPERTIES OF ATTRACTORS

Attr.	Number of electrons total	spin	Charge
1	2.079170	0.000000	0.920830
2	9.921736	0.000000	-0.921736
Total	12.000906	0.000000	-0.000906

In accordance with the NBO analysis, the AIM charges agree with the ionic bond model in Li^+F^- . (Mulliken analysis overestimates the covalent character: $q(\text{Li}) = 0.614e$).

Attr.	Kinetic energy			Dipole moment		
	G	K	L	X	Y	Z
1	0.756642E+01	0.756111E+01	-0.531E-02	0.000000	0.000000	0.029026
2	0.996403E+02	0.996421E+02	0.186E-02	0.000000	0.000000	0.205255
Total	0.107207E+03	0.107203E+03	-0.345E-02	0.000000	0.000000	0.234281

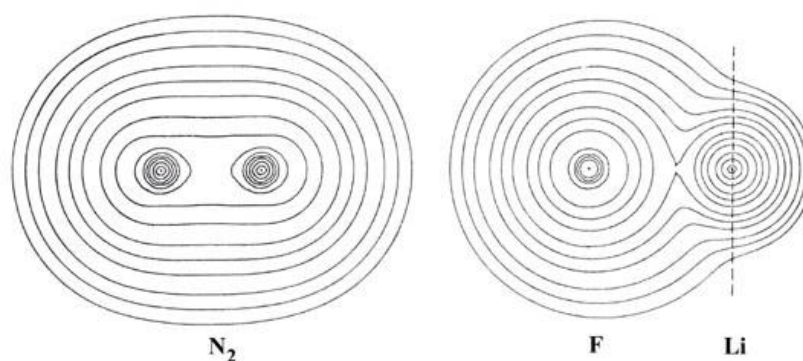
...

```
1|1|UNPC-UNK|SP|RHF|6-31G(d)|F1Li1|PCUSER|26-Jan-2004|0|#HF/6-31G(D)
AIM SCF=TIGHT|lif|0,1|Li|F,1,1.3|Version=x86-Win32-G03RevB.03|State
=1-SG|HF=-106.8950603|RMSD=1.643e-009|Dipole=0.,0.,-2.028179|PG=C*V [C
*(Li1F1)]|@
```


Ionic and Covalent Binding

The distribution of negative charge in a molecule will exhibit varying degrees of asymmetry depending on the relative abilities of the nuclei in the molecule to attract and bind the electronic charge density. The symmetry or asymmetry of the charge distribution plays a fundamental role in determining the chemical properties of the molecule and consequently this property of the charge distribution is used as a basis for the classification of chemical bonds.

We can envisage two extremes for the distribution of the valence charge density. An example of one of the extremes is obtained when a bond is formed between two identical atoms. The charge density of the valence electrons will in this case necessarily be delocalized equally over corresponding regions of each nucleus since both nuclei will attract the electron density with equal force. Such an equal *sharing of the charge* density is an example of *covalent binding* and is exemplified by the molecular charge distribution of N_2 .



Contour maps of the molecular charge distributions of N_2 and LiF at their equilibrium internuclear separations. The space to the right of the dashed line through the Li nucleus denotes the region of nonbonded charge density. The values of the contours increase from the outermost one to the innermost one.

The charge distribution of LiF provides an example of the other extreme, termed *ionic binding*, obtained when a bond is formed between two atoms with very different affinities for the electronic charge density. The very unsymmetrical distribution of charge in LiF is not simply a reflection of the fluorine atom possessing seven valence electrons to lithium's one. Instead the formation of the bond in LiF corresponds to the nearly **complete transfer of the valence charge density of lithium to fluorine** resulting in a molecule best described as Li^+F^- . We need only recall that initially a lithium atom is considerably larger than a fluorine atom to realize that a considerable transfer of charge has occurred in the formation of the LiF molecule.

In N_2 the valence charge density is delocalized over the whole molecule. The electronic charge is heavily concentrated in the internuclear region where it forms a bridge of high density between the two nuclei. Only the density of the $1s$ inner shell or "core" orbitals is strongly localized in the regions of the nuclei. In contrast to this, practically all of the charge density in the lithium fluoride molecule is localized in nearly spherical contours on the two nuclei in the manner characteristic of two separate closed-shell distributions. Only contours of very small value encompass both nuclei and the bridge of charge density joining the two spherical distributions is very low in value, being approximately one tenth of the value observed for N_2 .