

Supporting information for: **New accurate reference energies for the G2/97 test set**

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All TURBOMOLE calculations used the revision 15240 of the development version from November 17, 2010. All CFOUR calculations employed the official release version 1.2 from June 2010.

The detailed F12 options used in TURBOMOLE are:

```
$rir12
  ansatz      2
  r12model    B
  comaprox    F+K
  cabs        svd  1.0000E-08
  examp       fixed  flip
  corrfac     LCG
  cabsingles  on

$lcg
  nlcg        6
  slater      1.1000
```

Closed-shell systems were calculated with `examp fixed noflip` rather than `examp fixed flip`.

MRCC was invoked by CFOUR via the keywords:

```
CC_PROG=MRCC,
INPUT_MRCC=1
```

The STG-6G Slater-type geminal with Slater exponent 1.1 a_0^{-1} is constructed as follows

Exponent	Contraction coefficient
0.267289	-0.285818181818
1.214840	-0.276090909091
4.382620	-0.152818181818
14.713600	-0.089190909091
55.502700	-0.054763636364

307.824000 -0.033872727273

Geometries for molecules and radicals of the G2/97 test set in Bohr (the format is x, y, and z coordinates and atom symbol):

- CO, Carbon monoxide:

0.0000000000000000	0.0000000000000000	0.91590490318248	o
0.0000000000000000	0.0000000000000000	-1.22120716748535	c

- CS, Carbon monosulfide:

0.0000000000000000	0.0000000000000000	-2.11777450315002	c
0.0000000000000000	0.0000000000000000	0.79416496624972	s

- H₂, Dihydrogen:

0.0000000000000000	0.0000000000000000	0.70183483712306	h
0.0000000000000000	0.0000000000000000	-0.70183483712306	h

- HF, Hydrogen fluoride:

0.0000000000000000	0.0000000000000000	0.17375275901430	f
0.0000000000000000	0.0000000000000000	-1.56377105167646	h

- P₂, Diphosphorus:

0.0000000000000000	0.0000000000000000	1.79081408763814	p
0.0000000000000000	0.0000000000000000	-1.79081408763814	p

- S₂, Disulfur:

0.0000000000000000	0.0000000000000000	1.80672558167704	s
0.0000000000000000	0.0000000000000000	-1.80672558167704	s

- HS, Hydrogensulfuryl radical:

0.0000000000000000	0.0000000000000000	0.15007449056925	s
0.0000000000000000	0.0000000000000000	-2.40118240047728	h

- OS, Triplet sulfur oxide:

0.0000000000000000	0.0000000000000000	-1.88571802375779	o
0.0000000000000000	0.0000000000000000	0.94285995674196	s

- C₂H, Acetyl radical:

0.02540736785665	-1.382988511447830	0.0000000000000000	c
0.025407367856650	.90201730583191	0.0000000000000000	c
-0.30489408345817	2.885821564517130	0.0000000000000000	h

- CF₄, Tetrafluoromethane:

0.0000000000000000	0.0000000000000000	0.0000000000000000	c
1.441730648288581	.44173064828858	1.44173064828858	f
-1.44173064828858	-1.441730648288581	.44173064828858	f
-1.44173064828858	1.44173064828858	-1.44173064828858	f
1.44173064828858	-1.44173064828858	-1.44173064828858	f

- CH₄, Methane:

0.0000000000000000	0.0000000000000000	0.0000000000000000	c
1.191249339100721	.19124933910072	1.19124933910072	h

-1.19124933910072	-1.19124933910072	1.19124933910072	h
1.19124933910072	-1.19124933910072	-1.19124933910072	h
-1.19124933910072	1.19124933910072	-1.19124933910072	h

- **CO₂, Carbon dioxide:**

0.0000000000000000	.0000000000000000	0.0000000000000000	c
0.0000000000000000	.0000000000000000	2.19752283568392	o
0.0000000000000000	.0000000000000000	-2.19752283568392	o

- **CS₂, Carbon disulfide:**

0.0000000000000000	.0000000000000000	2.94051779770737	s
0.0000000000000000	.0000000000000000	0.0000000000000000	c
0.0000000000000000	.0000000000000000	-2.94051779770737	s

- **OF₂, Difluorine monoxide:**

0.0000000000000002	.07596809191219	-0.50052987109129	f
0.0000000000000000	.0000000000000000	1.12619173752386	o
0.0000000000000000	-2.07596809191219	-0.50052987109129	f

- **BeH, Beryllium hydride:**

0.0000000000000000	.0000000000000000	0.50788468520048	be
0.0000000000000000	.0000000000000000	-2.03154252025418	h

- **H₂O, Water:**

0.0000000000000000	.0000000000000000	0.22457505363213	o
0.0000000000000001	.42991985995804	-0.89830210425465	h
0.0000000000000000	-1.42991985995804	-0.89830210425465	h

- H₂S, Hydrogen sulfide:

0.0000000000000000	0.0000000000000000	0.19548083009022	s
0.0000000000000001	.83520375449963	-1.56384664072178	h
0.0000000000000000	-1.83520375449963	-1.56384664072178	h

- Cl₂, Dioxygen:

0.0000000000000000	0.0000000000000000	1.90529936594675	cl
0.0000000000000000	0.0000000000000000	-1.90529936594675	cl

- CNH, Hydrogen cyanide:

0.0000000000000000	0.0000000000000000	-0.94426969243710	c
0.0000000000000000	0.0000000000000000	1.23220726330488	n
0.0000000000000000	0.0000000000000000	-2.95982890905933	h

- CHO, Hydrogen carbonyl:

0.117826314111551	.10586773296468	0.0000000000000000	c
0.11782631411155	-1.116847041796740	0.0000000000000000	o
-1.64955705920494	2.299569936585880	0.0000000000000000	h

- HCl, Hydrogen chloride:

0.0000000000000000	0.0000000000000000	0.13476581916674	cl
0.0000000000000000	0.0000000000000000	-2.29102459501297	h

- N₂O, Nitrous oxide:

0.0000000000000000	0.0000000000000000	-2.26786978070672	n
0.0000000000000000	0.0000000000000000	-0.13674436242787	n
0.0000000000000000	0.0000000000000000	2.10403808389007	o

- **NF₃, Trifluoroamine:**

0.0000000000000000	0.0000000000000000	0.91024517341449	n
0.0000000000000002	.32751520663899	-0.23598899947476	f
2.01568771799927	-1.16375760331950	-0.23598899947476	f
-2.01568771799927	-1.16375760331950	-0.23598899947476	f

- **NO₂, Doublet nitrosyl radical:**

0.0000000000000000	0.0000000000000000	0.61013776625092	n
0.0000000000000002	.08234024843228	-0.26693515462689	o
0.0000000000000000	-2.08234024843228	-0.26693515462689	o

- **Li₂, Dilithium:**

0.0000000000000000	0.0000000000000000	2.57123696544952	li
0.0000000000000000	0.0000000000000000	-2.57123696544952	li

- **LiF, Lithiumfluoride:**

0.0000000000000000	0.0000000000000000	-2.21607616685660	li
0.0000000000000000	0.0000000000000000	0.73869205561887	f

- **LiH, Lithiumhydride:**

0.0000000000000000	0.0000000000000000	0.76275393846890	li
0.0000000000000000	0.0000000000000000	-2.28826370513283	h

- **PF₃, Phosphorus trifluoride:**

0.0000000000000000	0.0000000000000000	0.94459850478422	p
0.0000000000000002	.59082397681688	-0.52477694710234	f
2.24371908072845	-1.29541104354537	-0.52477694710234	f
-2.24371908072845	-1.29541104354537	-0.52477694710234	f

- PH₃, Phosphane:

0.0000000000000000	0.0000000000000000	0.24359703688576	p
0.0000000000000002	.25506688615642	-1.21798707415492	h
1.95294692066133	-1.12753344307821	-1.21798707415492	h
-1.95294692066133	-1.12753344307821	-1.21798707415492	h

- Na₂, Disodium:

0.0000000000000000	0.0000000000000000	2.84872246107632	na
0.0000000000000000	0.0000000000000000	-2.84872246107632	na

- O₂S, Sulfur dioxide:

0.0000000000000000	0.0000000000000000	0.68948547684466	s
0.0000000000000002	.35152984633571	-0.68948547684466	o
0.0000000000000000	-2.35152984633571	-0.68948547684466	o

- SiO, Singlet silicon monoxide:

0.0000000000000000	0.0000000000000000	1.03957236077078	si
0.0000000000000000	0.0000000000000000	-1.81925257621194	o

- C₅H₈, Spiropentane:

0.0000000000000000	0.0000000000000000	0.0000000000000000	c
0.0000000000000001	.44394162786405	2.39850654827311	c
0.0000000000000000	-1.443941627864052	2.39850654827311	c
1.443941627864050	0.0000000000000000	-2.39850654827311	c
-1.44394162786405	0.0000000000000000	-2.39850654827311	c
-1.72364944142312	2.397448301638692	.97368627079178	h

1.723649441423122.39744830163869	2.97368627079178	h
-1.72364944142312 -2.397448301638692.97368627079178		h
1.72364944142312 -2.397448301638692.97368627079178		h
2.39744830163869 -1.72364944142312 -2.97368627079178		h
2.397448301638691.72364944142312 -2.97368627079178		h
-2.39744830163869 -1.72364944142312 -2.97368627079178		h
-2.39744830163869 1.72364944142312 -2.97368627079178		h

• **C₃H₄, Allene:**

0.0000000000000000.0000000000000000	0.0000000000000000	c
0.0000000000000000.0000000000000000	2.45928769961124	c
0.0000000000000000.0000000000000000	-2.45928769961124	c
0.0000000000000001.74953679971752	3.53271072460041	h
0.0000000000000000 -1.749536799717523.53271072460041		h
1.749536799717520.0000000000000000	-3.53271072460041	h
-1.74953679971752 0.0000000000000000	-3.53271072460041	h

• **C₂H₃, Ethenyl radical:**

0.09074464890117 -1.106559372729310.0000000000000000		c
0.090744648901171.36054612389368 0.0000000000000000		c
-1.65909828644988 -2.208437893827470.0000000000000000		h
1.82769209312141 -2.209070952081990.0000000000000000		h
-1.25754093184235 2.893588338923290.0000000000000000		h

• **C₂H₅, Ethyl radical:**

-0.02074541348682 -1.309731388180380.0000000000000000		c
-0.02074541348682 1.501502685871750.0000000000000000		c

1.91221387386698	-2.094496856645130	.0000000000000000	h
-0.95999977276724	-2.082196629246181	.67575055313287	h
-0.95999977276724	-2.08219662924618	-1.67575055313287	h
0.128367206480792	.55413305422077	1.75068197375405	h
0.128367206480792	.55413305422077	-1.75068197375405	h

- **CCl₄, Tetrachloromethane:**

0.0000000000000000	.0000000000000000	0.0000000000000000	c
1.946652242912691	.94665224291269	1.94665224291269	cl
-1.94665224291269	-1.946652242912691	.94665224291269	cl
-1.94665224291269	1.94665224291269	-1.94665224291269	cl
1.94665224291269	-1.94665224291269	-1.94665224291269	cl

- **CH₃O, Methyl oxo radical:**

-0.02114036624859	-1.079404008199750	.0000000000000000	c
-0.02114036624859	1.494418102599560	.0000000000000000	o
2.00183413571908	-1.639707806600340	.0000000000000000	h
-0.85292977980407	-1.919608372224961	.71696359036497	h
-0.85292977980407	-1.91960837222496	-1.71696359036497	h

- **CH₃S, Methyl sulfo radical:**

-0.00859447445236	2.097890804779790	.0000000000000000	c
-0.00859447445236	-1.311653239657530	.0000000000000000	s
1.982043033929372	.68129083597652	0.0000000000000000	h
-0.89648796716708	2.858906195206441	.70034155930011	h
-0.89648796716708	2.85890619520644	-1.70034155930011	h

- **CHF₃, Trifluoromethane:**

0.0000000000000000	0.0000000000000000	0.63493475256665	c
0.0000000000000000	0.0000000000000000	2.70495776606478	h
0.0000000000000002	.36285686477622	-0.24128023264684	f
2.04629372244748	-1.18142843238811	-0.24128023264684	f
-2.04629372244748	-1.18142843238811	-0.24128023264684	f

- **COF₂, Carbonyl fluoride:**

0.0000000000000000	0.0000000000000000	2.48633912920350	o
0.0000000000000000	0.0000000000000000	0.26634367034730	c
0.0000000000000002	.00416038858867	-1.19382125636757	f
0.0000000000000000	-2.00416038858867	-1.19382125636757	f

- **AlF₃, Aluminum trifluoride:**

0.0000000000000000	0.0000000000000000	0.0000000000000000	al
0.0000000000000003	.08313542895625	0.0000000000000000	f
2.67007342165171	-1.541566769615060	0.0000000000000000	f
-2.67007342165171	-1.541566769615060	0.0000000000000000	f

- **CH₂O, Formaldehyde:**

0.0000000000000000	0.0000000000000000	1.27470909375961	o
0.0000000000000000	0.0000000000000000	-0.99288667665784	c
0.0000000000000001	.77087936666233	-2.12017256561265	h
0.0000000000000000	-1.77087936666233	-2.12017256561265	h

- **H₂O₂, Hydrogen peroxide:**

0.0000000000000001	.36610947762889	-0.11119715483739	o
0.0000000000000000	-1.36610947762889	-0.11119715483739	o

1.493161434721191.69761846394262 0.88957912842525 h
-1.49316143472119 -1.697618463942620.88957912842525 h

• **F₃Cl, Chlorine trifluoride:**

0.0000000000000000.0000000000000000 0.68952138164118 cl
0.0000000000000000.0000000000000000 -2.38313551590822 f
0.00000000000000003.23632229846636 0.54035395961572 f
0.0000000000000000 -3.236322298466360.54035395961572 f

• **NOCl, Nitrosylchloride:**

-0.99783208994761 -1.777880801984670.0000000000000000 cl
0.00000000000000001.84609991538185 0.0000000000000000 n
2.120395553296332.16265927825832 0.0000000000000000 o

• **HOCl, Hydroxyl chloride:**

0.068700993561062.09452898198939 0.0000000000000000 o
-1.71751350066964 2.489415603347840.0000000000000000 h
0.06870099356106 -1.132097131689130.0000000000000000 cl

• **NaCl, Sodiumchloride:**

0.0000000000000000.0000000000000000 -2.70858415051378 na
0.0000000000000000.0000000000000000 1.75261327386186 cl

• **SiF₄, Silicon tetrafluoride:**

0.0000000000000000.0000000000000000 0.0000000000000000 si
1.707240949411281.70724094941128 1.70724094941128 f

-1.70724094941128	-1.70724094941128	1.70724094941128	f
-1.70724094941128	1.70724094941128	-1.70724094941128	f
1.70724094941128	-1.70724094941128	-1.70724094941128	f

• **SiH₃, Silyl radical:**

0.0000000000000000	0.0000000000000000	0.15211350506663	si
0.0000000000000002	.67019625385034	-0.70986806291396	h
2.31245786881216	-1.33509907178824	-0.70986806291396	h
-2.31245786881216	-1.33509907178824	-0.70986806291396	h

• **SiH₄, Silane:**

0.0000000000000000	0.0000000000000000	0.0000000000000000	si
1.617371243709631	.61737124370963	1.61737124370963	h
-1.61737124370963	-1.617371243709631	.61737124370963	h
-1.61737124370963	1.61737124370963	-1.61737124370963	h
1.61737124370963	-1.61737124370963	-1.61737124370963	h

• **C₃H₇Cl, 1-Propyl chloride:**

1.72239088381862	-1.190897850040000	0.0000000000000000	c
4.51562531645502	-0.418409932260610	0.0000000000000000	c
0.0000000000000001	.11166730246650	0.0000000000000000	c
1.30157533019085	-2.351696142235401	.66065353105725	h
1.30157533019085	-2.35169614223540	-1.66065353105725	h
5.73400923309784	-2.087877146001630	0.0000000000000000	h
-3.31165056157545	0.223879634415230	0.0000000000000000	cl
4.989496820989680	.70634939285453	-1.67176323099248	h
4.989496820989680	.70634939285453	1.67176323099248	h

0.276911018882402.27923459366990	1.67762138200443	h
0.276911018882402.27923459366990	-1.67762138200443	h

- N_2H_4 , Hydrazine:

0.0000000000000001.35765295318423	-0.14944143231473	n	
0.0000000000000000	-1.35765295318423	-0.14944143231473	n
0.427990843754342.06690118592660	1.58875890033161	h	
-1.79352962409110	1.91196254029131	-0.54267454330690	h
-0.42799084375434	-2.06690118592660	1.58875890033161	h
1.79352962409110	-1.91196254029131	-0.54267454330690	h

- CH_2O_2 , Formic acid:

-1.94515557981544	-0.841260720933500.0000000000000000	o
0.0000000000000000.79321254427875	0.0000000000000000	c
2.190591320228500.22026647804915	0.0000000000000000	o
-1.22111268117871	-2.526826511600580.0000000000000000	h
-0.74237891130412	2.735503299276740.0000000000000000	h

- C_2H_4 , Ethylene:

0.0000000000000000.0000000000000000	1.25401092342612	c	
0.0000000000000000.0000000000000000	-1.25401092342612	c	
0.0000000000000001.74098389924008	2.33979464705049	h	
0.0000000000000000	-1.74098389924008	2.33979464705049	h
0.0000000000000001.74098389924008	-2.33979464705049	h	
0.0000000000000000	-1.74098389924008	-2.33979464705049	h

- C_4H_8 , Cyclobutane:

0.0000000000000002	.04926815138065	0.23557325972552	c
0.0000000000000000	-2.049268151380650	.23557325972552	c
-2.04926815138065	0.0000000000000000	-0.23557325972552	c
2.049268151380650	.0000000000000000	-0.23557325972552	c
0.0000000000000003	.71348381619838	-0.98731954347036	h
0.0000000000000002	.68665009928938	2.20267611884830	h
0.0000000000000000	-3.71348381619838	-0.98731954347036	h
0.0000000000000000	-2.686650099289382	.20267611884830	h
-3.71348381619838	0.0000000000000000	.98731954347036	h
-2.68665009928938	0.0000000000000000	-2.20267611884830	h
3.713483816198380	.0000000000000000	0.98731954347036	h
2.686650099289380	.0000000000000000	-2.20267611884830	h

• C_4H_6 , Cyclobutene:

0.0000000000000001	.26388663219658	1.53923106811481	c
0.0000000000000000	-1.263886632196581	.53923106811481	c
0.0000000000000001	.48543245483769	-1.32138910869415	c
0.0000000000000000	-1.48543245483769	-1.32138910869415	c
0.0000000000000002	.67972425301235	3.02024345352768	h
0.0000000000000000	-2.679724253012353	.02024345352768	h
1.678630495759392	.35566078766219	-2.16364760502582	h
-1.67863049575939	2.35566078766219	-2.16364760502582	h
-1.67863049575939	-2.35566078766219	-2.16364760502582	h
1.67863049575939	-2.35566078766219	-2.16364760502582	h

• C_2H_6OS , Dimethyl sulfoxide:

-0.00000377945227	0.46179237509326	-0.82636212010183	s
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-0.00003968424879	2.807295884791200	.73190415934954	o
2.56610446927260	-1.538603679038690	.33757122774803	c
-2.56606478502381	-1.538662260548810	.33756933802189	c
2.39993329150344	-1.733702784450072	.38671087775164	h
-4.32898651494056	-0.57751542401892	-0.13394189857280	h
2.49944626966120	-3.38048761541807	-0.59491413252439	h
4.32901297110642	-0.57743227606907	-0.13393811912054	h
-2.49936879088975	-3.38053485857139	-0.59493302978572	h
-2.39991061478984	-1.733782152947652	.38670898802550	h

• **NH₃, Ammonia:**

0.0000000000000000	.0000000000000000	0.22774223463085	n
0.0000000000000001	.76596229926456	-0.53140043719811	h
1.52936858742728	-0.88298209449535	-0.53140043719811	h
-1.52936858742728	-0.88298209449535	-0.53140043719811	h

• **C₂H₆, Ethane:**

0.0000000000000000	.0000000000000000	1.44567450672791	c
0.0000000000000000	.0000000000000000	-1.44567450672791	c
0.0000000000000001	.92665894042676	2.19972058717647	h
-1.66853557875751	-0.963329470213382	.19972058717647	h
1.66853557875751	-0.963329470213382	.19972058717647	h
0.0000000000000000	-1.92665894042676	-2.19972058717647	h
-1.66853557875751	0.96332947021338	-2.19972058717647	h
1.668535578757510	.96332947021338	-2.19972058717647	h

• **C₂NF₃, Trifluoroacetonitril:**

0.0000000000000000	0.0000000000000000	-0.61905916332427	c
0.0000000000000000	0.0000000000000000	2.18848994476873	c
0.0000000000000002	.35950449061648	-1.48071947786227	f
2.04339110310737	-1.17975224530824	-1.48071947786227	f
-2.04339110310737	-1.17975224530824	-1.48071947786227	f
0.0000000000000000	0.0000000000000000	4.36611774372563	n

• BCl_3 , Boron trichloride:

0.0000000000000000	0.0000000000000000	0.0000000000000000	b
0.0000000000000003	.30819425247840	0.0000000000000000	cl
2.86497977499753	-1.654096181376130	0.0000000000000000	cl
-2.86497977499753	-1.654096181376130	0.0000000000000000	cl

• CH_2F_2 , Difluoromethane:

0.0000000000000000	0.0000000000000000	0.93751203178590	c
0.0000000000000002	.07829434478177	-0.54579070170003	f
0.0000000000000000	-2.07829434478177	-0.54579070170003	f
-1.71794813768021	0.0000000000000002	.09958966857326	h
1.717948137680210	0.0000000000000000	2.09958966857326	h

• $\text{C}_2\text{H}_3\text{O}$, Carbonyl methane:

-1.82590630192583	-1.260003244993500	0.0000000000000000	c
0.0000000000000000	.94702491313884	0.0000000000000000	c
-0.82634133311437	-3.072855318793350	0.0000000000000000	h
-3.04369495483679	-1.108804367375181	.66312340311293	h
-3.04369495483679	-1.10880436737518	-1.66312340311293	h
2.233646840440170	.89604010207359	0.0000000000000000	o

- **CH₃Cl, Chloromethane:**

0.0000000000000000	0.0000000000000000	-2.14807437196471	c
0.0000000000000000	0.0000000000000000	1.25127271025956	cl
0.0000000000000001	.95340612411162	-2.79439661420812	h
1.69169984169442	-0.97670306205581	-2.79439661420812	h
-1.69169984169442	-0.97670306205581	-2.79439661420812	h

- **CH₄S, Thiomethanol:**

-0.09063504478546	2.193061192284180	0.0000000000000000	c
-0.09063504478546	-1.263984897955490	0.0000000000000000	s
2.43311688239691	-1.578495797703910	0.0000000000000000	h
-2.07295397873024	2.762352528172780	0.0000000000000000	h
0.816911599711272	.94077669018758	1.69277887531630	h
0.816911599711272	.94077669018758	-1.69277887531630	h

- **CHCl₃, Trichloromethane:**

0.0000000000000000	0.0000000000000000	0.86311540366032	c
0.0000000000000000	0.0000000000000000	2.91260654272465	h
0.0000000000000003	.20636635980785	-0.15865384721255	cl
2.77679381528029	-1.60318317990393	-0.15865384721255	cl
-2.77679381528029	-1.60318317990393	-0.15865384721255	cl

- **AlCl₃, Aluminum trichloride:**

0.0000000000000000	0.0000000000000000	0.0000000000000000	al
0.0000000000000003	.93099129409352	0.0000000000000000	cl
3.40433784894122	-1.965494702183690	0.0000000000000000	cl
-3.40433784894122	-1.965494702183690	0.0000000000000000	cl

- CH_3O , Methylene hydroxide:

1.291030658369350	.05329972557804	-0.13838842416348	c
-1.26563840832176	-0.236805361164170	.04732063209359	o
-2.06118665410076	1.38820037612233	-0.13158352035896	h
2.117545846287941	.86448506092869	0.36568468342697	h
2.32256601389697	-1.678035232027530	.21766243543803	h

- $\text{C}_4\text{H}_4\text{O}$, Furan:

0.0000000000000000	.0000000000000000	2.18666446932436	o
0.0000000000000002	.06335039052291	0.65630377567732	c
0.0000000000000000	-2.063350390522910	.65630377567732	c
0.0000000000000001	.35539095100316	-1.81019889830928	c
0.0000000000000000	-1.35539095100316	-1.81019889830928	c
0.0000000000000003	.86449183147727	1.60535825468288	h
0.0000000000000000	-3.864491831477271	.60535825468288	h
0.0000000000000002	.59426894755713	-3.42863972701013	h
0.0000000000000000	-2.59426894755713	-3.42863972701013	h

- $\text{C}_3\text{H}_8\text{O}$, Ethyl methyl ether:

0.03025640511363	-1.338971120634520	.0000000000000000	o
0.0000000000000001	.32899714610515	0.0000000000000000	c
2.48901687113380	-2.343388906155230	.0000000000000000	c
-2.73091504422609	2.214965007890460	.0000000000000000	c
1.006976474704642	.06040241775561	1.67451467224196	h
1.006976474704642	.06040241775561	-1.67451467224196	h
2.32086903982964	-4.401911046408620	.0000000000000000	h

3.56667288266063	-1.75955234822182	-1.68423731319566	h
3.56667288266063	-1.75955234822182	1.68423731319566	h
-3.71927393706954	1.51395787081360	-1.67434081743774	h
-3.71927393706954	1.51395787081360	1.67434081743774	h
-2.82028019305025	4.280618974569360	.000000000000000	h

• **C₆H₆, Benzene:**

0.0000000000000002	.63345997782705	0.000000000000000	c
2.28064243963890	1.31672904405046	0.000000000000000	c
2.28064243963890	-1.31672904405046	0.000000000000000	c
0.000000000000000	-2.63345997782705	0.000000000000000	c
-2.28064243963890	-1.31672904405046	0.000000000000000	c
-2.28064243963890	1.31672904405046	0.000000000000000	c
0.0000000000000004	.68416621079482	0.000000000000000	h
4.05660705932483	2.34208310539741	0.000000000000000	h
4.05660705932483	-2.34208310539741	0.000000000000000	h
0.000000000000000	-4.68416621079482	0.000000000000000	h
-4.05660705932483	-2.34208310539741	0.000000000000000	h
-4.05660705932483	2.34208310539741	0.000000000000000	h

• **COS, Monothio carbon oxide:**

0.000000000000000	.000000000000000	-3.18359704963272	o
0.000000000000000	.000000000000000	-0.99594803299312	c
0.000000000000000	.000000000000000	1.96527927340454	s

• **C₂H₆S, Thioethanol:**

2.874165733729491	.32419346227536	0.000000000000000	c
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0.0000000000000001	.57554404548434	0.000000000000000	c
-1.43241996763185	-1.596973539831270	.000000000000000	s
-3.86315579510132	-0.848088301451610	.000000000000000	h
-0.64253334134698	2.594110210561971	.67658581208360	h
-0.64253334134698	2.59411021056197	-1.67658581208360	h
3.749046572293163	.19831234702950	0.000000000000000	h
3.536459941248050	.30734316852639	1.67379657631147	h
3.536459941248050	.30734316852639	-1.67379657631147	h

- **Si₂H₆, Disilane:**

0.0000000000000000	.000000000000000	2.22441363855489	si
0.0000000000000000	.000000000000000	-2.22441363855489	si
0.0000000000000002	.62941029472427	3.20746429069106	h
-2.27713699766240	-1.314705147362143	.20746429069106	h
2.27713699766240	-1.314705147362143	.20746429069106	h
0.0000000000000000	-2.62941029472427	-3.20746429069106	h
-2.27713699766240	1.31470514736214	-3.20746429069106	h
2.27713699766240	1.31470514736214	-3.20746429069106	h

- **SiCl₄, Silicon tetrachloride:**

0.0000000000000000	.000000000000000	0.000000000000000	si
2.226705876354082	.22670587635408	2.22670587635408	cl
-2.22670587635408	-2.226705876354082	.22670587635408	cl
2.22670587635408	-2.22670587635408	-2.22670587635408	cl
-2.22670587635408	2.22670587635408	-2.22670587635408	cl

- **C₄H₉, *tert*-Butyl radical:**

0.0000000000000000	0.0000000000000000	0.25474453134365	c
0.0000000000000002	.81172351312055	-0.02529587401481	c
2.43502361606499	-1.40586175656027	-0.02529587401481	c
-2.43502361606499	-1.40586175656027	-0.02529587401481	c
0.0000000000000003	.40779793749053	-2.02798416594596	h
-1.67791995873342	3.669438079493080	.83513422881068	h
1.677919958733423	.66943807949308	0.83513422881068	h
2.95124010378536	-1.70389991360833	-2.02798416594596	h
4.01678675025266	-0.381598067192000	.83513422881068	h
2.33886679151924	-3.287840012301090	.83513422881068	h
-2.95124010378536	-1.70389991360833	-2.02798416594596	h
-2.33886679151924	-3.287840012301090	.83513422881068	h
-4.01678675025266	-0.381598067192000	.83513422881068	h

• **C₂H₂O, Ketene:**

0.0000000000000000	0.0000000000000000	-2.28081251499086	c
0.0000000000000000	0.0000000000000000	0.19159933261328	c
0.0000000000000001	.77320561953191	-3.29296305984734	h
0.0000000000000000	-1.77320561953191	-3.29296305984734	h
0.0000000000000000	0.0000000000000000	2.39015017931349	o

• **C₄H₁₀, *n*-Butane:**

1.330414440704823	.46467680436426	0.0000000000000000	c
1.330414440704820	.57175553876588	0.0000000000000000	c
-1.33041444070482	-0.571755538765880	0.0000000000000000	c
-1.33041444070482	-3.464676804364260	0.0000000000000000	c
3.254384300844484	.22432214334456	0.0000000000000000	h

-3.25438430084448	-4.224322143344560	.000000000000000	h
0.359635670075604	.21258883378547	1.66937839661278	h
0.359635670075604	.21258883378547	-1.66937839661278	h
-0.35963567007560	-4.212588833785471	.66937839661278	h
-0.35963567007560	-4.21258883378547	-1.66937839661278	h
2.37036663642831	-0.12269802808213	-1.65654337671822	h
2.37036663642831	-0.122698028082131	.65654337671822	h
-2.37036663642831	0.12269802808213	-1.65654337671822	h
-2.37036663642831	0.122698028082131	.65654337671822	h

• **C₂H₄O₂, Acetic acid:**

0.000000000000000	.29954048932370	0.000000000000000	c
0.366979145827992	.54404191667116	0.000000000000000	o
-2.35234620802511	-0.714949536485290	.000000000000000	o
-3.51362638038440	0.700770921310250	.000000000000000	h
1.99717029162312	-1.731926441885160	.000000000000000	c
3.86253029575134	-0.863521694778890	.000000000000000	h
1.77550541623564	-2.937836276324801	.66386606548315	h
1.77550541623564	-2.93783627632480	-1.66386606548315	h

• **FCl, Singlet chlorine monofluoride:**

0.000000000000000	.000000000000000	-2.02976617768927	f
0.000000000000000	.000000000000000	1.07458331683476	cl

• **C₂H₄O, Acetaldehyde:**

2.271065307597430	.74719960266912	0.000000000000000	o
0.000000000000000	.87212561786192	0.000000000000000	c

-0.97735690729779	2.738672370001590	.0000000000000000	h
-1.75443496985396	-1.372595017716960	.0000000000000000	c
-0.68349693472954	-3.134573774293400	.0000000000000000	h
-2.99052562036192	-1.289437619239321	.66153225370904	h
-2.99052562036192	-1.28943761923932	-1.66153225370904	h

• **C₂H₄O, Oxirane:**

0.0000000000000001	.38621427395666	-0.69929504520047	c
0.0000000000000000	.0000000000000000	1.61022052002279	o
0.0000000000000000	-1.38621427395666	-0.69929504520047	c
1.737816718241372	.40410958625712	-1.12255401471806	h
-1.73781671824137	2.40410958625712	-1.12255401471806	h
-1.73781671824137	-2.40410958625712	-1.12255401471806	h
1.73781671824137	-2.40410958625712	-1.12255401471806	h

• **NO, Nitric oxide:**

0.0000000000000000	.0000000000000000	-1.16026916887819	n
0.0000000000000000	.0000000000000000	1.01523457790535	o

• **NH, Triplet nitrogen monohydride:**

0.0000000000000000	.0000000000000000	0.24678311514580	n
0.0000000000000000	.0000000000000000	-1.72747613684221	h

• **C₂H₄O₂, Methyl formate:**

-1.75695208506296	-0.173501425438630	.0000000000000000	c
-1.36039494580305	-2.406292219940600	.0000000000000000	o
0.0000000000000001	.64757662621768	0.0000000000000000	o

-3.63772280580486	0.715892509825600	0.000000000000000	h
2.571397592170820	.77549447205681	0.000000000000000	c
3.737184761357032	.47253656952890	0.000000000000000	h
2.94851511870174	-0.365331304640121	.67932780470242	h
2.94851511870174	-0.36533130464012	-1.67932780470242	h

• **C₄H₆, 2-Butyne:**

0.000000000000000	0.000000000000000	3.88903370476506	c
0.000000000000000	0.000000000000000	1.13722395868765	c
0.000000000000000	0.000000000000000	-1.13722395868765	c
0.000000000000000	0.000000000000000	-3.88903370476506	c
0.000000000000001	.92803655077763	4.64472006749696	h
-1.66972799594736	-0.964017330525754	.64472006749696	h
1.66972799594736	-0.964017330525754	.64472006749696	h
0.000000000000001	.92803655077763	-4.64472006749696	h
1.66972799594736	-0.96401733052575	-4.64472006749696	h
-1.66972799594736	-0.96401733052575	-4.64472006749696	h

• **CNH₅, Methyl amine:**

0.097753643128041	.32989098656601	0.000000000000000	c
0.09775364312804	-1.437928519309210	0.000000000000000	n
-1.78136167752145	2.230130060106870	0.000000000000000	h
-0.86407349480969	-2.083617703298111	.52993172581488	h
-0.86407349480969	-2.08361770329811	-1.52993172581488	h
1.119360377553482	.01162858626583	1.66506037239913	h
1.119360377553482	.01162858626583	-1.66506037239913	h

• **OCl, Doublet chlorine monoxide:**

0.0000000000000000	0.0000000000000000	0.96308191608997	cl
0.0000000000000000	0.0000000000000000	-2.04654883547542	o

• C_3H_8 , Propane:

0.0000000000000000	0.0000000000000000	1.10797666732898	c
0.0000000000000002	.41182722778382	-0.49075053835360	c
0.0000000000000000	-2.41182722778382	-0.49075053835360	c
-1.65593299517730	0.0000000000000002	.35598960000932	h
1.655932995177300	0.0000000000000000	2.35598960000932	h
0.0000000000000004	.10896381156256	0.69204605575472	h
0.0000000000000000	-4.108963811562560	.69204605575472	h
1.669219659617622	.49675340992183	-1.71373404840387	h
-1.66921965961762	2.49675340992183	-1.71373404840387	h
-1.66921965961762	-2.49675340992183	-1.71373404840387	h
1.66921965961762	-2.49675340992183	-1.71373404840387	h

• C_3H_6 , Propene:

2.438266386109020	.29019201414432	0.0000000000000000	c
0.0000000000000000	.89402565401593	0.0000000000000000	c
3.06362211690807	-1.665986338204250	0.0000000000000000	h
3.908603708597221	.71873804320375	0.0000000000000000	h
-0.53530272166252	2.882293445827030	0.0000000000000000	h
-2.14657203968906	-0.956664406142690	0.0000000000000000	c
-1.46641803048859	-2.908689140451180	0.0000000000000000	h
-3.36033557593698	-0.695834956651151	.66058361119033	h
-3.36033557593698	-0.69583495665115	-1.66058361119033	h

• C_3H_4 , Propyne:

0.0000000000000000	0.0000000000000000	0.41324531073943	c
0.0000000000000000	0.0000000000000000	2.68367378063008	c
0.0000000000000000	0.0000000000000000	-2.33623629274226	c
0.0000000000000000	0.0000000000000000	4.68955193027354	h
0.0000000000000001	.92974486320176	-3.08455083382978	h
1.67120765150941	-0.96487337646395	-3.08455083382978	h
-1.67120765150941	-0.96487337646395	-3.08455083382978	h

• C_4H_6 , Methylene cyclopropane:

0.0000000000000000	0.0000000000000000	0.59937577592414	c
0.0000000000000001	.45377954211186	-1.75836937966263	c
0.0000000000000000	-1.45377954211186	-1.75836937966263	c
0.0000000000000000	0.0000000000000000	3.08703582369452	c
1.721859870775282	.41380766077108	-2.33520072282144	h
-1.72185987077528	2.41380766077108	-2.33520072282144	h
-1.72185987077528	-2.41380766077108	-2.33520072282144	h
1.72185987077528	-2.41380766077108	-2.33520072282144	h
0.0000000000000001	.74827824211302	4.16138481448880	h
0.0000000000000000	-1.74827824211302	4.16138481448880	h

• SiH_2 , Singlet silene:

0.0000000000000000	0.0000000000000000	0.25180978665928	si
0.0000000000000002	.06241686581326	-1.76266661688881	h
0.0000000000000000	-2.06241686581326	-1.76266661688881	h

• SiH_2 , Triplet silene:

0.0000000000000000	0.0000000000000000	0.17976586756915	si
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0.0000000000000002.41317082306430 -1.25835540380562 h
0.0000000000000000 -2.41317082306430 -1.25835540380562 h

• **C₂H₄S, Thiirane:**

0.0000000000000001.39980896375664 -1.51660726685190 c
0.0000000000000000.0000000000000000 1.64646168779927 s
0.0000000000000000 -1.39980896375664 -1.51660726685190 c
1.727672668360032.37411774280209 -2.03602306091525 h
-1.72767266836003 2.37411774280209 -2.03602306091525 h
-1.72767266836003 -2.37411774280209 -2.03602306091525 h
1.72767266836003 -2.37411774280209 -2.03602306091525 h

• **CNH₃O₂, Nitromethane:**

-2.50103363961282 -0.00219019258801 -0.00639672295982 c
0.332542666508420.00002078698746 -0.01745917974173 n
1.38033722568339 -2.054037820140050.00481880163886 o
1.375936053519902.05632816821311 0.00481124273433 o
-3.08979860330080 0.018044994842931.97042310793826 h
-3.14198528018657 1.70218215255354 -0.96026244469971 h
-3.13999350884251 -1.72554672646054 -0.92661209145141 h

• **C₃H₇, Isopropyl radical:**

0.021512642296771.00779094666791 0.0000000000000000 c
0.02151264229677 -0.372126759813972.45572556585075 c
0.02151264229677 -0.37212675981397 -2.45572556585075 c
-0.44295369527453 3.006909545934040.0000000000000000 h
0.506074327565170.86540953118564 4.04077115433125 h

0.506074327565170	.86540953118564	-4.04077115433125	h
-1.84200109939962	-1.205057567953712	.89459178349985	h
1.36379456311611	-1.954424686497252	.44128049929098	h
-1.84200109939962	-1.20505756795371	-2.89459178349985	h
1.36379456311611	-1.95442468649725	-2.44128049929098	h

• C_2NH_5O , Acetamide:

-2.59475838662555	-0.56092362857218	-0.00109415143094	c
0.153226553758900	.29188331903325	-0.01430900627821	c
0.782097175165122	.49794015793329	0.00839983266068	o
1.87867879391279	-1.63624582832489	-0.05202416043834	n
3.71617478621161	-1.186829269675900	.15412039421975	h
1.36582790843509	-3.452446496832220	.15681892313752	h
-2.91361565647961	-2.18439112878650	-1.24078473022205	h
-3.14770359146469	-1.105741121313781	.91824776940929	h
-3.77903274656979	1.01385696755448	-0.59901861768502	h

• C_4NH_5 , Pyrrole:

0.0000000000000000	.0000000000000000	4.01327752882389	h
0.0000000000000000	.0000000000000000	2.11518935780023	n
0.0000000000000002	.12213788079085	0.62545021710569	c
0.0000000000000000	-2.122137880790850	.62545021710569	c
0.0000000000000001	.34490486069178	-1.85462069051503	c
0.0000000000000000	-1.34490486069178	-1.85462069051503	c
0.0000000000000003	.98403212719135	1.45237547559512	h
0.0000000000000000	-3.984032127191351	.45237547559512	h
0.0000000000000002	.56695106658014	-3.48715509671493	h
0.0000000000000000	-2.56695106658014	-3.48715509671493	h

- C_2H_3OF , Acetyl fluoride:

0.0000000000000000	.35420837662195	0.0000000000000000	c
0.326162951083802	.56959479344004	0.0000000000000000	o
-2.36114099344756	-0.612671888995120	.0000000000000000	f
1.92123542642538	-1.730386315086860	.0000000000000000	c
3.81886628372488	-0.934467682985820	.0000000000000000	h
1.64734796935560	-2.925588961257571	.66406826617937	h
1.64734796935560	-2.92558896125757	-1.66406826617937	h

- C_2H_2 , Acetylene:

0.0000000000000000	.0000000000000000	1.13280388926283	c
0.0000000000000000	.0000000000000000	-1.13280388926283	c
0.0000000000000000	.0000000000000000	-3.14001240610384	h
0.0000000000000000	.0000000000000000	3.14001240610384	h

- C_2H_3F , Vinyl fluoride:

0.0000000000000000	.80572253127845	0.0000000000000000	c
2.24036670656871	-0.297480687838860	.0000000000000000	c
-2.16521607771611	-0.488881599208180	.0000000000000000	f
-0.32087360763785	2.832535067022020	.0000000000000000	h
2.43485354071303	-2.334535539222660	.0000000000000000	h
3.930766416683710	.85248380443671	0.0000000000000000	h

- C_2N_2 , Cyanogen:

0.0000000000000000	.0000000000000000	3.48826625568107	n
0.0000000000000000	.0000000000000000	1.29988213557578	c

0.0000000000000000	0.0000000000000000	-1.29988213557578	c
0.0000000000000000	0.0000000000000000	-3.48826625568107	n

• C₂H₅Cl, Ethyl chloride:

0.0000000000000001	.54870237549283	0.0000000000000000	c
2.854608957980261	.27328990943381	0.0000000000000000	c
-1.55805463012449	-1.509074818486220	0.0000000000000000	cl
-0.68631262666754	2.529498584352481	.67743240939114	h
-0.68631262666754	2.52949858435248	-1.67743240939114	h
3.724570839420023	.15309498012181	0.0000000000000000	h
3.503656185307290	.25511113821343	1.67526867296898	h
3.503656185307290	.25511113821343	-1.67526867296898	h

• CH₂, Singlet carbene:

0.0000000000000000	0.0000000000000000	0.33999574637652	c
0.0000000000000001	.61661346353035	-1.01998723912956	h
0.0000000000000000	-1.61661346353035	-1.01998723912956	h

• CH₂, Triplet carbene:

0.0000000000000000	0.0000000000000000	0.20020703514857	c
0.0000000000000001	.87922114531293	-0.60062299517184	h
0.0000000000000000	-1.87922114531293	-0.60062299517184	h

• HO, Hydroxyl radical:

0.0000000000000000	0.0000000000000000	0.20495780664664	o
0.0000000000000000	0.0000000000000000	-1.63966623262542	h

- CH, Carbonhydride radical:

0.0000000000000000	0.0000000000000000	0.30522478553142	c
0.0000000000000000	0.0000000000000000	-1.83134871318854	h

- C₅NH₅, Pyridine:

0.0000000000000000	0.0000000000000000	2.67859230705876	n
0.0000000000000000	0.0000000000000000	-2.61258606296319	c
0.0000000000000002	.15345631199116	1.36137193421375	c
0.0000000000000000	-2.15345631199116	1.36137193421375	c
0.0000000000000000	-2.25932821858608	-1.26858449136293	c
0.0000000000000002	.25932821858608	-1.26858449136293	c
0.0000000000000000	0.0000000000000000	-4.66321103770725	h
0.0000000000000003	.88679248957146	2.46631559109944	h
0.0000000000000000	-3.88679248957146	2.46631559109944	h
0.0000000000000000	-4.06977278129264	-2.22875244975599	h
0.0000000000000004	.06977278129264	-2.22875244975599	h

- Si₂, Triplet disilicon:

0.0000000000000000	0.0000000000000000	2.14524356221764	si
0.0000000000000000	0.0000000000000000	-2.14524356221764	si

- C₃H₆, Cyclopropane:

0.0000000000000001	.64434897398271	0.0000000000000000	c
1.42404659113703	-0.822174486991350	0.0000000000000000	c
-1.42404659113703	-0.822174486991350	0.0000000000000000	c
0.0000000000000002	.76065555410545	1.71854907059046	h

0.0000000000000002	.76065555410545	-1.71854907059046	h
2.39079835537707	-1.38032777705272	-1.71854907059046	h
2.39079835537707	-1.38032777705272	1.71854907059046	h
-2.39079835537707	-1.38032777705272	1.71854907059046	h
-2.39079835537707	-1.38032777705272	-1.71854907059046	h

• C_3H_4 , Cyclopropene:

0.0000000000000000	.0000000000000000	1.62606587364704	c
0.0000000000000001	.21941759683751	-0.94629925830381	c
0.0000000000000000	-1.21941759683751	-0.94629925830381	c
-1.72322047359096	0.0000000000000002	.76323503027684	h
1.72322047359096	0.0000000000000000	2.76323503027684	h
0.0000000000000002	.97923450671793	-1.96363899112120	h
0.0000000000000000	-2.97923450671793	-1.96363899112120	h

• N_2 , Dinitrogen:

0.0000000000000000	.0000000000000000	1.03820797850284	n
0.0000000000000000	.0000000000000000	-1.03820797850284	n

• F_2 , Difluorine:

0.0000000000000000	.0000000000000000	1.31140001635572	f
0.0000000000000000	.0000000000000000	-1.31140001635572	f

• $SiCH_6$, Methyl silane:

0.0000000000000000	.0000000000000000	-2.35330429917448	c
0.0000000000000000	.0000000000000000	1.20043151838041	si
0.0000000000000000	-1.93094672902228	-3.09220422466797	h

-1.67224889060863	0.96547430937421	-3.09220422466797	h
1.672248890608630	.96547430937421	-3.09220422466797	h
0.0000000000000002	.62573666712194	2.19679340139663	h
-2.27395469885462	-1.312868333560972	.19679340139663	h
2.27395469885462	-1.312868333560972	.19679340139663	h

• CH₃, Methyl radical:

0.0000000000000000	.0000000000000000	0.0000000000000000	c
0.0000000000000002	.04337598529831	0.0000000000000000	h
1.76961513987943	-1.021687992649150	.0000000000000000	h
-1.76961513987943	-1.021687992649150	.0000000000000000	h

• PH₂, Doublet phosphanyl radical:

0.0000000000000000	.0000000000000000	0.22119244385426	p
0.0000000000000001	.93291771337888	-1.65893954945472	h
0.0000000000000000	-1.93291771337888	-1.65893954945472	h

• C₃NH₉, Trimethyl amine:

0.0000000000000000	.0000000000000000	0.69257706879806	n
0.0000000000000002	.62341986288303	-0.11284121657300	c
2.27194969942762	-1.31170993144151	-0.11284121657300	c
-2.27194969942762	-1.31170993144151	-0.11284121657300	c
0.0000000000000002	.84894355903386	-2.19527028213352	h
1.674754667460843	.58594430976380	0.62815441520185	h
-1.67475466746084	3.585944309763800	.62815441520185	h
2.46725667471362	-1.42447177951693	-2.19527028213352	h
2.26814190126986	-3.243352079680690	.62815441520185	h

3.94289656873070	-0.342592230083100	.62815441520185	h
-2.46725667471362	-1.42447177951693	-2.19527028213352	h
-3.94289656873070	-0.342592230083100	.62815441520185	h
-2.26814190126986	-3.243352079680690	.62815441520185	h

• C_2H_6O , Ethanol:

2.21303370778265	-0.783238569749380	.000000000000000	c
0.0000000000000001	.04755078450383	0.000000000000000	c
-2.26423772707932	-0.394871503549390	.000000000000000	o
-3.66978011992314	0.756593431275690	.000000000000000	h
0.102748189297262	.28063488073437	1.67514395104421	h
0.102748189297262	.28063488073437	-1.67514395104421	h
4.007714175088680	.24359892661189	0.000000000000000	h
2.14612984377397	-1.994188303785431	.67397987974635	h
2.14612984377397	-1.99418830378543	-1.67397987974635	h

• C_2NH_7 , Dimethyl amine:

-0.05086575831888	-0.418196393207592	.29203748822020	c
-0.05086575831888	1.101355066959350	.000000000000000	n
-0.05086575831888	-0.41819639320759	-2.29203748822020	c
1.50650101149323	-1.807967131746352	.40362392664096	h
0.063152757634910	.81358568171739	3.94888133139355	h
-1.82853113152441	-1.475507613187772	.41642304173900	h
1.484213581481982	.24866260429207	0.000000000000000	h
1.50650101149323	-1.80796713174635	-2.40362392664096	h
0.063152757634910	.81358568171739	-3.94888133139355	h
-1.82853113152441	-1.47550761318777	-2.41642304173900	h

- O₂, Dioxygen:

0.0000000000000000	0.0000000000000000	1.13987335472596	o
0.0000000000000000	0.0000000000000000	-1.13987335472596	o

- NH₂, Doublet aminyl radical:

0.0000000000000000	0.0000000000000000	0.27278574673431	n
0.0000000000000001	1.51365551463234	-0.95475011357008	h
0.0000000000000000	-1.51365551463234	-0.95475011357008	h

- C₂F₄, Tetrafluoroethylene:

0.0000000000000000	0.0000000000000000	1.25052059925868	c
0.0000000000000000	0.0000000000000000	-1.25052059925868	c
0.0000000000000002	0.07580557546476	2.61419988908068	f
0.0000000000000000	-2.07580557546476	2.61419988908068	f
0.0000000000000002	0.07580557546476	-2.61419988908068	f
0.0000000000000000	-2.07580557546476	-2.61419988908068	f

- CH₄O, Methanol:

-0.08791005970184	1.245357867463630	0.0000000000000000	c
-0.08791005970184	-1.429111057173170	0.0000000000000000	o
-2.06462406593648	1.847464297649790	0.0000000000000000	h
1.64121013887599	-1.985973664285770	0.0000000000000000	h
0.827076436580062	0.04961964044136	1.68519729407116	h
0.827076436580062	0.04961964044136	-1.68519729407116	h

- C₄H₆, 1,3-Butadiene:

1.133093017361163.30254964051947	0.0000000000000000	c
1.133093017361160.77721412283774	0.0000000000000000	c
-1.13309301736116 -0.777214122837740	.0000000000000000	c
-1.13309301736116 -3.302549640519470	.0000000000000000	c
2.871661846603424.38580680030417	0.0000000000000000	h
-0.61783084133790 4.373835385252340	.0000000000000000	h
2.92452504544476 -0.236177972088050	.0000000000000000	h
-2.92452504544476 0.236177972088050	.0000000000000000	h
0.61783084133790 -4.373835385252340	.0000000000000000	h
-2.87166184660342 -4.385806800304170	.0000000000000000	h

• C_2H_5O , Ethyl oxo radical:

1.96734852352005 -1.149102777158970	.0000000000000000	c
0.0000000000000000.96572186349761	0.0000000000000000	c
-2.46222811347401 0.206424234125760	.0000000000000000	o
0.259368691190822.25239103395226	1.63723226536626	h
0.259368691190822.25239103395226	-1.63723226536626	h
3.88612730597268 -0.373808616072240	.0000000000000000	h
1.74443453915873 -2.341041866298191	.67399877700768	h
1.74443453915873 -2.34104186629819	-1.67399877700768	h

• C_2H_6S , Dimethyl thioether:

0.0000000000000002.62641129935138	-0.96953344110764	c
0.0000000000000000.0000000000000000	1.24781451143638	s
0.0000000000000000 -2.62641129935138	-0.96953344110764	c
0.0000000000000004.35986652967805	0.14968898643814	h
1.689821453918342.59762699089527	-2.15750410536780	h

-1.68982145391834	2.59762699089527	-2.15750410536780	h
0.0000000000000000	-4.359866529678050	.14968898643814	h
-1.68982145391834	-2.59762699089527	-2.15750410536780	h
1.68982145391834	-2.59762699089527	-2.15750410536780	h

• C_2NH_5 , Aziridine:

-0.07218186909783	-0.749841439802891	.40125271452217	c
-0.07218186909783	1.651960790845970	.0000000000000000	n
-0.07218186909783	-0.74984143980289	-1.40125271452217	c
1.695258196002652	.40355778622631	0.0000000000000000	h
-1.80453160963676	-1.147105336636512	.42815257184582	h
-1.80453160963676	-1.14710533663651	-2.42815257184582	h
1.64263310265405	-1.337489575346342	.36715977118080	h
1.64263310265405	-1.33748957534634	-2.36715977118080	h

• C_4H_6 , Bicyclo[1.1.0]butane:

0.0000000000000002	.14550434442398	0.59447949551383	c
0.0000000000000000	-2.145504344423980	.59447949551383	c
1.404446351686740	.0000000000000000	-0.60721813937561	c
-1.40444635168674	0.0000000000000000	-0.60721813937561	c
0.0000000000000002	.33718493526097	2.64984579312530	h
0.0000000000000003	.93718203690485	-0.41317728059865	h
0.0000000000000000	-2.337184935260972	.64984579312530	h
0.0000000000000000	-3.93718203690485	-0.41317728059865	h
2.722645602668590	.0000000000000000	-2.16024231853436	h
-2.72264560266859	0.0000000000000000	-2.16024231853436	h

• C_3NH_3 , Acrylonitrile:

2.487542884750151.86494237465285	0.0000000000000000	c
0.0000000000000001.45382111608678	0.0000000000000000	c
-1.08903405257293 -1.011528824958760	.0000000000000000	c
3.836057122355740.32349087833190	0.0000000000000000	h
3.234842642904313.77167793246059	0.0000000000000000	h
-1.33528048549700 3.012183771570920	.0000000000000000	h
-2.01809522909257 -2.992965256799480	.0000000000000000	n

• C_3H_8O , Isopropyl alcohol:

0.075008899392632.58659099027922	-0.30665152876175	o
-0.00322954196110 0.083079919706180	.68850659870782	c
1.670311921322423.32412086432636	0.16065128773501	h
0.010941514309410.15503880112034	2.77255326983809	h
-2.50712044748684 -1.05193872858439	-0.16941016836093	c
2.27141490693202 -1.46623094760144	-0.19468525538828	c
-2.56846662693871 -1.17259585244300	-2.23391707127717	h
2.30503313483605 -1.57960695667005	-2.26030709672292	h
-4.08195395594522 0.130906998403390	.45419945549133	h
4.04705071427082 -0.601998715796580	.43311011184833	h
-2.75791734093890 -2.950132724271490	.61009052309760	h
2.20853426986025 -3.387931246655510	.57037225923661	h

• C_4H_4S , Thiophene:

0.0000000000000000.0000000000000000	2.25367793744875	s
0.0000000000000002.34354197397200	-0.01615337898391	c
0.0000000000000000 -2.34354197397200	-0.01615337898391	c
0.0000000000000001.34734260740320	-2.39684736872844	c

0.0000000000000000	-1.34734260740320	-2.39684736872844	c
0.0000000000000004	.30452589987649	0.54395955707727	h
0.0000000000000000	-4.304525899876490	.54395955707727	h
0.0000000000000002	.48784713065754	-4.09538234984551	h
0.0000000000000000	-2.48784713065754	-4.09538234984551	h

- **BF₃, Boron trifluoride:**

0.0000000000000000	.0000000000000000	0.0000000000000000	b
0.0000000000000002	.47330190861272	0.0000000000000000	f
2.14194221066349	-1.236651899169430	.0000000000000000	f
-2.14194221066349	-1.236651899169430	.0000000000000000	f

- **C₂Cl₄, Tetrachloro ethylene:**

0.0000000000000000	.0000000000000000	1.26949911881125	c
0.0000000000000000	.0000000000000000	-1.26949911881125	c
0.0000000000000002	.74863122672190	3.01801735614314	cl
0.0000000000000000	-2.748631226721903	.01801735614314	cl
0.0000000000000000	-2.74863122672190	-3.01801735614314	cl
0.0000000000000002	.74863122672190	-3.01801735614314	cl

- **C₄H₁₀, Isobutane:**

0.0000000000000000	.0000000000000000	0.70480737633009	c
0.0000000000000000	.0000000000000000	2.78215685804542	h
0.0000000000000002	.76058563423853	-0.18086757790462	c
0.0000000000000002	.87076422669029	-2.25079043591770	h
-1.67275722693838	3.771825331098960	.49949619089660	h
1.672757226938383	.77182533109896	0.49949619089660	h

2.39073599441468	-1.38029187225620	-0.18086757790462	c
2.48615393604248	-1.43538116848208	-2.25079043591770	h
4.10287511396240	-0.437263729888410	.49949619089660	h
2.43011788702402	-3.334563490936680	.49949619089660	h
-2.39073599441468	-1.38029187225620	-0.18086757790462	c
-2.48615393604248	-1.43538116848208	-2.25079043591770	h
-2.43011788702402	-3.334563490936680	.49949619089660	h
-4.10287511396240	-0.437263729888410	.49949619089660	h

● C_4H_8 , Isobutene:

0.0000000000000000	.0000000000000000	2.75332719616212	c
0.0000000000000000	.0000000000000000	0.23540318437356	c
0.0000000000000001	.74468776246054	3.83203200569270	h
0.0000000000000000	-1.744687762460543	.83203200569270	h
0.0000000000000002	.40933467901454	-1.28113416261142	c
0.0000000000000004	.08122263193179	-0.06888996617435	h
1.659924096769952	.50809365644528	-2.52126693731763	h
-1.65992409676995	2.50809365644528	-2.52126693731763	h
0.0000000000000000	-2.40933467901454	-1.28113416261142	c
0.0000000000000000	-4.08122263193179	-0.06888996617435	h
-1.65992409676995	-2.50809365644528	-2.52126693731763	h
1.65992409676995	-2.50809365644528	-2.52126693731763	h

● CNH_3O_2 , Methyl nitrite:

-2.49400952757688	0.610880428621140	.0000000000000000	c
0.0000000000000001	.67472443184271	0.0000000000000000	o
-3.75825520773871	2.235428852183480	.0000000000000000	h

-2.79669452118571	-0.552510567828571	.68112682398093	h
-2.79669452118571	-0.55251056782857	-1.68112682398093	h
1.97030405519189	-0.072074154708260	.000000000000000	n
1.31544780973236	-2.211121304936170	.000000000000000	o

• C_3H_6O , Acetone:

0.000000000000000	.000000000000000	2.64191083309331	o
0.000000000000000	.000000000000000	0.35787255559362	c
0.000000000000002	.43798481691522	-1.16078884356473	c
0.000000000000000	-2.43798481691522	-1.16078884356473	c
0.000000000000004	.05859127176436	0.11199650899160	h
0.000000000000000	-4.058591271764360	.11199650899160	h
-1.66181382290284	2.51905217828988	-2.39426033365252	h
1.66181382290284	.51905217828988	-2.39426033365252	h
1.66181382290284	-2.51905217828988	-2.39426033365252	h
-1.66181382290284	-2.51905217828988	-2.39426033365252	h

• $C_2H_2O_2$, Glyoxal:

-0.61695400841224	1.303192935760600	.000000000000000	c
0.61695400841224	-1.303192935760600	.000000000000000	c
0.61695400841224	.21120594843417	0.000000000000000	o
-2.71375633093949	1.258944998359080	.000000000000000	h
-0.61695400841224	-3.211205948434170	.000000000000000	o
2.71375633093949	-1.258944998359080	.000000000000000	h

• C_2H_3OCl , Acetyl chloride:

0.000000000000001	.03280903094119	0.000000000000000	c
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2.817254741511501.36655734272239	0.0000000000000000	c
-0.86539063392432 -2.321500208358020	.0000000000000000	cl
-1.58726034750823 2.599739704711840	.0000000000000000	o
3.263067592425093.37953330372096	0.0000000000000000	h
3.621567537094820.44591678585089	1.66489218677331	h
3.621567537094820.44591678585089	-1.66489218677331	h

• CN, Cyano radical:

0.0000000000000000.0000000000000000	-1.18996999450875	c
0.0000000000000000.0000000000000000	1.01997401104663	n

• C₂NH₇, Ethyl amine:

2.29626480557946 -0.681612877775050	.0000000000000000	c
0.0000000000000001.08559664073721	0.0000000000000000	c
-2.47951343841152 -0.150155748792960	.0000000000000000	n
4.072501545828530.38383361320720	0.0000000000000000	h
2.29113986830708 -1.903732782982591	.67274021940318	h
2.29113986830708 -1.90373278298259	-1.67274021940318	h
0.081560579895342.32974697320193	-1.65578748626507	h
0.081560579895342.32974697320193	1.65578748626507	h
-2.61945332773010 -1.304334330344861	.53023786144841	h
-2.61945332773010 -1.30433433034486	-1.53023786144841	h

• C₂H₃Cl, Vinyl chloride:

0.0000000000000001.44339549701165	0.0000000000000000	c
2.444298391925191.97424035472669	0.0000000000000000	c
-1.18312162700318 -1.635272619366460	.0000000000000000	cl

-1.49107517707049	2.843385874477050	.0000000000000000	h
3.884326396968040	.51975972421953	0.0000000000000000	h
3.054037425962083	.93069082763839	0.0000000000000000	h

• O₃, Ozone:

0.0000000000000002	.03281997512001	-0.40755723507945	o
0.0000000000000000	.0000000000000000	0.81511447015889	o
0.0000000000000000	-2.03281997512001	-0.40755723507945	o

• C₂NH₃, Acetonitrile:

0.0000000000000000	.0000000000000000	-2.22350845973723	c
0.0000000000000000	.0000000000000000	0.52971858093984	c
0.0000000000000000	.0000000000000000	2.71238627949315	n
0.0000000000000001	.93742848965808	-2.94132471076611	h
1.67786137722330	-0.96871329996597	-2.94132471076611	h
-1.67786137722330	-0.96871329996597	-2.94132471076611	h

• CH₂Cl₂, Dichloromethane:

0.0000000000000000	.0000000000000000	1.45320884481972	c
0.0000000000000002	.81298962962958	-0.40950554272245	cl
0.0000000000000000	-2.81298962962958	-0.40950554272245	cl
-1.70136957031640	0.0000000000000002	.60196958154864	h
1.701369570316400	.0000000000000000	2.60196958154864	h

• C₂H₆O, Dimethyl ether:

0.0000000000000002	.20863253561916	-0.36627427798043	c
0.0000000000000000	.0000000000000000	1.11091141201335	o

0.0000000000000000	-2.20863253561916	-0.36627427798043	c
0.0000000000000000	3.81981303651746	0.92569935372923	h
1.684677619384622	.32577098941834	-1.58584872208697	h
-1.68467761938462	2.32577098941834	-1.58584872208697	h
0.0000000000000000	-3.81981303651746	0.92569935372923	h
-1.68467761938462	-2.32577098941834	-1.58584872208697	h
1.68467761938462	-2.32577098941834	-1.58584872208697	h