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Electronic Supplementary Information

Calculations of current densities for neutral and doubly charged persubstituted benzenes using effective core potentials

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Implementation Details

Once the density matrix and the magnetically perturbed density matrices have been obtained from a NMR magnetic shielding calculation, the density matrices have to be transformed into the appropriate format for GIMIC calculations. The density matrices in the Gaussian code are expressed in real spherical-harmonic atomic orbital basis (spherical AO), whereas the GIMIC code use Cartesian basis sets (Cartesian AO). The basis functions are also sorted differently in the two codes. Thus, the elements of the density matrices have to be reordered and transformed from the spherical AO basis to the Cartesian representation. The expression for the transformation coefficients is derived in detail here.

Spherical-harmonic atomic orbital

In most quantum chemistry packages, the AOs are written as a linear combination of contracted Gaussian Type Orbitals (CGTOs) [1]:

$$\chi^{\mathrm{CGTO}}_{\mu,\ell,m}(\vec{r}) = \sum_{\nu} d_{\nu\mu}\chi^{\mathrm{GTO}}_{\ell,m}(\alpha_\nu,\vec{r}) \tag{1}$$

A normalised primitive GTO is defined as [1]:

$$\chi^{\mathrm{GTO}}_{\ell,m}(\alpha_\nu,r,\theta,\phi) = \sqrt{\frac{8\,2^{3\ell+\frac{3}{2}}\alpha_\nu^{\ell+\frac{3}{2}}(\ell+1)!}{\pi^{\frac{1}{2}}(2\ell+2)!}}\, r^\ell e^{-\alpha_\nu r^2} Y_{\ell m}(\theta,\phi) \tag{2}$$

$$= \frac{R^{\mathrm{GTO}}_\ell(\alpha_\nu,r)}{r^\ell}\mathscr{Y}_{\ell m}(r,\theta,\phi) \tag{3}$$

where $\mathscr{Y}_{\ell m}(r,\theta,\phi) = r^\ell Y_{\ell m}(\theta,\phi)$ is a complex solid harmonic. The contraction coefficients $d_{\nu\mu}$ are the same for all the angular components are therefore the contraction only involve the radial part of the orbital. A CGTO can thus be separated into two parts:

$$\chi^{\mathrm{CGTO}}_{\mu,\ell,m}(r,\theta,\phi) = \left[\frac{\sum_\nu d_{\nu\mu}R^{\mathrm{GTO}}_\ell(\alpha_\nu,r)}{r^\ell}\right]\mathscr{Y}_{\ell m}(r,\theta,\phi) \tag{4}$$

$$= \frac{R^{\mathrm{CGTO}}_\ell(r)}{r^\ell}\mathscr{Y}_{\ell m}(r,\theta,\phi) \tag{5}$$

From the normalisation of the radial function, the contracted coefficients are related by:

$$1 = \int_0^\infty \left[R^{\mathrm{CGTO}}_\ell(r)\right]^2 r^2\,\mathrm{d}r$$

$$= \sum_{\nu,\eta} d_{\nu\mu}d_{\eta\mu}\frac{2^{\ell+\frac{3}{2}}}{(\alpha_\nu+\alpha_\eta)^{\ell+\frac{3}{2}}}\sqrt{\alpha_\nu^{\ell+\frac{3}{2}}\alpha_\eta^{\ell+\frac{3}{2}}} \tag{6}$$

The complex solid harmonics are defined by introducing the real-valued solid harmonics ($S_{\ell m}$):

$$\mathscr{Y}_{\ell 0} = \sqrt{\frac{2\ell+1}{4\pi}}S_{\ell 0} \tag{7}$$

$$\mathscr{Y}_{\ell|m|} = (-1)^{|m|}\sqrt{\frac{2\ell+1}{8\pi}}\left[S_{\ell|m|} + iS_{\ell,-|m|}\right] \quad m \neq 0 \tag{8}$$

$$\mathscr{Y}_{\ell,-|m|} = \sqrt{\frac{2\ell+1}{8\pi}}\left[S_{\ell|m|} - iS_{\ell,-|m|}\right] \quad m \neq 0 \tag{9}$$

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Since it is generally easier to deal with real atomic orbitals, we also use real normalised spherical-harmonic CGTOs which are defined as:

$$\chi^{CGTO,R}_{\mu,\ell,|m|}(r,\theta,\phi) = \frac{R^{\mathrm{CGTO}}_{\ell}(r)}{r^{\ell}}(-1)^{|m|}\sqrt{\frac{2\ell+1}{4\pi}}S_{\ell|m|} \tag{10}$$

$$\chi^{CGTO,R}_{\mu,\ell,-|m|}(r,\theta,\phi) = \frac{R^{\mathrm{CGTO}}_{\ell}(r)}{r^{\ell}}(-1)^{|m|}\sqrt{\frac{2\ell+1}{4\pi}}S_{\ell,-|m|} \tag{11}$$

Note that the $(-1)^{|m|}$ phase factor is often omitted and will not be considered in the following.

The real-valued solid harmonics ($S_{\ell m}$) for $\ell \leq 4$ are given in Table 1.

Table 1 The real solid harmonics $S_{\ell m}(\vec{r})$ for $\ell \leq 4$

m / ℓ	0	1	2	3	4
4					$\frac{1}{8}\sqrt{35}\left[x^4-6x^2y^2+y^4\right]$
3				$\frac{1}{2}\sqrt{\frac{5}{2}}\left[x^3-3xy^2\right]$	$\frac{1}{2}\sqrt{\frac{35}{2}}\left[x^3z-3xy^2z\right]$
2			$\frac{1}{2}\sqrt{3}\left[x^2-y^2\right]$	$\frac{1}{2}\sqrt{15}\left[x^2z-y^2z\right]$	$\frac{1}{4}\sqrt{5}\left[7z^2-r^2\right]\left[x^2-y^2\right]$
1		x	$\sqrt{3}xz$	$\frac{1}{2}\sqrt{\frac{3}{2}}\left[4xz^2-x^3-xy^2\right]$	$\frac{1}{2}\sqrt{\frac{5}{2}}\left[4xz^3-3x^3z-3xy^2z\right]$
0	1	z	$\frac{1}{2}\left[2z^2-x^2-y^2\right]$	$\frac{1}{2}\left[2z^3-3x^2z-3y^2z\right]$	$\frac{1}{8}\left[35z^4-30z^2r^2+3r^4\right]$
-1		y	$\sqrt{3}yz$	$\frac{1}{2}\sqrt{\frac{3}{2}}\left[4yz^2-x^2y-y^3\right]$	$\frac{1}{2}\sqrt{\frac{5}{2}}\left[4yz^3-3x^2yz-3y^3z\right]$
-2			$\sqrt{3}xy$	$\sqrt{15}xyz$	$\frac{1}{2}\sqrt{5}\left[6xyz^2-x^3y-xy^3\right]$
-3				$\frac{1}{2}\sqrt{\frac{5}{2}}\left[3x^2y-y^3\right]$	$\frac{1}{2}\sqrt{\frac{35}{2}}\left[3x^2yz-y^3z\right]$
-4					$\frac{1}{8}\sqrt{35}\left[x^3y-xy^3\right]$

Cartesian atomic orbital

Even though spherical AOs have many advantages as compared to Cartesian AOs, quantum chemistry codes often employ Cartesian AOs in the algorithms for computational reasons. Transformations between the two representations are an integrated part of many electronic structure codes. A Cartesian GTO is defined as:

$$\begin{aligned}\chi^{\text{Cart, GTO}}_{\ell_x,\ell_y,\ell_z}(\alpha_v,x,y,z) &= \frac{R^{\mathrm{GTO}}_{\ell}(\alpha_v,r)}{r^{\ell}}\sqrt{\frac{\ell_x!\ell_y!\ell_z!(2\ell+2)!}{8\pi(2\ell_x)!(2\ell_y)!(2\ell_z)!(\ell+1)!}}x^{\ell_x}y^{\ell_y}z^{\ell_z} \\ &= \sqrt{\frac{2^{3\ell+\frac{3}{2}}\alpha_v^{\ell+\frac{3}{2}}\ell_x!\ell_y!\ell_z!}{\pi^{\frac{3}{2}}(2\ell_x)!(2\ell_y)!(2\ell_z)!}}x^{\ell_x}y^{\ell_y}z^{\ell_z}e^{-\alpha_v r^2} \quad \ell_x+\ell_y+\ell_z=\ell\end{aligned} \tag{12}$$

A normalised Cartesian CGTO is therefore defined as:

$$\chi^{\text{Cart, CGTO}}_{p,\ell_x,\ell_y,\ell_z}(x,y,z) = \frac{R^{\mathrm{CGTO}}_{\ell}(r)}{r^{\ell}}\sqrt{\frac{\ell_x!\ell_y!\ell_z!(2\ell+2)!}{8\pi(2\ell_x)!(2\ell_y)!(2\ell_z)!(\ell+1)!}}x^{\ell_x}y^{\ell_y}z^{\ell_z} \tag{13}$$

GIMIC as well as many quantum chemistry codes do not use normalised CGTOs but instead they use the same normalisation factor for all the Cartesian orbitals of a given ℓ:

$$\begin{aligned}\chi'^{\text{Cart, CGTO}}_{p,\ell_x,\ell_y,\ell_z}(x,y,z) &= \frac{R^{\mathrm{CGTO}}_{\ell}(r)}{r^{\ell}}\sqrt{\frac{(2\ell+2)!}{8\pi 2^{\ell}(\ell+1)!}}x^{\ell_x}y^{\ell_y}z^{\ell_z} \\ &= \sqrt{\frac{(2\ell_x)!(2\ell_y)!(2\ell_z)!}{\ell_x!\ell_y!\ell_z!2^{\ell}}}\chi^{\text{Cart, CGTO}}_{p,\ell_x,\ell_y,\ell_z}(x,y,z)\end{aligned} \tag{14}$$

Relation from Cartesian to spherical-harmonic functions

A shell of normalised Cartesian CGTO of a given ℓ value can be transformed into real normalised CGTOs:

$$\chi^{\text{CGTO, R}}_{\mu,\ell,m}(r,\theta,\phi) = \sum_{p\in\ell_x+\ell_y+\ell_z=\ell} c_{\ell,m,\ell_x,\ell_y,\ell_z}\chi^{\text{Cart, CGTO}}_{p,\ell_x,\ell_y,\ell_z}(x,y,z) \tag{15}$$

The coefficients for $m>0$, $m<0$ and $m=0$ are given by[2]:

$$\begin{aligned} c_{\ell,|m|,\ell_x,\ell_y,\ell_z} &= \sqrt{\frac{(2\ell_x)!(2\ell_y)!(2\ell_z)!\ell!(\ell-|m|)!}{(2\ell)!\ell_x!\ell_y!\ell_z!(\ell+|m|)!}}\frac{1}{2^\ell\ell!} \\ &\times\left[\sum_{\alpha=0}^{(\ell-|m|)/2}\binom{\ell}{\alpha}\binom{\alpha}{\tau}\frac{(-1)^\alpha(2\ell-2\alpha)!}{(\ell-|m|-2\alpha)!}\right] \\ &\times\left[\sum_{\beta=0}^{\tau}\binom{\tau}{\beta}\binom{|m|}{\ell_x-2\beta}\left\{(-1)^{(|m|-\ell_x+2\beta)/2}+(-1)^{-(|m|-\ell_x+2\beta)/2}\right\}\frac{1}{\sqrt{2}}\right] \end{aligned} \tag{16}$$

$$\begin{aligned} c_{\ell,-|m|,\ell_x,\ell_y,\ell_z} &= \sqrt{\frac{(2\ell_x)!(2\ell_y)!(2\ell_z)!\ell!(\ell-|m|)!}{(2\ell)!\ell_x!\ell_y!\ell_z!(\ell+|m|)!}}\frac{1}{2^\ell\ell!} \\ &\times\left[\sum_{\alpha=0}^{(\ell-|m|)/2}\binom{\ell}{\alpha}\binom{\alpha}{\tau}\frac{(-1)^\alpha(2\ell-2\alpha)!}{(\ell-|m|-2\alpha)!}\right] \\ &\times\left[\sum_{\beta=0}^{\tau}\binom{\tau}{\beta}\binom{|m|}{\ell_x-2\beta}\left\{(-1)^{(|m|-\ell_x+2\beta)/2}-(-1)^{-(|m|-\ell_x+2\beta)/2}\right\}\frac{1}{i\sqrt{2}}\right] \end{aligned} \tag{17}$$

$$\begin{aligned} c_{\ell,0,\ell_x,\ell_y,\ell_z} &= \sqrt{\frac{(2\ell_x)!(2\ell_y)!(2\ell_z)!\ell!}{(2\ell)!\ell_x!\ell_y!\ell_z!}}\frac{1}{2^\ell\ell!}\left[\sum_{\alpha=0}^{\ell/2}\binom{\ell}{\alpha}\binom{\alpha}{(\ell_x+\ell_y)/2}\frac{(-1)^\alpha(2\ell-2\alpha)!}{(\ell-2\alpha)!}\right] \\ &\times\frac{((\ell_x+\ell_y)/2)!}{(\ell_x/2)!(\ell_y/2)!} \end{aligned} \tag{18}$$

where $\tau=(\ell_x+\ell_y-|m|)/2$ and is an integer. If τ is a half-integer, $c_{\ell,m,\ell_x,\ell_y,\ell_z}=0$. α and β are also integers. Note that the binomial term $\binom{a}{b}$ is zero for $b<0$ and for $b>a$.

Relation from spherical-harmonic to Cartesian functions

The inverse relation, from real normalised CGTO to normalised Cartesian CGTO reads:

$$\chi^{\text{Cart, CGTO}}_{p,\ell_x,\ell_y,\ell_z}(x,y,z) = \sum_{\mu\in\ell=\ell_x+\ell_y+\ell_z,m} c^{-1}_{\ell,m,\ell_x,\ell_y,\ell_z}\chi^{\text{CGTO, R}}_{\mu,\ell,m}(r,\theta,\phi) \tag{19}$$

where the $c^{-1}_{\ell,m,\ell_x,\ell_y,\ell_z}$ coefficients must fulfil the following relation:

$$\sum_{\ell_x+\ell_y+\ell_z=\ell} c_{\ell,m1,\ell_x,\ell_y,\ell_z}c^{-1}_{\ell,m2,\ell_x,\ell_y,\ell_z} = \delta_{m1,m2} \tag{20}$$

When S denotes the overlap matrix for Cartesian AOs, $c^\dagger Sc=1$ is the overlap matrix for spherical-harmonic orbitals. Therefore, $c^{-1}=c^\dagger S$:

$$c^{-1}_{\ell,m,\ell_{x1},\ell_{y1},\ell_{z1}} = \sum_{\ell_{x2},\ell_{y2},\ell_{z2}=\ell} S_{\ell_{x1},\ell_{y1},\ell_{z1},\ell_{x2},\ell_{y2},\ell_{z2}}c_{\ell,m,\ell_{x1},\ell_{y1},\ell_{z1}} \tag{21}$$

The overlap between normalised Cartesian orbitals of the same total angular momentum is:

$$S_{\ell_{x1},\ell_{y1},\ell_{z1},\ell_{x2},\ell_{y2},\ell_{z2}} = \left[\frac{(\ell_{x1}+\ell_{x2})!(\ell_{y1}+\ell_{y2})!(\ell_{z1}+\ell_{z2})!}{((\ell_{x1}+\ell_{x2})/2)!((\ell_{y1}+\ell_{y2})/2)!((\ell_{z1}+\ell_{z2})/2)!)}\right] \times \left[\frac{\ell_{x1}!\ell_{y1}!\ell_{z1}!\ell_{x2}!\ell_{y2}!\ell_{z2}!}{(2\ell_{x1})!(2\ell_{y1})!(2\ell_{z1})!(2\ell_{x2})!(2\ell_{y2})!(2\ell_{z2})!}\right]^{1/2} \quad (22)$$

and $(\ell_{x1}+\ell_{x2})/2$, $(\ell_{y1}+\ell_{y2})/2$, $(\ell_{z1}+\ell_{xz})/2$ are integers or $S=0$.

Transformation of the density matrix

Equations 15 and 19 can be generalised to express the relation between all the normalised real spherical-harmonic CGTOs and normalised Cartesian CGTOs for a molecule in a given basis set:

$$\chi_{\mu}^{\text{CGTO, R}}(r,\theta,\phi) = \sum_{p} c_{p,\mu}\chi_{p}^{\text{Cart, CGTO}}(x,y,z) \quad (23)$$

$$\chi_{p}^{\text{Cart, CGTO}}(x,y,z) = \sum_{\mu} c_{\mu,p}^{-1}\chi_{\mu}^{\text{CGTO, R}}(r,\theta,\phi) \quad (24)$$

where μ, ν are used to refer to spherical-harmonic CGTO and p, q to Cartesian CGTO.

By introducing the LCAO coefficients ($C_{\mu i}^{\text{CGTO, R}}$) of the molecular orbitals ($\phi_i(r,\theta,\phi)$) one obtains:

$$\phi_i(r,\theta,\phi) = \sum_{\mu} C_{\mu i}^{\text{CGTO, R}}\chi_{\mu}^{\text{CGTO, R}}(r,\theta,\phi) \quad (25)$$

$$= \sum_{p} C_{pi}^{\text{Cart, CGTO}}\chi_{p}^{\text{Cart, CGTO}}(x,y,z) \quad (26)$$

Inserting Equations 23 and 24 into the two previous equations gives the two sets of LCAO coefficients:

$$C_{pi}^{\text{Cart, CGTO}} = \sum_{\mu} c_{p,\mu}C_{\mu i}^{\text{CGTO, R}} \quad (27)$$

$$C_{\mu i}^{\text{CGTO, R}} = \sum_{p} c_{\mu,p}^{-1}C_{pi}^{\text{Cart, CGTO}} \quad (28)$$

Finally, the definition of the density matrices expressed in both type of orbitals are given by:

$$D_{\mu\nu}^{\text{CGTO, R}} = \sum_{i}^{\text{occ}} C_{\mu i}^{\text{CGTO, R}}C_{\nu i}^{*,\text{CGTO, R}} = \sum_{i}^{\text{occ}}\sum_{p,q} c_{\mu,p}^{-1}c_{\nu,q}^{-1*}C_{pi}^{\text{Cart, CGTO}}C_{qi}^{*,\text{Cart, CGTO}} \quad (29)$$

$$D_{pq}^{\text{Cart, CGTO}} = \sum_{i}^{\text{occ}} C_{pi}^{\text{Cart, CGTO}}C_{qi}^{*\text{Cart, CGTO}} = \sum_{i}^{\text{occ}}\sum_{\mu,\nu} c_{p,\mu}c_{q,\nu}^{*}C_{\mu i}^{\text{CGTO, R}}C_{\nu i}^{*,\text{CGTO, R}} \quad (30)$$

The relation between the two density matrices are therefore:

$$D_{pq}^{\text{Cart, CGTO}} = \sum_{\mu,\nu} c_{p,\mu} c_{q,\nu}^{*} D_{\mu\nu}^{\text{CGTO, R}} \tag{31}$$

$$D_{\mu\nu}^{\text{CGTO, R}} = \sum_{p,q} c_{\mu,p}^{-1} c_{\nu,q}^{-1*} D_{pq}^{\text{Cart, CGTO}} \tag{32}$$

where Eq. 31 is the key expression used in Gaussian2Gimic.py to transform the density matrices obtained using the Gaussian quantum chemistry program to the input density matrices of the GIMIC code.

Cartesian coordinates of the studied molecules

```
12
 c6f6 neutral, -827.6361893627 H
 C    1.2029717618   -0.6945316150    0.0000000055
 C    1.2029717630    0.6945316155   -0.0000000070
 C   -0.0000000000    1.3890593511    0.0000000016
 C   -1.2029717622    0.6945316135    0.0000000055
 C   -1.2029717612   -0.6945316147   -0.0000000068
 C   -0.0000000013   -1.3890593501    0.0000000014
 F    2.3564569812   -1.3604981255    0.0000000251
 F    2.3564569822    1.3604981243   -0.0000000317
 F   -0.0000000008    2.7209876484    0.0000000072
 F   -2.3564569817    1.3604981215    0.0000000239
 F   -2.3564569788   -1.3604981233   -0.0000000307
 F   -0.0000000022   -2.7209876457    0.0000000061

12
c6f6 dicat singlet -826.7163769216 H
 C    1.1761424411   -0.7677708407    0.0000043347
 C    1.1761761890    0.7678160455    0.0000160067
 C    0.0000229032    1.5126990405   -0.0001064723
 C   -1.1761469109    0.7677653935   -0.0000074900
 C   -1.1761806469   -0.7678105957    0.0000278328
 C   -0.0000328802   -1.5126990384   -0.0000736096
 F    2.3155372696   -1.3022554995    0.0000659485
 F    2.3156101554    1.3022396191    0.0001988979
 F   -0.0000507626    2.8019457859   -0.0001877252
 F   -2.3155216583    1.3022404101    0.0000759214
 F   -2.3155945086   -1.3022245346    0.0001889341
 F    0.0000384092   -2.8019457857   -0.0002025790

12
c6cl6 neutral, -2989.5278990300 H
C     1.2115217   -0.6994724    0.0000000
C     1.2115217    0.6994724    0.0000000
C    -0.0000000    1.3989447    0.0000000
C    -1.2115217    0.6994724    0.0000000
C    -1.2115217   -0.6994724    0.0000000
C    -0.0000000   -1.3989447    0.0000000
Cl    2.7043248   -1.5613426    0.0000000
Cl    2.7043248    1.5613426    0.0000000
Cl    0.0000000    3.1226853    0.0000000
Cl   -2.7043248    1.5613426    0.0000000
Cl   -2.7043248   -1.5613426    0.0000000
Cl    0.0000000   -3.1226853    0.0000000
```

```
12
c6cl6 dication singlet,  -2988.7108023150 H
C     1.2007293   -0.7549028   -0.0000684
C     1.2006788    0.7549155    0.0000097
C    -0.0000282    1.4780155   -0.0000228
C    -1.2007309    0.7549023   -0.0000244
C    -1.2006804   -0.7549150    0.0000700
C     0.0000259   -1.4780155    0.0000302
Cl    2.6530691   -1.5404387   -0.0002655
Cl    2.6530162    1.5405077    0.0002602
Cl   -0.0000514    3.1724733    0.0000450
Cl   -2.6530668    1.5404385   -0.0002790
Cl   -2.6530142   -1.5405075    0.0002259
Cl    0.0000528   -3.1724733    0.0000191

12
c6br6 neutral,-15672.7976747800 H
C     1.2126367   -0.7001161    0.0000000
C     1.2126367    0.7001161    0.0000000
C    -0.0000000    1.4002323    0.0000000
C    -1.2126367    0.7001161    0.0000000
C    -1.2126367   -0.7001161    0.0000000
C    -0.0000000   -1.4002323    0.0000000
Br    2.8543839   -1.6479793    0.0000000
Br    2.8543839    1.6479793    0.0000000
Br    0.0000000    3.2959587    0.0000000
Br   -2.8543839    1.6479793    0.0000000
Br   -2.8543839   -1.6479793    0.0000000
Br    0.0000000   -3.2959587    0.0000000

12
c6br6 dicat,   -15671.9903025700 H
C     1.1990584   -0.6922780    0.0000000
C     1.1990584    0.6922780    0.0000000
C    -0.0000000    1.3845592   -0.0000000
C    -1.1990584    0.6922780    0.0000000
C    -1.1990584   -0.6922780    0.0000000
C     0.0000000   -1.3845592   -0.0000000
Br    2.8275389   -1.6324902    0.0000000
Br    2.8275389    1.6324902    0.0000000
Br    0.0000000    3.2649721   -0.0000000
Br   -2.8275389    1.6324902    0.0000000
Br   -2.8275389   -1.6324902    0.0000000
Br   -0.0000000   -3.2649721   -0.0000000

12
c6i6 neutral,  -2015.1509068 H
C     0.0000000000    1.4051159234   -0.0000000000
C     1.2168660862    0.7025579617   -0.0000000000
C     1.2168660862   -0.7025579617   -0.0000000000
C    -0.0000000000   -1.4051159234   -0.0000000000
C    -1.2168660862   -0.7025579617   -0.0000000000
C    -1.2168660862    0.7025579617   -0.0000000000
I     0.0000000000    3.5243498760   -0.0000000000
I     3.0521765267    1.7621749380    0.0000000000
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```
I     3.0521765267   -1.7621749380    0.0000000000
I     0.0000000000   -3.5243498760    0.0000000000
I    -3.0521765267   -1.7621749380   -0.0000000000
I    -3.0521765267    1.7621749380    0.0000000000

12
c6i6 dication, -2014.456054
C    -1.2034403673    0.6953567431    0.0000185867
C    -1.2039147376   -0.6945335814    0.0000020867
C    -0.0004797656   -1.3899290232   -0.0000194133
C     1.2034402032   -0.6953631461    0.0000162867
C     1.2039187753    0.6945356716    0.0000044867
C     0.0004732012    1.3899308224   -0.0000222133
I    -3.0087799230    1.7384545731    0.0000681867
I    -3.0099602423   -1.7363975871    0.0000502867
I    -0.0012180997   -3.4748505515   -0.0001344133
I     3.0087960417   -1.7385076866    0.0001013867
I     3.0099980890    1.7364381697    0.0000169867
I     0.0011644392    3.4748633628   -0.0001024133

12
c6at6 neutral, -1803.3981133270 H
C     1.2157385   -0.7019070    0.0000000
C     1.2157385    0.7019070    0.0000000
C     0.0000000    1.4038139    0.0000000
C    -1.2157385    0.7019070    0.0000000
C    -1.2157385   -0.7019070    0.0000000
C     0.0000000   -1.4038139    0.0000000
At    3.1528191   -1.8202809    0.0000000
At    3.1528191    1.8202809    0.0000000
At    0.0000000    3.6405619    0.0000000
At   -3.1528191    1.8202809    0.0000000
At   -3.1528191   -1.8202809    0.0000000
At    0.0000000   -3.6405619    0.0000000

12
c6at6 dicat, -1802.7653484400 H
C     1.2034841144   -0.6949736187    0.0000137989
C     1.2036050896    0.6947648848   -0.0000150011
C     0.0001207973    1.3897687301    0.0000119989
C    -1.2034842784    0.6949740791   -0.0000102011
C    -1.2036048620   -0.6947644244    0.0000089989
C    -0.0001207661   -1.3897679681   -0.0000095011
At    3.1028867464   -1.7916972763    0.0001110989
At    3.1031992255    1.7911572774   -0.0001187011
At    0.0003114112    3.5830565882    0.0001046989
At   -3.1028878153    1.7916966360   -0.0000887011
At   -3.1031981936   -1.7911579177    0.0000810989
At   -0.0003113800   -3.5830554240   -0.0000895011

18
c6seh6 neutral, -14640.8345301100 H
 C   -0.8457607527   -1.1312653893   -0.0349906124
 C    0.5487257438   -1.2689082057   -0.0260108554
 C    1.4035973964   -0.1585903696   -0.0304614456
 C    0.8457165092    1.1312370911    0.0349974998
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 C   -0.5487808245    1.2688763795    0.0260524067
 C   -1.4036403682    0.1585676562    0.0304032837
SE   -3.3004753194    0.5099409523    0.2017428406
 H   -3.5839701211   -0.7972298142    0.8261436214
SE   -1.8880551219   -2.7537345432   -0.2124153134
 H   -3.0353544067   -2.0628694987   -0.8332668494
SE    1.3181928281   -3.0498123064    0.1567971026
 H    1.4343936588   -3.3154593707   -1.2893114206
SE    3.3004310927   -0.5098252807   -0.2021326437
 H    3.5838556051    0.7975307777   -0.8261697753
SE    1.8880339712    2.7536735809    0.2126018613
 H    3.0355306325    2.0626791685    0.8329343942
SE   -1.3184269236    3.0497257585   -0.1565294324
 H   -1.4340135998    3.3154634136    1.2896153381

18
c6seh6 dicat singlet, -14640.1801356500 H
 C   -0.8340183840   -1.1328396615   -0.0005336682
 C    0.5513841199   -1.2760266397    0.0139140670
 C    1.3965942483   -0.1689108475    0.0023263469
 C    0.8340307989    1.1328326221    0.0005705174
 C   -0.5513734908    1.2760184517   -0.0139628366
 C   -1.3965830503    0.1689014974   -0.0023205263
SE   -3.2723433796    0.4873136569   -0.0083072760
 H   -3.5602410053   -0.5169165399    1.0462075380
SE   -1.8875181947   -2.7172062014    0.0012876587
 H   -2.8136963409   -2.2376983221   -1.0549408618
SE    1.3210534429   -3.0574883149    0.0512198786
 H    1.3823862422   -3.1893712760   -1.4214939744
SE    3.2723479505   -0.4873618294    0.0083378933
 H    3.5602853905    0.5169044614   -1.0461328265
SE    1.8875118167    2.7172121750   -0.0010674067
 H    2.8136400253    2.2376385912    1.0551765954
SE   -1.3210237643    3.0574848280   -0.0514895971
 H   -1.3824364251    3.1895133486    1.4212084783

18
c6secl6 neutral, -17398.2573656300 H
 C   -1.0415546272    0.9402645023    0.0170785660
 C   -1.3350806170   -0.4319243576   -0.0167382813
 C   -0.2934818534   -1.3722841607    0.0159820457
 C    1.0416312881   -0.9403491600   -0.0171529748
 C    1.3351420934    0.4318401178    0.0168112910
 C    0.2935466895    1.3721860623   -0.0160917150
SE    0.7106415836    3.2498051932   -0.1720670463
CL   -0.7007554851    3.7228676593   -1.8363113281
SE   -2.4591173259    2.2400299465    0.1750003066
CL   -3.5717844142    1.2533570264    1.8405436554
SE   -3.1696237833   -1.0094884799   -0.1739793509
CL   -2.8735016809   -2.4635297606   -1.8423908541
SE   -0.7106349477   -3.2499013905    0.1712588944
CL    0.6998460100   -3.7235734489    1.8360130256
SE    2.4590981291   -2.2402068379   -0.1745397374
CL    3.5730481256   -1.2534667225   -1.8391495994
SE    3.1696646290    1.0093327165    0.1744312362
CL    2.8729161863    2.4650410943    1.8413018666
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18
secl6 dication singlet,  -17397.5813589000
 C   -1.2039435011    0.7026934483    0.0054446150
 C   -1.2105244341   -0.6912810869   -0.0054664153
 C   -0.0065855363   -1.3939124911    0.0053784110
 C    1.2039325638   -0.7026734520   -0.0054168895
 C    1.2105137151    0.6912993852    0.0054684349
 C    0.0065761827    1.3939318396   -0.0054076129
SE    0.0160878154    3.3299411673   -0.0173934784
CL    0.0041906886    3.6454219567   -2.1499678985
SE   -2.8757664398    1.6789885658    0.0174386127
CL   -3.1555151279    1.8259904516    2.1500270126
SE   -2.8918166942   -1.6512020085   -0.0172919033
CL   -3.1595980201   -1.8195986939   -2.1498308402
SE   -0.0160915590   -3.3299225864    0.0172271591
CL   -0.0042166511   -3.6455633505    2.1497779546
SE    2.8757564842   -1.6789662140   -0.0172835605
CL    3.1556452718   -1.8260149793   -2.1498490426
SE    2.8918065297    1.6512171649    0.0173028747
CL    3.1595487122    1.8196508833    2.1498425668

18
c6seme6 neutral, -14876.6147754300 H
 C   -1.0067593188   -0.9823883386    0.0150388363
 C    0.3473716117   -1.3629979624   -0.0166213953
 C    1.3540454936   -0.3806805359    0.0164037906
 C    1.0067421325    0.9823773118   -0.0150544585
 C   -0.3473889252    1.3629868780    0.0166312021
 C   -1.3540622430    0.3806710988   -0.0163966959
SE   -3.1997475466    0.8997202211   -0.3661517069
SE   -2.3790897388   -2.3214146974    0.3644205213
SE    0.8209520406   -3.2208220004   -0.3665863589
SE    3.1997283044   -0.8997053437    0.3662019838
SE    2.3790933921    2.3213715178   -0.3644793626
SE   -0.8210002753    3.2208047138    0.3665952053
 C    2.8837373941    2.8145763878    1.4668536208
 H    2.0211992735    3.2312277813    1.9811951837
 H    3.2786723343    1.9422448515    1.9818300319
 H    3.6601799630    3.5719525282    1.3679027653
 C   -0.9968889093    3.9040391848   -1.4647742258
 H   -0.0440073715    3.8105973034   -1.9800468449
 H   -1.7886357682    3.3645217813   -1.9787294765
 H   -1.2654110868    4.9549402340   -1.3659628671
 C   -3.8786094228    1.0915922999    1.4652556519
 H   -3.8087064989    0.1364890350    1.9801522958
 H   -3.3198443830    1.8696102548    1.9796196850
 H   -4.9225676370    1.3859489983    1.3664458606
 C   -2.8837243122   -2.8145833752   -1.4669245735
 H   -3.2786691464   -1.9422453253   -1.9818831384
 H   -2.0211810935   -3.2312145019   -1.9812744044
 H   -3.6601601009   -3.5719693856   -1.3679917509
 C    0.9968497687   -3.9040763923    1.4647755831
 H    1.7886151117   -3.3645796805    1.9787242714
 H    0.0439759489   -3.8106190987    1.9800603245
 H    1.2653471947   -4.9549826224    1.3659490439
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 C    3.8786557698   -1.0915363374   -1.4651863905
 H    3.3199210033   -1.8695571666   -1.9795786702
 H    3.8087507918   -0.1364258727   -1.9800691977
 H    4.9226162495   -1.3858737447   -1.3663443393

18
c6seme6 dication singlet, -14876.0479687800 H
C    -0.9968182   -0.9729047   -0.0081669
C     0.3443517   -1.3497524    0.0071455
C     1.3412517   -0.3766523   -0.0077772
C     0.9969425    0.9732312    0.0084316
C    -0.3442244    1.3500789   -0.0073775
C    -1.3411256    0.3769816    0.0077456
Se   -3.1961844    0.8982200   -0.0313541
Se   -2.3756289   -2.3188412    0.0310734
Se    0.8206012   -3.2168628   -0.0325336
Se    3.1963077   -0.8979166    0.0311754
Se    2.3757793    2.3191810   -0.0295709
Se   -0.8204965    3.2172083    0.0312113
C     2.6724504    2.6094658    1.8980502
H     1.7566974    2.9708589    2.3560554
H     3.0192665    1.6875310    2.3549417
H     3.4475711    3.3720493    1.9455507
C    -0.9258370    3.6200912   -1.8960983
H     0.0498758    3.4774621   -2.3505636
H    -1.6845444    2.9949528   -2.3570254
H    -1.2172711    4.6677307   -1.9425643
C    -3.5965956    1.0150464    1.8957932
H    -3.4836303    0.0353064    2.3499325
H    -2.9491003    1.7543885    2.3573157
H    -4.6349823    1.3379521    1.9418990
C    -2.6732563   -2.6098694   -1.8962857
H    -3.0203022   -1.6881113   -2.3533603
H    -1.7577310   -2.9714369   -2.3546093
H    -3.4483986   -3.3724733   -1.9431026
C     0.9264310   -3.6207162    1.8945442
H     1.6852600   -2.9958128    2.3555895
H    -0.0491642   -3.4783079    2.3493319
H     1.2178707   -4.6683802    1.9404109
C     3.5966827   -1.0143479   -1.8960040
H     2.9491712   -1.7535869   -2.3576685
H     3.4837152   -0.0345114   -2.3499329
H     4.6350653   -1.3372522   -1.9422027

18
c6teh6 neutral, -1840.1688690870 H
C    -0.8408040626   -1.1304424879   -0.0174462013
C     0.5581891424   -1.2935513997    0.0180935014
C     1.3989774038   -0.1635752123   -0.0179601013
C     0.8407793659    1.1295768862    0.0169621013
C    -0.5582271426    1.2926893964   -0.0175523013
C    -1.3990107049    0.1627030123    0.0179075013
Te   -3.4748225633    0.4038108307    0.5860301417
H    -4.1074319077    0.4848960366   -0.9503697727
Te   -2.0874566577   -2.8071562104   -0.5871324444
H    -2.4723503850   -3.3178188487    0.9485290720
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Te    1.3861102050   -3.2117386440    0.5883942464
H     1.6398265228   -3.7991516846   -0.9471188728
Te    3.4744314642   -0.4066431307   -0.5865911437
H     4.1088537117   -0.4765974361    0.9496107738
Te    2.0889975584    2.8063724089    0.5827003415
H     2.4663434877    3.3180206505   -0.9544876713
Te   -1.3873626035    3.2115827430   -0.5834013426

18
c6teh6 dication singlet,  -1839.6268720200 H
C    -0.8336975   -1.1203322    0.0031917
C     0.5533921   -1.2821817   -0.0029902
C     1.3871207   -0.1618331    0.0029149
C     0.8337003    1.1203319   -0.0031911
C    -0.5533897    1.2821804    0.0029865
C    -1.3871171    0.1618319   -0.0029117
Te   -3.5124360    0.4096013    0.0963271
H    -3.6898022    0.4311988   -1.5607328
Te   -2.1110207   -2.8369059   -0.0963197
H    -2.2184670   -2.9800002    1.5606506
Te    1.4012343   -3.2467126    0.0963137
H     1.4713160   -3.4110932   -1.5606984
Te    3.5124393   -0.4096027   -0.0963084
H     3.6897949   -0.4312011    1.5607519
Te    2.1110198    2.8369068    0.0963257
H     2.2184695    2.9800016   -1.5606433
Te   -1.4012352    3.2467086   -0.0963385
H    -1.4713217    3.4111013    1.5606719

36
c6teme6 neutral,-2076.0002880650 H
C    -0.0010862001    1.4086513037    0.0183841014
C    -1.2204746940    0.7034436509   -0.0167987013
C    -1.2194294896   -0.7052742550    0.0164316012
C     0.0010638001   -1.4086601039   -0.0181233014
C     1.2204779908   -0.7034234522    0.0166228013
C     1.2193975908    0.7052983537   -0.0165001013
Te    3.0334272265    1.7548642326   -0.5445442436
Te   -0.0030123002    3.5039927659    0.5479587439
Te   -3.0360289264    1.7501123320   -0.5453400415
Te   -3.0338878277   -1.7543882324    0.5438985415
Te    0.0027589002   -3.5044897639   -0.5457642405
Te    3.0366583298   -1.7496901332    0.5438086396
C     0.0019515001   -4.3977999308    1.4185233063
H     0.9021902692   -4.0917664090    1.9450217484
H    -0.8992459693   -4.0926001066    1.9438583470
H     0.0025637002   -5.4761167240    1.2646656934
C     3.8105890888   -2.1982965631   -1.4199998061
H     3.0956194335   -2.8259365151   -1.9455166456
H     3.9968161036   -1.2661163958   -1.9468437480
H     4.7441647600   -2.7376775078   -1.2651463980
C     3.8107185891    2.1999509670    1.4187352048
H     3.0964895332    2.8262795120    1.9468299471
H     3.9982323036    1.2667705964    1.9433406476
H     4.7438076554    2.7400178048    1.2633126930
C    -0.0016392001    4.3997190291   -1.4152341046
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H     0.8997251658    4.0951666110   -1.9406644448
H    -0.9017190686    4.0943107091   -1.9423736449
H    -0.0023175002    5.4778677186   -1.2601473928
C    -3.8124362878    2.1977795675    1.4177075055
H    -3.9993128994    1.2653301971    1.9438475465
H    -3.0981310357    2.8251675148    1.9444311443
H    -4.7458248579    2.7372486044    1.2620026935
C    -3.8091634853   -2.2014070670   -1.4197378051
H    -3.9962660027   -1.2687584931   -1.9454348454
H    -3.0943306329   -2.8281539107   -1.9465151448
H    -4.7423457556   -2.7414160075   -1.2646963962

36
c6teme6 dication singlet, -2075.4976129350 H
C    -0.0018391    1.3977864   -0.0041520
C    -1.2114446    0.6973296    0.0041923
C    -1.2096044   -0.7004808   -0.0041665
C     0.0018361   -1.3977591    0.0041310
C     1.2114416   -0.6973023   -0.0041802
C     1.2096014    0.7005082    0.0041748
Te    3.0583393    1.7699477   -0.0606827
Te   -0.0038180    3.5334712    0.0606323
Te   -3.0622250    1.7632349   -0.0605566
Te   -3.0583394   -1.7699226    0.0607348
Te    0.0038153   -3.5334406   -0.0607604
Te    3.0622188   -1.7632092    0.0606326
C     0.0055787   -3.9250825    2.0648172
H     0.9214139   -3.5380460    2.5005771
H    -0.8761782   -3.4774758    2.5127496
H    -0.0306791   -5.0088711    2.1577492
C     3.4029861   -1.9573241   -2.0649259
H     2.5747818   -2.4973332   -2.5131394
H     3.5256012   -0.9705913   -2.5004985
H     4.3236514   -2.5303550   -2.1574258
C     3.3971223    1.9675739    2.0648548
H     2.6042293    2.5673785    2.5006336
H     3.4502732    0.9801750    2.5128277
H     4.3539787    2.4778841    2.1573461
C    -0.0055843    3.9250116   -2.0649640
H     0.8761720    3.4773835   -2.5128763
H    -0.9214202    3.5379544   -2.5007041
H     0.0306735    5.0087958   -2.1579480
C    -3.4029280    1.9573396    2.0650131
H    -3.5255289    0.9706048    2.5005851
H    -2.5747106    2.4973476    2.5132038
H    -4.3235912    2.5303691    2.1575437
C    -3.3971716   -1.9675468   -2.0647951
H    -3.4503340   -0.9801474   -2.5127654
H    -2.6042881   -2.5673500   -2.5005932
H    -4.3540295   -2.4778580   -2.1572646

24
c6sbh2 neutral, -1677.0805236280 H
C    -0.6295621461   -1.2463629923    0.0180266014
C     0.7786439608   -1.1730801879    0.0371013028
C     1.4188662079    0.0809969063    0.0447724034
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C     0.6295758465    1.2463929913   -0.0180695014
C    -0.7786348589    1.1731071866   -0.0371971028
C    -1.4188622073   -0.0809722059   -0.0448385034
Sb    1.4831686097    3.2300379425   -0.5126621388
H     2.1957102675    3.5883824715    1.0054704754
H     2.9545447214    2.5722200915   -1.1161206866
Sb    3.5415250644    0.3674182276    0.5900432421
H     3.7331000821   -1.2156467930    1.2218202912
H     4.2291684193   -0.1026977075   -0.9122690690
Sb    1.7853928332   -3.0942324335   -0.3942023297
H     3.1580496380   -2.3862525799   -1.1303882842
H     2.6035950952   -3.3239371484    1.0938462827
Sb   -1.4830389137   -3.2299661437    0.5128290387
H    -2.1962295650   -3.5882809700   -1.0050269772
H    -2.9541401231   -2.5720117914    1.1168893854
Sb   -3.5416228669   -0.3676377276   -0.5897071457
H    -3.7336863840    1.2155063917   -1.2211369911
H    -4.2288875162    0.1020822077    0.9129046691
Sb   -1.7853788364    3.0943848312    0.3933975295
H    -2.6030274944    3.3237225512   -1.0949979841
H    -3.1582699398    2.3868267795    1.129515485

24
c6sbh2 dication singlet, -1676.4467260910 H
C    -0.6258252   -1.2607636    0.0568829
C     0.7720214   -1.1450675    0.0509723
C     1.4090159    0.0933850   -0.0286780
C     0.6255652    1.2605093   -0.0570989
C    -0.7722589    1.1447901   -0.0512474
C    -1.4093529   -0.0936235    0.0283093
Sb    1.4734336    3.2768186   -0.1954757
H     1.7407260    3.4706622    1.4789347
H     3.0717522    2.6414085   -0.5325126
Sb    3.5883739    0.2975050   -0.0010028
H     3.9015942   -1.1667843    0.8526632
H     3.8931516   -0.3230446   -1.5610325
Sb    1.8005586   -3.0794786    0.1270204
H     3.1395701   -2.8459735   -0.9025078
H     2.6138633   -3.0219280    1.6192328
Sb   -1.4728384   -3.2773733    0.1957602
H    -1.7438138   -3.4707866   -1.4780734
H    -3.0706320   -2.6448511    0.5374881
Sb   -3.5889154   -0.2973890    0.0004156
H    -3.9010000    1.1665060   -0.8542136
H    -3.8929390    0.3254703    1.5597215
Sb   -1.7998647    3.0796179   -0.1279072
H    -2.6135208    3.0221929   -1.6198909
H    -3.1386651    2.8481978    0.9022401
```

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